## Model systems for heterogeneous catalysts at the atomic level

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Our understanding of catalysis, and in particular heterogeneous catalysis, is to a large extent based on the investigation of model systems. Increasing the complexity of the models towards oxide supported nanoparticles, resembling a real disperse metal catalyst, allows one to catch in the model some of the important aspects that cannot be covered by metal or oxide single crystals per se.

The main purpose of our studies is to provide conceptual insight into questions concerned with a variety of topics in catalysis, including support nanoparticle interaction, reactivity at the particle-support interface, strong metal support interaction, reactions in confined space and development of new instrumentation for surface science studies.

The talk will address some of those issues.

# Special metallic gasket sealing for the non-circular profile flanges

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Various types of the metallic gaskets for the non-circular profile flanges and the potential applications will be introduced. The sealing surface of flange is flat to accommodate the special metallic gasket with knife edges for the sealing. Both the flange and gasket are made of aluminum alloys and produced by the oil-free Ethanol-CNC-machining process that any non-circular profile, e. g. race-track, rectangular, key-hole, etc., flanges can be made. All the flanges and gaskets after oil-free machining can be assembled immediately without any chemical cleaning. The quality of ultrahigh vacuum at pressure < 20 nPa after vacuum baking has been approved. The as mentioned non-circular metallic flange-sealing can be applied for the high radiation reactors, accelerators, wave guides, aluminum ultrahigh vacuum systems, large aluminum chambers for industrial, et al. The non-circular metallic gaskets can be reused few more times while the flanges won't take any risk of damage on sealing surfaces that result in the consequent advantages of high systematic reliability and low manufacturing cost.

## Microstructural design for enhancing both hardness and toughness in transition-metal diboride thin films

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Transition-metal (TM) diborides have received increasing attention as next-generation ceramic thin films for replacing TM nitrides. They exhibit high hardness; however, this is not always sufficient to prevent failure in applications involving high stresses since hardness is typically accompanied by brittleness leading to crack formation and propagation. Toughness, the combination of hardness and ductility, is required to avoid brittle fracture. We propose a strategy for increasing both the hardness and ductility of ZrB2, selected as a model TM diboride, thin films grown by hybrid high-power impulse and dc magnetron (HiPIMS/DCMS) cosputering in pure Ar at 450°C on Al2O3(0001). A Ta target operated in HiPIMS mode supplies pulsed energetic Ta ions to the growing film, while a ZrB2 target operated in DCMS mode provides a continuous flux of Zr and B atoms. The average power (and pulse frequency) applied to the HiPIMS Ta target are varied from 0 to 1800 W (300 Hz) in increments of 600 W (100 Hz); all other deposition parameters are maintained constant. The resulting boron-to-metal ratio, y = B/(Zr + Ta), in Zr1-xTaxBy films continuously decreases from 2.4 to 1.5 as the power is increased; x increases from 0 to 0.3. All films have the hexagonal AlB2 crystal structure with a columnar microstructure. Films with x < 0.2 have B-rich column boundaries, while those with x  $\ge 0.2$  have Ta-rich column boundaries. As a result, hardness increases from 35 to 42 GPa, ~20%, with a simultaneous increase in nanoindentation toughness from 4 to 5.2 MPa $\sqrt{m}$ , ~30%.

# Tunable Mo-O(-N) films prepared using reactive deep oscillation magnetron sputtering

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A modified version of HiPIMS, called Deep Oscillation Magnetron Sputtering, with a pulsed reactive gas flow control and tosubstrate reactive gas injection into a high-density plasma in front of the sputtered molybdenum target was used for lowtemperature deposition of Mo-O(-N) films. The depositions were performed using a strongly unbalanced magnetron with a planar molybdenum target of 100 mm diameter in argon-oxygen(-nitrogen) gas mixtures at the total pressure close to 1 Pa. Voltage macropulses, composed of 5 voltage micropulses (pulse-on time of 23 us and pulse-off time of 27 us), with a total length of 250 us and repetition frequency of 400 Hz were used for all depositions with a maximum target power density up to 1150 Wcm-2 during pulses at a deposition-averaged target power density of 10 Wcm-2. The substrate temperatures were less than 120 °C (no external heater) during the depositions of films on floating glass and Si substrates at the distance of 100 mm from the target. A pulsed reactive gas flow control made it possible to produce high-quality MoOx and MoOxNy films with a tunable composition, and optical and electrical properties. The luminous absorption of 4% for 1 um thick non-conductive MoO3 films (the luminous transmittance of 80%) was smoothly changed into 88% for conductive (electrical resistivity decreased by up to 10 orders of magnitude) MoOx or MoOxNy films, keeping hardness of 3-5 GPa and very low macrostress (less than 200 MPa).

# Design of high-performance VO2-based thermochromic coatings, and pathway for their low-temperature preparation

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The contribution deals with thermochromic multilayer VO2-based coatings for smart window applications prepared by reactive magnetron sputtering. First, we show that and how reactive high-power impulse magnetron sputtering with a pulsed O2 flow control allows reproducible preparation of crystalline VO2 of the correct stoichiometry under exceptionally industry-friendly deposition conditions: on soda-lime glass substrates without any substrate bias at a low temperature of around 300 °C [1]. Second, doping of VO2 by W is employed in order to shift the thermochromic transition temperature (68°C for bulk, 57°C for thin film VO2) towards the room temperature (39°C for V0.988W0.012O2, 20°C for V0.982W0.018O2), without concessions in terms of transmittance and its modulation. Third, we employ ZrO2 antireflection layers both below and above the thermochromic V1-xWxO2 layer, and present an optimum design of the resulting ZrO2/V1-xWxO2/ZrO2 coatings [2]. Most importantly, we show that while utilizing a first-order interference on ZrO2 leads to a tradeoff between the luminous transmittance (Tlum) and the modulation of the solar transmittance (dTsol), utilizing a second-order interference allows one to optimize both Tlum and dTsol in parallel. The properties achieved under the aforementioned industry-friendly deposition conditions and at lowered transition temperature include e.g. Tlum=42% and dTsol=12%, or Tlum=59% and dTsol=6% (depending on the V1-xWxO2 thickness). The experimental transmittance values are in agreement with those predicted during the multilayer coating design.

- [1] J. Vlcek et al., J. Phys. D Appl. Phys. 50, 38LT01 (2017).
- [2] J. Houska et al., Sol. Energy Mater. Sol. Cells 191, 365-371 (2019).

# Vacuum System Design, Construction and Commissioning for Cornell Brookhaven ERLTest Accelerator (CBETA)

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A novel electron accelerator, Cornell Brookhaven Energy-Recovery LINAC (ERL) Test Accelerator (CBETA), is developed by collaboration between CLASSE and Brookhaven National Laboratory. Many unique accelerator technologies will be tested in CBETA, including photo-cathode electron injector, 4-turn superconducting RF (SRF) Energy Recover LINAC (ERL), non-scaling Fixed-Field Alternating Gradient (NS-FFAG) optics with 4x energy acceptance. With a total circumference ~80-m, the CBETA consists of an photo-cathode injector and a LINAC SRF cryomodule, a NS-FFAG loop to transport electron beams of four energies (42, 78, 114 and 150 MeV) in single bore beampipe, and two splitter sections where the four energy beams are separately manipulated. CBETA vacuum system is designed to provide adequate level of vacuum and physical aperture for transporting electron beams at four energies, while stay clear of 300+ complex magnets. Furthermore, the vacuum system also accommodate a high density of beam diagnostics tools. Beam path length adjustment is required in the splitter sections. CBETA beampipes are mostly constructed of aluminum alloy (6061-T6), including 80+ metal knife-edge seal flanges made of non-coated aluminum alloy (type 6013-T6). Compact NEG pumps are used due to the space constraints. In this presentation, we report the status of CBETA vacuum system design, chamber fabrications and many stages of beamline installations and operations. Measurements of aluminum alloy outgassing and vacuum simulation, and experiences of using aluminum knife-edge flanges will also be discussed.

# Surface Functionalization of RF Magnetron Sputtering Titanium Dioxide Thin Films

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Nanostructured titanium dioxide (TiO2) has been employed as surface modifiers in medical and dental implants, promoting improvements in biocorrosion resistance of the material and increasing the oxides bioactivity, with promising results in the interaction with living tissue. Although these materials have good mechanical properties, the thin native oxide layer (5-6nm) on their surfaces is not capable of protecting them from long-term corrosion. The surface modification with TiO2 can promote improvement in the biocorrosion resistance of the material and increase the oxides bioactivity, presenting promising results in the interaction with the tissue, since the biocompatibility is determined by chemical processes that occur at the interface between the implant and the proteins of the biological fluids.

In this contribution, X-ray Photoelectron Spectroscopy (XPS) and Atomic Force Microscopy (AFM) were used to examine the adsorption of 3-mercaptopropionic acid (MPA) on anatase and rutile TiO2 thin films surfaces grown by RF magnetron sputtering.

Obtained results showed that by the change of the deposition parameters, it was possible to grow monophasic anatase and rutile films on Ti substrates. AFM results determined the differences in morphology and grain size related to the anatase and rutile phases. Although the similarities of roughness and thickness, the anatase and rutile phases, functionalization was seen to occur only for the rutile phase.

## Observation of pronounced electron-phonon coupling in a point defect in monolayer WS2 on the single atom scale

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Two-dimensional transition metal dichalcogenides (2D-TMDs) are a novel class of materials with many potential applications including electronic and opto-electronic devices, quantum information systems, and catalysis. Properties of these materials are significantly impacted by atomic-scale local morphology and defects within the lattice. Particularly, the formation of electronic resonances that lie within the valence and conduction bands, referred to as in-gap states, result in significantly different opto-electronic than from a pristine lattice. High resolution scanning probe microscopy has the unique capability to resolve both geometric and electronic structure of materials on relevant length scales. Previously [1] using scanning tunneling microscopy/ spectroscopy (STM/STS) in combination with high-resolution NC-AFM imaging we identified and characterized point defects in monolayer tungsten disulfide (WS2) on graphene on silicon carbide.

Commonly observed was a negatively charged defect sitting at the chalcogen site with a sharp in-gap resonance just above the valence band. Remarkably, after applying a local electric field (achieved by tunneling with a high current setpoint and bias), this defect can be reproducibly converted to a new type of defect. This new defect shows striking in-gap vibrionic signatures that can be reproducibly fit with a Frank-Condon model resulting in Huang-Rhys (HR) factors of ~5 and a lifetime broadening of 6 meV. Here, using STS we directly observe electron-phonon coupling of a single defect that we have created with an electric field. SPM techniques allow for an unprecedented view of the relationship between atomic structure therefore crucial optoelectronic properties.

[1] Schuler, B. et al. arXiv:1810.02896v1

## Fundamental Properties of Transition-metal Nitrides: Materials Design Strategies for Extreme Properties

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Transition-metal (TM) nitrides exhibit an enormous range of useful properties. Cubic TM nitrides have wide single-phase compound fields that can be exploited. Results are presented for vacancy hardening in 3d Group-IV TiNx(001) and Group-V VNx (001); the hardness H (and resistivity) of epitaxial layers increases, while the elastic modulus E and the relaxed lattice constant decrease linearly with decreasing x. In contrast, H(x), E(x), and resistivity(x) for 5d Group-V TaNx(001) remain constant due primarily to the presence of isoelectronic antisites.

All Group-IV TM nitrides are very good metallic conductors with room-temperature resistivities of 12-14 micro-ohm-cm. 3d Group-III ScN(001) is a transparent semiconductor with an indirect  $\Gamma$ -X gap of 1.3 eV.

Group-IV TM nitrides are superconducting, but not the Group-IV rare-earth nitride CeN. The results are consistent with electron/phonon coupling parameters. Acoustic phonon modes soften monotonically with increasing cation mass; optical mode energies remain approximately constant for the TM nitrides, but are significantly lower for CN due a lower interatomic force constant.

While TM nitrides are very hard, they are also brittle, leading to failure by crack formation and propagation. We show several approaches for obtaining TM nitride layers that are both hard and ductile (i.e., tough). IV-VI and V-VI alloys, e.g. Ti1 xWxN and V1 xMoxN, exhibit dramatic delocalization of electron density leading to a more ductile response to shear stress while exhibiting increased hardness under tensile and compressive loading. Vacancy-induced toughening is also observed.

# Operation of turbo-molecular pumps in magnetic fields with passive shielding

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Operating turbo-molecular pumps (TMP) in an external magnetic field can induce eddy currents in the fast moving rotor, which leads to an undetected increase of the rotor temperature. The upper limit of the magnetic field for long-term safe operation is of the order of a few mT. It depends not only on the type of the TMP, but also on the direction of the field, the throughput of gas, and on the cooling of the TMP housing. For TMPs with active magnetic bearings, high magnetic fields can also cause a failure of the bearing, with the rotor plunging into the touchdown bearings at full speed.

The KATRIN neutrino experiment operates more than 20 TMPs in the vicinity of super-conducting magnets with fields ranging from a few mT up to 18 mT at the location of the pumps. In order to ensure the safe operation of the TMPs, pumping radioactive tritium gas from the beam-line of the experiment, we studied the rotor temperature as a function of the magnetic field and developed an empirical model, describing the rotor temperature over time. Since the fields are far too strong for most of the TMPs, passive magnetic shieldings were installed around the pumps. This talk describes the temperature model, the measurement of the model parameters, the design of the passive shielding, and the experience with the TMPs operated at the beam-line of the KATRIN experiment.

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# Performance of III–V//Si triple-junction solar cells fabricated by mechanical stacking and wire bonding

Ray-Hua Horng

The integration of III–V and Si triple-junction solar cells as photovoltaic devices have been studied in order to achieve high photovoltaic conversion efficiency. However, there exists a large difference in the coefficients of thermal expansion and the lattice parameters of GaAs and Si, which has made it difficult to obtain high-efficiency solar cells grown as epilayers on Si substrates. In this paper, the GaInP/GaAs stacked on Si (GaInP/GaAs//Si) was fabricated via mechanical stacking and wire bonding technologies. Mechanically stacked GaInP/GaAs//Si triple-junction solar cells are prepared via glue bonding. Current-voltage measurements of the sample are made at room temperature. The short-circuit current density of the GaInP/GaAs//Si solar cell is 13.37 mA/cm2, while the open-circuit voltage of the sample is measured to be 2.71 V. After bonding the GaInP/GaAs dual-junction with the Si solar cell, the conversion efficiency is relatively improved by 32.6%, compared to the efficiency of the GaInP/GaAs dual-junction solar cell alone. This study demonstrates the high potential of combining mechanical stacked with wire bonding and ITO films to achieve high conversion efficiency in solar cells with three or more junctions.

# Titanium Oxide thin films deposited by sputtering mimic the biological response of bulk titanium

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Orthopaedic and dental implant durability depends on successful bone regeneration and osseointegration. Commercially pure titanium (cpTi) and its alloys are currently the standard metallic materials for such implants and it has been shown that the appropriate biological response is greatly consequence of the native oxide layer. In this paper, we show that sputtered titanium oxide (TiO2) films are able to mimic the biological response of the cpTi in-vitro, opening the possibility to use these films to coat bulk implants which might have mechanical properties more similar to the bone than cpTi. Titanium oxide (TiO2) coatings were produced by magnetron sputtering using a Ti target and a reactive Ar/O2 atmosphere. The coatings were deposited on commercially pure titanium and stainless steel substrates with a thickness of about 60-70 nm. The biological response of the coatings was evaluated using human osteoblast and mesenchymal stem cells, including short-term and long-term cell adhesion, differentiation and inflammatory response. The results clearly show that the TiO2 surfaces presented the highest expression of integrins and production of osteogenic proteins in comparison to the uncoated substrates.

# **Pulsed-Power Applications for Farming and Food Processing**

Repetitively operated compact pulsed power generators with a moderate peak power were developed for the applications in several stages of agriculture, fishery and food processing. Pulsed high-voltage produces intense high-electric field which can cause some biological effects such as stress response (stimulation) and electroporation. Types of pulsed power that also have biological effects are caused with gas discharges which include reactive species such as ROS and RNS. The repetitive pulse discharge were used for promoting growth of plants. The growth of vegetables and sugar content in the harvested strawberry increased by plasma irradiation to the hydroponic solution. Number of R. solanacearum in the liquid fertilizer decreased from 10^7 to 10^2 CFU/mL using the plasma treatment. Seedlings with discharge plasma treatment were relatively healthy; in contrast, all seedlings in the positive control wilted and died. The yielding rate of Shiitake mushroom (L. edodes) was also improved with the high-voltage stimulation in fruit-body formation phase. The AC high-voltage can be used to keep freshness of agricultural and marine products. The electrostatic effects can be used to remove airborne bacteria and fungi spore in storage house and container. This removal contributed to reduce an infection risk by fungi and bacteria. Some kinds of fruit and vegetable emit the ethylene gas which accelerate a degradation of other kind fruits and vegetables. The repetitive DBD remediation of air inhibits degradation of agricultural products owing to the ethylene removal. These applications can contribute a food supply chain in the world.

# Toward a Thinking Microscope: Deep Learning-enabled Computational Microscopy and Sensing

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Deep learning is a class of machine learning techniques that uses multi-layered artificial neural networks for automated analysis of signals or data. The name comes from the general structure of deep neural networks, which consist of several layers of artificial neurons, each performing a nonlinear operation, stacked over each other. Beyond its main stream applications such as the recognition and labeling of specific features in images, deep learning holds numerous opportunities for revolutionizing image formation, reconstruction and sensing fields. In fact, deep learning is mysteriously powerful and has been surprising optics researchers in what it can achieve for advancing optical microscopy, and introducing new image reconstruction and transformation methods. From physics-inspired optical designs and devices, we are moving toward data-driven designs that will holistically change both optical hardware and software of next generation microscopy and sensing, blending the two in new ways. Today, we sample an image and then act on it using a computer. Powered by deep learning, next generation optical microscopes and sensors will understand a scene or an object and accordingly decide on how and what to sample based on a given task – this will require a perfect marriage of deep learning would be the key to scale up its impact on various areas of science and engineering, where access to labeled image data might not be immediately available or very costly, difficult to acquire. In this presentation, I will provide an overview of some of our recent work on the use of deep neural networks in advancing computational microscopy and sensing systems, also covering their biomedical applications.

# Growth pressure effects on functionality of complex AI-Ga oxide thin films using pulsed laser deposition

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The synthesis of complex oxide materials in the form of thin films has widely employed the epitaxial growth techniques, but which are limited in the range of compositions that can be accessed because of kinetic phenomena such as surface diffusion and phase separation. Precise control over the functionality of complex oxides arises from microstructural features such as interfaces, defects, lattice deformation, and domain boundaries. In this report, the 100-nm-thick aluminum-gallium oxide (AGO) thin films with bandgaps higher than 5.0 eV were grown on c-plane sapphire substrates using pulsed laser deposition with the oxygen growth pressure ranging from 0.7 to 200 mTorr. The oxygen pressure during the deposition process has a great impact on the lattice deformation in AGO materials as examined by X-ray photoelectron spectroscopy, X-ray diffraction, and transmission electron microscopy. Higher oxygen pressure results in the decrease of the AGO (-201) d-spacing. The measured transmittance spectra of AGO films demonstrate that the absorption edge shifts toward higher energy with increasing the oxygen pressure due to the d-spacing narrowing of main plane. The AGO films were also utilized as the active layers of metal-semiconductor-metal photodetectors. The presented lattice deformation seems to benefit the enhancement of photocurrent and the reduction of dark current. It is found that the responsivity of lattice-deformed AGO device is over 20 times higher than that with the normal lattice. The separated piezopotential induced by the lattice deformation could contribute to assist the photogenerated carrier recombination more efficiently, resulting in the reduction of decay time.

# A comprehensive solution for vacuum monitoring with a new total and partial pressure gauge

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For today's experiments in vacuum it is no longer sufficient to "just" know the pressure. Instead, precise inline process monitoring is required to assess information about the vacuum quality. This is the only way to react adequately to disturbances such as heat-induced outgassing or leaky connections.

We present a novel and yet simple, recently developed, multi-tool for exploring these conditions. However, our pressure gauge has a nice twist: Instead of directly measuring the ion current like normal pressure gauges do, ions are accumulated inside an electron space charge region. The total pressure in the chamber is determined by the accumulation time that is necessary to collect a certain amount of ions.

In this talk the underlying physical principles of the novel ion source are presented along with numerous experimental results. Interesting use cases for the new ion gauge will be shown. We will show how the gauge is capable of a precise total pressure measurement over a wide range and, simultaneously, the determination of partial pressures. The gauge achieves a high dynamic range without the utilization of a cost-intensive electron multiplier, even in the UHV. Fast partial pressure reads give access to important vacuum conditions, such as air- or water-leaks and heavy hydrocarbon contamination. The Helium signal can be separated from other residual gas components, whereby helium leak detection can be carried out without additional apparatus.

## Atomic-Level Catalyst Precise Design using Atomic Layer Deposition

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Catalyst synthesis with precise control over the structure of catalytic active sites at the atomic level is of essential importance for the scientific understanding of reaction mechanisms and for rational design of advanced catalysts with high performance. Such precise control is achievable using atomic layer deposition (ALD). ALD is similar to chemical vapor deposition (CVD), except that the deposition is split into a sequence of two self-limiting surface reactions between gaseous precursor molecules and a substrate. The unique self-limiting feature of ALD allows conformal deposition of catalytic materials on a high surface area catalyst support at the atomic level. The deposited catalytic materials can be precisely constructed on the support by varying the number and type of ALD cycles. As an alternative to the wet-chemistry based conventional methods, ALD, facilitated by area-selective deposition, provides a cycle-by-cycle "bottom-up" approach for nanostructuring supported catalysts with near atomic precision. In this presentation, we will discuss synthesis of single-atom catalysts, bimetallic catalysts and nanostructured catalysts using ALD. Such atomic-level catalyst synthesis offered by ALD greatly facilitates our understanding of the structure-activity relations, and provides knowledge for rational catalyst design.

# Mechanisms of molecular machines

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Molecular machines are gaining increasing interest and have earned the Chemistry Nobel Prize in 2016. They have the potential to spawn the next technological revolution after microelectronics and optoelectronics. Central issues in molecular machines are energy intake, conversion, output and transmission. Molecular machines promise to convert energy and control mechanical motion at length scales down to the nanometer. This talk will discuss basic issues of the operation of molecular motors, including energy conversion steps, continuous energy supply, the role of thermal energy, intentional start and stop of motion, unidirectionality of motion and transmission of rotation among gear-like molecules. Without intentional control of these aspects, motors create random motion and are largely useless. Some molecular machines cause reciprocal motion, as in muscles and switches, while others cause rotational motion, as in flagellae: we discuss mechanisms and theoretical models of both.

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## Cytometry is advanced by new materials and microfluidic design

Amy Herr

From fundamental biosciences to applied biomedicine, high dimensionality data is increasingly important. In single-cell measurement tools, microfluidic design has underpinned the throughput, multiplexing and quantitation needed for this rich data. Genomics and transcriptomics are leading examples. Yet, measurement of proteins lags. Here, I will describe our 'electrophoretic cytometry' tools that increase target selectivity beyond simple immunoassays. Enhanced selectivity is essential for targets that lack high quality immunoreagents – as is the case for the vast majority of protein forms (proteoforms). I will share our results on highly multiplexed single-cell western blotting and single-cell isoelectric focusing that resolves single charge-unit proteoform differences. In fundamental engineering and design, I will discuss how the physics and chemistry accessible in microsystems allows both the "scale-down" of electrophoresis to single cells and the "scale-up" to concurrent analyses of large numbers of cells. Particular emphasis will be placed on precision control of fluids and materials transport in passive systems, with no pumps or valves. Precise reagent control allows for integration of cytometry with sophisticated sample preparation – the unsung hero of measurement science. I will discuss compartment-specific, single-cell western blotting for nucleo-cytoplasmic profiling, which eliminates the need for complex image segmentation algorithms. Lastly, I will link our bioengineering research to driving cytology needs, including understanding the role of protein signaling and truncated isoforms in development of breast cancer drug resistance and understanding protein signaling in individual circulating tumor cells. Taken together, we view microfluidic design strategies as key to advancing protein measurement performance needed to address unmet gaps in quantitative biology and precision medicine.

# A binary two-dimensional honeycomb lattice with strong spin-orbit coupling and electron-hole asymmetry

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Two-dimensional (2D) materials consisting of heavy atoms with particular arrangements may host exotic quantum properties. In this talk, I will present a unique 2D semiconducting binary compound, Sn2Bi atomic layer on Si(111), in which hexagons are formed by bonding Bi with a triangular network of Sn. Due to the unique honeycomb configuration, the heavy elements and the energy-dependent hybridization between Sn and Bi, 2D Sn2Bi not only shows strong spin-orbit coupling effects, but also exhibits high electron-hole asymmetry: nearly free hole bands and dispersionless flat electron band co-exist in the same system. By tuning the Fermi level, it is possible to preserve both nearly free and strongly localized charge carriers in the same 2D material, which provides an ideal platform for the studies of strongly correlated phenomena and possible applications in nanodevices.

# Advanced surface functionalization based on chemical gradients in plasma polymer films

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<sup>1</sup> Empa, Swiss Federal Laboratories for Materials Science and Technology

Plasma polymer deposition making use of non-equilibrium conditions during film growth yields surface functionalization that generally undergo reorganization processes to approach equilibrium state. Most of all, when material's surfaces are exposed to aqueous environments, water molecules might not only adsorb on the surface but can also react with the surface material or penetrate into it. This interaction might be detrimental yielding oxidation and degradation reactions, but it is also substantial e.g. for the interaction with biomolecules. Plasma process conditions and film structures are thus investigated to enhance the stability of plasma polymer films in water with respect to oxygen- or amine-rich functional surfaces as well as for siloxane coatings. Therefore, a controlled change in deposition conditions during film growth is conducted resulting in vertical gradient structures affecting chemical composition, crosslinking, density, porosity, wettability etc. of the outermost few nanometers of the plasma polymer film. The response of such surfaces in water as well as in aqueous media containing biomolecules is reported with respect to protein adsorption and surface functionalization for bio sensors.

# Advances in nanotoxicology using ion probes

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The increasing use of engineered nanoparticles and metallic nanosized complexes in a variety of applications, from technological to medical areas, raised concerns on their potential toxicity. It is therefore urgent to understand how these nanosized entities interact with biological systems. Due to their small size, the identification and localization within cells is extremely challenging. Various cutting edge techniques are required to detect electron-dense nanoparticles and quantify metals inside the cells. However, few of these techniques are able to peer into cells combining nanometre probe-formation with several other specifications such as, precise elemental quantification, depth profile of the element of interest, and subwavelength fluorescence imaging. This is the prospect of nuclear microscopy techniques using MeV ion beams.

Such type of ion probes can be used for whole-cell investigations delivering unique and relevant information for nanotoxicology studies. The main issues are (2): i) visualization of individual and small clusters of nanoparticles; ii) and production of 3D maps of their distribution inside cells. This will help to unravel the internalization efficiency, the mechanisms of action and eventually shed light on the toxicity of nanosized materials to cells (1).

An overview of ion probes contribution to nanotoxicology advances will be given concerning visualization and quantification systems, their limitations and pitfalls.

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# Tribological and mechanical properties and oxidation resistance of tungsten and tungsten nitride films at temperatures up to $500 \square^{\circ}$ C

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The presentation deals with the structure, microstructure, mechanical and tribological properties and oxidation resistance of WNx films with a stoichiometry x=[N]/[W] ranging from 0 to 1.5 prepared by magnetron sputtering. The as-deposited films exhibit high hardness H=22-34 GPa and (1) columnar microstructure and alpha-W phase at x lower or equal to 0.20 or (2) fine-grained microstructure, and a mixture of alpha-W and beta-W2N phase at x between 0.20 and 0.64, beta-W2N phase at x=0.64 and delta-WN phase at x=1.5. It was found that the tribological properties of the films are strongly influenced by (1) the relative humidity RH of ambient air ranging from 5 % (dry nitrogen) to 82 % (moist environment), the coefficient of friction (CoF) decreasing from 0.75 to 0.16 and wear rate k increasing from 0.004 to 2×10E-6 mm3/Nm, respectively, due to the surface hydration at temperature T≈22 ° C, (2) the mechanical properties of WNx, where the films with alpha-W phase exhibit low ratio hardness to effective Young's modulus H/E lower to 0.1 and high k up to 5×10E-6 mm3/Nm, the films with beta-W2N and/or delta-WN phase exhibit H/E higher to 0.1 and low k up to 0.01×10E-6 mm3/Nm at T ranging from 22 to 150 °C, and (3) the WO3 surface scale with columnar microstructure created at T increasing from 150 °C to 500 °C acts as an lubricant where CoF decreasing to ≈0.5 due to its low H=4 -5 GPa but k increasing above 6×10E-6 mm3/Nm due to its low H/E=0.05.

# Performance improvement of nanomesh electrode and nanorod array in III-V solar cells

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In the renewable energy category, the solar cells have attracted great attention for alleviating the energy shortage problem. Among the highly anticipated solar cells, the III-V compound solar cells revealed the highest conversion efficiency due to their high carrier mobility and high absorption coefficient. In this study, the AuGeNi/Au nanomesh electrode structure with various intervals were designed on InGaP/InGaAs/Ge triple-junction solar cells to replace the conventional bus-bar electrodes with interval of 125 um The conversion efficiency of the solar cells using nanomesh electrode with the interval of 100 um was 35.25% that was better than that of 30.84% for the solar cells with conventional bus-bar metal electrode. The performance improvement was attributed to that the block ratio of the shadow area and the series resistance of the solar cells using nanomesh electrode structure with interval of 100 um were reduce form 7.50 to 0.66% and 9.1 to 7.9 ohm-cm2, respectively, in comparison with the solar cells with conventional bus-bar metal electrode. To further improve the performance of the solar cells with AuGeNi/Au nanomesh electrode of 100 um, the TiO2 nanorod array with period of 1.00 um was used to replace the standard TiO2/SiO2 antireflection layers. The conversion efficiency was further improved from 35.25% to 37.00%. Consequently, the designed nanomesh electrode and nanostructured antireflection structures were promising candidate for improving conversion efficiency of solar cells.

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## Post-Li-ion batteries: promises and challenges

M. Rosa Palacin

Current societal challenges in terms of energy storage have prompted to an intensification in the research aiming at unravelling new high energy density battery technologies with the potential of having disruptive effects in the world transition towards a less carbon dependent energy economy through transport electrification and renewable energy integration. Aside from controversial debates on lithium supply, the development of new sustainable battery chemistries based on abundant elements is appealing, especially for large scale stationary applications. Interesting alternatives are to use sodium, magnesium or calcium instead of lithium.

While for the Na-ion case fast progresses are expected as a result of chemical similarities with lithium and the cumulated Li-ion battery know how over the years, for Ca and Mg the situation is radically different. On one hand, the possibility to use Ca or Mg metal anodes which would bring a breakthrough in terms of energy density, on the other, development of suitable electrolytes and cathodes with efficient multivalent ion diffusion are bottlenecks to overcome.

The presentation will serve to discuss such promises and challenges and describe current state-of-the-art of research in the field.

# Bioinspired approach to functional hybrid materials by vapor phase infiltration

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The ALD process can be seen from various perspectives. On the one hand, it allows controlled deposition of thin films on a variety of substrates and in this way enables a modification of a given functionality of a surface or even introduction of a new functionality. On the other hand, it may be seen as a chemical reactor that allows precise dosing of a chemical, allowing for chemical interaction and modification of the substrate. In this talk, some approaches will be discussed that show great promise for establishing ALD as the method-of-choice for innovation in technological fields beyond the microelectronics industry. Rather than growing thin conformal films, the ALD process technology is applied to controllably grow nanoparticles on functional substrates adding value to their chemical or electrochemical properties. In an adapted processing mode, the ALD processing technology also allows infusing metals into polymeric substrates, which leads to novel material blends that cannot easily be obtained in other ways. In either of those cases the chemical or physical properties of the initial substrate are improved or new functionalities added. With some showcases, this talk will discuss approaches towards non-traditional application of ALD to fabricate novel materials with great promise in energy storage, catalysis, personal protection or flexible electronics.

# The vacuum system of MAX IV 3 GeV storage ring.

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The vacuum system of the 3 GeV storage ring of MAX IV laboratory is innovative in the way it has been designed and constructed. It is the only storage ring that has its full circumference coated with non-evaporable getter (NEG). The vacuum performance of the storage ring proved to be very good: with low pressure levels and long beam lifetime. A brief description of the design, installation and operational results of the vacuum system are introduced.

# Imaging with XPS: Advanced Characterization for Advanced Materials and Devices

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X-ray Photoelectron Spectroscopy (XPS), as a surface sensitive technique with the sensitivity down to single atomic layer, provides unique information about elemental composition and chemical and electronic states of elements in the material. For some research goals, however, this knowledge is not sufficient as it does not provide the entire information required for a comprehensive characterization of the investigated system. In addition to the basic functions of standard XPS, our instrument is equipped with advanced capabilities such as XPS imaging, which is particularly valuable in the analysis of patterned or inhomogeneous specimens. Following image acquisition, specific areas can thus be chosen and small spot XP spectra acquired at sites of particular interest.

We present here two examples where XPS imaging is successfully used providing crucial information for understanding the investigated systems.

In the first example bunches of GaN nanowires (50-100 nm each) randomly spread on Si substrate were monitored with XPS imaging. Then, focusing on the GaN bunch itself, small area XP spectra were obtained. This allowed to get precise top surface composition of the bunches significantly consuming the analysis time.

In the second example variations in chemical composition though dimensions of the

CsxMa1-xPbBr3 (MA = CH3NH3) crystal were studied using XPS imaging. Significant changes in the N/Cs ratio, depending on the distance from the crystal edge/center, were observed on the top surface. Variations in the N/Cs and Pb/(N+Cs) ratios were also observed along the crystal bulk.

# Cavitas biosensors (soft contact lens & mouthguard type sensors) with deposited Pt and Ag/AgCl electrodes on biocompatible polymer

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#### <sup>1</sup> Tokyo Medical and Dental University

"Cavitas sensors" attached to body cavities such as a contact lens type and a mouthguard ("no implantable", "no wearable") are attracted attention for preventive medicine. In this contribution, the soft contact lens (SCL) glucose sensor for tear sugar monitoring and the mouthguard (MG) biosensor with dental materials integrated with Bluetooth low energy (BLE) wireless module would be introduced.

The SCL biosensor for tear glucose was fabricated using biocompatible 2-methacryloyloxyethyl phosphorylcholine (MPC) polymer and polydimethyl siloxane (PDMS) as the biosensor material. The biosensor consists of a flexible Pt working electrode and an Ag/AgCl reference/counter electrode, which were formed by ion-beam sputtering. The sensing region was modified with glucose oxidase (GOD). The calibration range of the SCL biosensor was from 0.03–5.0mM. As the result of the sensor application to a rabbit, the basal tear glucose was estimated to 0.11mM. Also, the change of tear glucose induced by the change of blood sugar level was assessed by the oral glucose tolerance test.

The MG biosensor with dental materials integrated with BLE wireless module was developed. The biosensor based on the integration of Pt and Ag/AgCl electrodes with an GOD membrane was fabricated on the MG surface of a polyethylene terephthalate glycol (PETG). In artificial saliva, the glucose sensor exhibits high-sensitive detection in a range of 5-1000 µmol/L.

The self-detachable cavitas sensors are expected to improve quality of life in view of the aging of society in the near future.

## Crystallographic Phase Transitions of AlCuMgZn Alloys

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The development of novel light-metal alloys represents an important task in the further evolution of technical materials. Multicomponent systems with more than 4 metals are very promising to outperform currently available alloys.

Thus a detailed structural investigation of the formed crystals is essential for the prediction of multicomponent systems properties. In this work we produced layers consisting of AI, Cu, Mg and Zn, all of which are promising constituents for novel light-metal alloys.

Multicomponent layers were co-deposited by magnetron sputtering. Using different geometrical arrangements of the sputter sources relative to one another, the generation of a composition gradient on the substrate was accomplished. The major advantage of this method is that combinations of materials that are difficult to produce by melting can be deposited together by separate sources on the sample. The starting materials were alloyed AlCu2 and MgZn2 discs. At these stoichiometric compositions, Laves-phases of the respective elements are formed. Mixing and varying the relative amount of the constituents may lead to the formation of new phases. Since sputter deposition is a highly non-equilibrium process, the formation of crystallographic ordering could be investigated by subsequent heat treatment and comparison of 'as-deposited' samples.

Grazing incidence XRD measurements showed a composition-dependent continuous change of different crystal structures with combined phases of all constituent materials including hexagonal and cubic systems. These results help answering the question, which metals are the driving elements for the formation of certain crystalline systems and how a simple structure without brittle intermetallic phases can be accomplished.

# Cooperative action for molecular debromination reaction on Cu(110)

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The metal-catalyzed coupling of halobenzene derivatives leading to biaryls and larger carbon-based structures is a fundamental reaction in chemical synthesis. Copper is the paradigmatic catalyzer of the Ullmann cross-coupling reaction. Despite this, its role in the reaction is still under debate. Here, we shed light on the mechanistic steps of the debromination, characterizing a prototypical molecule, namely 4,7-dibromobenzo[c]-1,2,5-thiadiazole (2Br-BTD), deposited on a Cu(110) surface.

By means of scanning probe techniques and first principle calculations, we demonstrate the oxidative addition of Cu atoms leading to a -C-Cu-Br metal-organic complex. The scission of the strongly bound bromine atoms requires the cooperative action of neighbouring complexes resulting in the formation of Cu coordinated BTD structures.

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## Long-lived vibrations in molecule-metal surface interaction

Igor Rahinov<sup>1</sup>, Pranav Shirhatti<sup>2,3</sup>, Kai Golibrzuch<sup>3,4</sup>, Jörn Werdecker<sup>5</sup>, Jan Geweke<sup>3,5</sup>, Jan Altschäffel<sup>3,4</sup>, Sumit Kumar<sup>4</sup>, Daniel Auerbach<sup>3,4</sup>, Christof Bartels<sup>3,6</sup>, Alec Wodtke<sup>3,4</sup>

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The most common mechanism of catalytic surface chemistry is that of Langmuir and Hinshelwood (LH). In the LH mechanism, reactants adsorb, thermalize with the surface and subsequently react. At the same time, molecular vibration is known to enhance the rates of gas-phase chemical reactions as the motion associated with bond stretching facilitates the reactant molecule approach to the transition state. However, for reactions occurring on via LH mechanism on metal surfaces, relevant for heterogeneous catalysis reactions, the ability of vibrational excitation to promote reactivity is hampered by rapid dissipation of the vibrational energy of the reactant into electronic excitation of the metal within several picoseconds. Our recent findings challenge this paradigm: we have demonstrated that excited vibrational states can survive longer than expected – suggesting vibrational excitation might promote or modify heterogeneously catalyzed LH-chemistry on metals [1]. In our experiments IR laser excitation was used to prepare short pulses of vibrationally excited CO(v=2) molecules that impinged and scattered from clean Au(111) surface. Our quantum-state-resolved scattering studied in temporally and spatially resolved fashion unambiguously demonstrated that vibrationally excited molecules, prepared in the v=2 state retain significant vibrational excitation, even after residing ~ 100 ps on Au(111). While previously studied CO on Pt(111) and Cu(100) is strongly chemisorbed to the surface and the molecular vibration induces electron flow between the metal and the 2pi\* orbitals of CO, on Au(111) a weaker physisorption results in longer vibrational lifetime.

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# The new static expansion system based on aluminium technology at PTB

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Static expansion is a well-established method for realising the pressure scale in medium and high vacuum by a fundamental method. The main component of uncertainty of the generated pressure in such a system is due to the temperature uncertainty of the vessels involved during an expansion. Stainless steel is a relatively poor heat conductor so that considerable gradients of temperature can develop across a larger vessel. For this reason, PTB developed a new, fully automated, static expansion system based on aluminium which has a high thermal conductivity. The temperature uniformity of the vessel is greatly improved compared to a stainless-steel vessel under the same conditions. The total uncertainty of the realized pressures is considerably reduced. The automatization and the use of very small volumes required a careful investigation of what happens during the closing of the valves in order to detect and correct any pressure differences across the valve plates. The validation and first comparisons of the new system with existing standards will be presented.

## Passivation of reflective silver thin films by surface nanolayers

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It is well known that silver (Ag) thin films have high electrical and optical properties but also low stability. We have developed a highly stable Ag thin film where thermal agglomeration can be suppressed, by utilizing nanometer thick surface Al layers. Then we have confirmed that Al surface nanolayer deposited Ag films show a high optical reflectance as well as Ag single film. In the present study, we investigate durability of the Ag films with surface nanolayers under high humidity condition. We prepared Ag single layer(150 nm), Ti(1, 3 -nm) / Ag films and Al(1, 3 -nm) / Ag films on glass substrate by rf magnetron sputtering in Ar discharge. The samples were kept for 16 hrs in a chamber where temperature and humidity was set to 55oC and 90%RH, respectively. After the test, agglomeration occurred in Ag single layer and optical reflectance was decreased. On the other hand, Ti or Al nanolayer covered Ag films kept smooth surface even after the test. The surface roughness observed using AFM was as small as 1.0 nm. As a result, we have found that both Al and Ti surface nanolayers can play significant role as passivation layer under high humidity condition. However, Ti / Ag films showed a lower reflectance due to light absorption by TiO2 layer formed on the surface, and the samples with Al surface nanolayer showed a higher optical reflectance.

# Characterization of external potential for field emission resonances and its applications on nanometer-scale measurements

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The form of the external potential (FEP) for generating field emission resonance (FER) in a scanning tunneling microscopy (STM) junction is usually assumed to be triangular. We demonstrate that this assumption can be examined using a plot that can characterize FEP. The plot is FER energies versus the corresponding distances between the tip and sample. Through this energy-distance relationship, we discover that the FEP is nearly triangular for a blunt STM tip. However, the assumption of a triangular potential form is invalid for a sharp tip. The disparity becomes more severe as the tip is sharper. We demonstrate that the energy-distance plot can be exploited to determine the barrier width in field emission and estimate the effective sharpness of an STM tip. Because FERs were observed on Pb islands grown on the Cu(111) surface in this study, determination of the tip sharpness enabled the derivation of the subtle expansion deformation of Pb islands due to electrostatic force in the STM junction.

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# Determination of virial coefficients used for optical pressure standard FLOC

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To measure the refractive index of gases with very high resolution we can use an optical resonator like Fabry-Perot interferometer. The National Institute of Standards and Technology is developing a new low-pressure sensor which is based on the measurements of (nitrogen) gas refractivity inside a Fabry-Perot cavity, so this allows a new realization of Pascal. In order to determine the pressure a laser is locked to the optical cavity while the laser frequency is interrogated. The frequency will change according to the pressure (density) of the gas which in our case was nitrogen [1]. For gases with simple electron structure (with mostly two electrons) such as helium the refractivity and density virial coefficients can be calculated through quantum mechanics [2]. For other gases, the value of density virial coefficients must be measured. In this research work, in order to determine the gas density virial coefficients, pressure determinations from the Fixed Length Optical Cavity – FLOC were compared with those of a piston gauge for four different temperatures (30 degree Celsius to 45 degree Celsius) in the pressure range from 50 kPa to 150 kPa.

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Opt. Lett. 40, 3945 (2015)

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#### high-resolution vibronic spectra of molecules on molybdenum disulfide allow for rotamer identification

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<sup>1</sup> Freie Universität Berlin, Berlin, Germany <sup>2</sup> University of Massachusetts, Amherst, United States Scanning tunneling spectroscopy (STS) is a tool that allows to address individual molecules in a precisely known surrounding. However, it bears the drawback that it requires a conductive substrate. Deposition of organic molecules on a metal substrate leads to strong hybridization of the electronic states. Preservation of the molecular character requires the inclusion of thin band-gapped materials. Here, we present STS experiments performed on 2,5-bis(3dodecylthiophen-2-yl)thieno[3,2-b]thiophene (BTTT) molecules adsorbed on a single layer molybdenum disulfide (MoS2) on Au(111). We show that it acts as an effective electronic decoupling layer that exhibits a small electron-phonon coupling strength. Differential conductance spectra of the molecules exhibit a multitude of sharp characteristic peaks, originating from vibronic states of BTTT. These vibronic fingerprints of different molecules allow for an identification of different rotamers. DFT calculations of the molecule in gas phase provide all details for an accurate simulation of the vibronic spectra of both investigated rotamers [1].

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# Quantum Simulation with Electrons in an STM

In a visionary colloquium nearly sixty years ago, Richard Feynman proposed to study complex and elusive quantum systems using more controllable analogues, an approach known as quantum simulation [later published, 1]. Quantum simulators based on ultracold atoms, nanophotonics, trapped ions, and superconducting circuits have been developed and successfully applied to study a host of different phenomena [2]. In contrast, electronic quantum simulators have been lacking behind.

In this talk, I will demonstrate that electron gases on well-defined metal surfaces form an excellent platform for quantum simulation. By patterning the surface with atomic scale precision using a scanning tunneling microscope, the electrons can be corralled into artificial lattices of nearly any geometry. The same microscope can then be used to measure the local density of states at all positions of interest and to probe the spatial extend and shape of the electronic states. I will show several examples of how we exploit the tunability of this platform. Particular emphasis will be given to our recent efforts to create and study topological insulators.

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# In-situ characterization of O-terminated copper tips for high-resolution atomic force microscopy

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The use of chemically inert tips allows to directly probe the repulsive interaction regime and thus to obtain high spatial resolution. Gross et al. found in 2009 [1] that CO-terminated metal tips enable intramolecular resolution imaging of organic molecules. Later, it was found that terminating the tip apex with noble gas atoms [2] achieves a similar spatial resolution. Recently, Mönig et al. [3] proposed to use oxygen-terminated Cu tips that apparently are also quite inert, but are stiffer in lateral directions than CO tips. So far, to verify tip functionalization with oxygen, the contrast of STM and AFM images of copper oxide domains has been compared to calculated images for different tip models. Here, we apply the COFI method [4] and force spectroscopy to characterize O-terminated Cu tips in-situ on a Cu(110) surface. Our approach is an efficient way to experimentally determine both the structural composition as well as the chemical species of the tip apex. Knowledge of these properties is of crucial importance, especially if the tips are used for experiments on other sample systems. The experimental data about the tip structure and composition is expected to improve the precision of theoretical studies about the interaction between tip and sample.

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# Self-assembly mechanism and control method of atomic-size tips

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The smartest method to fabricate nanostructures is to use self-assembly mechanism which forms desired configurations as a consequence of specific, local interactions among the components themselves, without external managements. Atomic-size tips can be widely used in a large number of scientific and technological applications, such as coherent electron sources to improve electron optics devices, field ion emitters to advance focused ion beam systems, and sharp probes to increase resolution for scanning probe microscopes, etc. After years of efforts, many atomic-size tips have been put into reality, including noble metal covered W or Mo single atom tips, oxygen induced Ir or Ni single atom tips, and CoPt alloy ultra-sharp tips, etc. Atomic dynamics, facet phenomena, surface reconstruction, and equilibrium shape, etc. are studied by field ion microscopy to illustrate the growth of several atomic-size tips. The conclusions provide the possible control methods for various atomic-size tips in practical applications.

# Ultra-Low Out Gas Residual Gas Analyzer, WATMASS

Shinsuke Kishikawa, Masahide Kuroiwa

In the ultra-high vacuum (UHV) and extremely-high vacuum (XHV) region of 10-7 Pa or lower, when conducting residual gas analyses with a standard quadrupole residual gas analyzer, outgassing from the sensor tip ion source cannot be ignored, and it is difficult to perform high-precision gas analyses under such conditions.

The most important element for solving this problem is a flange-integrated ion source in which radiant heat from the thermionic cathode filament cannot reach the other electrode. A thermionic cathode filament/grid is surrounded by a low-thermal-radiation, high-thermal-conductivity 0.2% beryllium-copper alloy (BeCu) as shown to the right in Figure 1. This is constructed such that heat generated from the filament does not flow to the quadrupole analyzer section and the secondary electron multiplier (EM).

As a result, WATMASS outgassing decreases to approximately 1/10000 that in a conventional residual gas analyzer (stainless steel material), and high precision gas analyses in the XHV region can be performed. Fig. 2

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# Redox Properties of Cu2O(100) and (111) Surfaces

Chunlei Wang, Jonas Weissenrieder

Intense research efforts are directed towards Cu and Cu2O based catalysts as they are viewed as potential replacements for noble metal catalysts. However, applications are hampered by deactivation, e.g. through facile complete oxidation to CuO. Despite the importance of the redox processes for Cu2O catalysts a molecular level understanding of the deactivation process is still lacking. Here we study the initial stages of oxidization of well-defined Cu2O bulk single crystals of (100) and (111) termination by means of synchrotron radiation X-ray photoemission spectroscopy (XPS) and scanning tunneling microscopy (STM). Exposure of the (100) surface to 1 mbar O2 at 25 °C results in formation of a 1.0 monolayers (ML) CuO surface oxide. The surface is covered by 0.7 ML OH groups from trace moisture in the reaction gas. In contrast, neither hydroxylation nor oxidation was observed on the (111) surface under similar mild exposure conditions. On Cu2O(111) the initial formation of CuO requires annealing to about 400 °C in 1 mbar O2, highlighting the marked different reactivity of the two Cu2O surfaces. Annealing of the (100) surface, under ultrahigh vacuum conditions, to temperatures up to 225 °C resulted in removal of the OH groups (0.46 ML decrease) at a rate similar to a detected increase in CuO coverage (0.45 ML increase), suggesting the reaction path 2OH + Cu2O = H2O + 2CuO. STM was used to correlate the observed changes in surface chemistry with surface morphology, confirming the surface hydroxylation and CuO formation.

# Scanning transmission x-ray microscopy investigation of lithium ion battery materials at the pohang light source

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A scanning transmission x-ray microscope (STXM) at the Pohang Light Source (PLS-II) is in flux-wise optimized for the investigation of transition metal (TM; such as Ni, Co, Fe, Mn) L-edges and O K-edge spectral features with a local space resolution of 30nm [J. Synchrotron Rad. 25, 878 (2018)]. There has been intense application activity on TM based lithium ion battery (LIB) materials with an aim to understand local valence, chemical state, and electronic structure of individual element or surrounding the element.

In the presentation, we will provide spectral feature changes and the resulting information of valence, chemical state changes of each element and hybridization changes between the TM 3d (t2g, eg) and O 2p orbitals for Ni, Co, Mn, and Fe based LIB materials. Depending on the sample recipe, elemental content ratio, lithiation and delithiation processes, the study provides diverse spectral features and spectral information; not only in the L-edges of TMs, such as Ni, Co, and Mn L-edges, but also in the O K-edge. As an example, 2+ to 4+ valence is in variety observed for the acting-role Ni element of the LiNiCoMnO LIB material; which is generally expected from previous reports, but also shows other detailed information. These spectral features also differ from depending on the local position inside individual particle. An attempt is being made to correlate the measured spectral features with the LIB materials' lithiation-delithiation environment.

# quantum tunneling mediated water partial dissociation on Pt(111) at low temperature

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The interaction of water with Pt(111) surface has been intensively investigated due to the crucial role of Pt(111) in electrochemistry and catalysis. The first water layer on Pt(111) is widely thought not to dissociate and forms root 37 and root 39 wetting phase. Here we report the structural change of the first layer hydrogen-bonding network from root 37 phase to complete hexagonal structure after annealing at 145K. Unlike the classic root 3 bilayer phase, the hexagonal network is a mixture of H2O and OH with a ratio of 5:1, which is identified with a combined noncontact atomic force microscopy and X-ray photoelectron spectroscopy techniques. To explore the reaction mechanism during the transition from intact to partial dissociation network, we tracked the transition rate of H2O and D2O, respectively, at the annealing temperature range of 120-145 K. At high temperature, the reaction follows the Arrhenius law presenting a linear plot, in which regime the reaction barrier is dominated by the classical dissociation energy of water molecules. Tunneling is most relevant at low temperature. However, the partial dissociation reaction of water network on Pt (111) is cooperated with the rotations and rearrangement of the water molecules. Therefore, we attributed the partial dissociation reaction mechanism at low temperature to the vibrational assisted tunneling, since the extracted activation energy barrier of H2O and D2O are 205 and 150 meV, respectively, which correspond to the bending mode of water molecule.

## adaptable PEI coating technique on silicon microsystems for generic bacteria capture

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In recent years, PolyEthylenImine has turned out to be an efficient cationic polymer for capturing bacteria by electrostatic interaction. In this work, zeta potential measurements and thickness measurement allowed us to optimize the conditions of the deposition and to characterize the PEI layers. For the first time different bacteria species were efficiently captured on PEI. The results of the membrane integrity assessments after capture indicated that the PEI/bacteria interactions did not damage bacteria membrane permeability. The deposition simplicity of the PEI layer facilitates its implementation in two main technological fabrication processes. First, localization of PEI micropatterns on silicon antennas was carried out combining photolithography and printing techniques, which enables strong control over the size and shape of functional areas and minimizes material waste. Localized bacterial capture on THz antennas was demonstrated showing the ability to trap bacteria in 2D arrays of features of arbitrary shape, independent of the topography of the sample. Then, to overcome the limitation of the capture performance due to the accessibility of cells to the surface, micropillar array reactors were coated with PEI. The presence of micropillars greatly increase the surface-to-volume ratio compared to planar substrates. The functionalized reactors proved highly efficient, capturing over 99 % of 108 bacteria per mL at 100  $\mu$ L/min. The reversible adhesion of the bacteria allows for the release and re-capture of adhered bacteria via adjustment of the buffer pH. Such surface functionalization with PEI layers have many applications in lab-on-chip systems and spectroscopic analysis for bacterial identification and diagnostic studies.

## On the formation of converted layers during erosion of composite AI-Cr arc cathodes

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Al-Cr composite cathodes are frequently employed for the cathodic arc deposition of Al-Cr-based oxide and nitride coatings. Due to local consecutive melting-solidification cycles caused by the motion of the cathode spot over the cathode surface, a so-called converted layer is formed that differs from the virgin cathode concerning microstructure, chemistry and phase composition [1]. A thorough characterization of the converted layer and a detailed understanding of its formation are essential as it determines the plasma properties and, hence, the thin film growth conditions.

Within the current work, composite cathodes with composition of Al0.5Cr0.5 were eroded in inert Ar gas at a pressure of 1 Pa applying a current of 60 A. The analysis of the eroded cathode surface by X-ray diffraction and scanning electron microscope revealed the presence of several intermetallic Al-Cr phases. Further details were obtained by differential scanning calorimetry and in-situ X-ray diffraction which confirmed the existence of, due to their different stoichiometry, unexpected phases like Al4Cr and provided insights regarding the formation mechanisms of the converted layer. Subsequently, selected areas of interest within the converted layer were lifted out using focused ion beam and their microstructure and phase composition were studied by conventional transmission electron microscopy, selected area electron diffraction and transmission Kikuchi diffraction. The combined results from the above-mentioned techniques aid the development of a model describing the formation of converted layers on eroded composite arc cathodes.

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# Spontaneous breaking of time-reversal symmetry at the edges of 1T' monolayer transition metal dichalcogenides.

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In this work[1], we use Density Functional Theory calculations and the Greens's function formalism to investigate the edges of 1T' phase monolayer transition metal dichalcogenides (TMDs). This is an interesting class of materials since many are known to be topological insulators. Previous electronic structure calculations on surfaces has either been using the traditional slab approach or a non-self-consistent Green's function method. We apply the novel Surface Green's Function method[2] implemented in QuantumATK. This allows for the self-consistent simulation of a single surface coupled to an infinite bulk of the material. Our results show that the time-reversal symmetry is spontaneously broken on some of the edges of MoS2, MoTe2 and WTe2 and that gapless magnetic states with a non-collinear spin texture appear. The breaking of the time-reversal symmetry means that the topological properties of the material are removed; there is no guarantee for finding gapless edge states and these states will no longer be topologically protected. The findings may therefore have an impact on the prospect of utilizing the 1T' TMDs as topological insulators. We furthermore apply an electric field perpendicular to the monolayers and treat the electronic response fully self-consistently. As previously suggested by Qian et al.[3], we find that the topological states of the monolayer 1T' TMDs can be switched off by an electric field but that the magnetic states remain gapless.

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- [3] X. Qian et. al., Science 346, 22 (2014), 1406.2749

# Investigation of tribomechanical surface properties of polymers filled with biochar

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The field of composite materials is always in quest of materials with improved properties. The most interesting properties are usually mechanical and electrical ones. Beside these also the surface properties are relevant because the surface interacts with the outer world from many points of view (chemical, tribological, ...). Carbon fillers such as carbon black are among the most widely used because of their low price and availability, although being obtained from oil they are impacting on the environment and depleting the resources. Biochars, i.e. carbon fillers derived from biomasses are actively investigated as a possible environment friendly alternative for current carbon fillers.

In this work we compare friction coefficient, surface hardness and wettability of polymer composites containing carbon black and a number of different biochars. We present a correlation between the type of biochar and its amount and the surface properties detailed above, with the support of XPS investigation, and a focus of the various mechanisms involved.

We show that a proper selection of biochar type and amount allows to achieve results close to or even exceeding those obtained with carbon black with the same easiness of dispersion and lower environmental impact.

# Electronic structure defects in SiC: What have we learned from joint DFT/DLTS studies?

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A wide and indirect band gap, high chemical and thermal stability, as well as radiation and electrical hardness, are among the merits that make silicon carbide (SiC), in particular its 4H polytype, an outstanding material for high-voltage and high-power electronics. SiC-based radiation detectors are highly sensitive to defects that introduce deep carrier traps, especially to those with large capture cross section for minority carriers. Among the most recombination-active defects in 4H-SiC we have the carbon vacancy, which may be created by ion and electron bombardment, but due to its low formation energy, it is also present in asgrown material. We report a joint work by means of density functional theory (DFT) calculations and space-charge techniques, including deep-level transient spectroscopy (DLTS) and Laplace-DLTS, to investigate the capture and emission kinetics of electrons involving the Z1/2 electron trap, which was assigned to the carbon vacancy in 4H-SiC. We show how first-principles calculations can be applied to unravel the positions of transition levels in the band gap, as well as the high of capture barriers. A direct comparison between calculations and measurements, allow us to demonstrate the negative-U ordering of the acceptor levels, as well as to assign Laplace-DLTS peaks to electron emissions from carbon vacancies in two symmetry-inequivalent lattice sites.

# Surface decorated biochar as highly tunable carbon bioderived material

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Carbon based materials gained more and more interest in recent years due to their outstanding properties. However high cost and difficult in isolation/purification is a strong limit to the massive use of graphene[1] and carbon nanotubes[2] leading to investigation of alternative routes. Biochar is one promising alternative and it is a well assessed route for producing carbon based material from biomasses scaffolds[3]. Differently from the assessed allotropic carbon phases (graphite, diamond, ...), biochar can retain the original structure of biomass and its properties can be easily tuned by specific treatments.

As high electrical conductivity and high specific surface can be achieved, biochar can be considered as a conductive support for nanoparticles to be used in sensors or other devices.

In this research we report on the use of inorganic salts (i.e. Na2CO3, KI, Fe(NO3)3, Bi(NO3)3) for decoration of olive rape seed derived biochar with metal and oxide nanoparticles. A carbon-on-carbon growth is also presented that allows to achieve improved properties without inorganic additives.

According to this purposes, we analyzed the hybrid materials produced using several techniques as Raman spectroscopy, surface area analysis, XPS and FESEM evaluating the morphology changes induced by the treatments. The electrical properties of the structures are also investigated in details.

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# Ti-Mg alloy coatings deposited on AISI 316L stainless steel for biomedical applications

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Two crucial criteria for manufacturing biomedical metallic implants are the absence of toxic elements and a low modulus of elasticity. Titanium and its alloys have better mechanical properties, biocompatibility, and corrosion resistance as compared to the most used metallic biomaterials, stainless steel (SS) and cobalt-based alloys [1]. Although Ti alloys are significantly more expensive than SS and Co-Cr alloys, they present better biocompatibility and have elastic modulus values closer to the human bones. An interesting option would be to coat an implant with Ti-based alloy thin films having adequate composition and thickness so that the coating would enhance the material biocompatibility [2]. Since magnesium is a lightweight metal, it is expected that alloying Ti with Mg produces a useful metallic biomaterial [3]. Due to the lack of complete solubility in the Ti-Mg phase diagram, high Mg content Ti-Mg alloys cannot be obtained by conventional melting processes [3], thus non-equilibrium processes, such as magnetron sputtering, have been employed for producing Ti-Mg alloys [4]. In this work, Ti-Mg alloy coatings have been deposited on AISI 316L SS by magnetron sputtering. The structure, morphology, and nanostructure of the coatings have been analyzed by x-ray diffraction, atomic force microscopy, scanning electron microscopy, and transmission electron microscopy, while the mechanical properties have been evaluated by nanoindentation, scratch, and nanowear tests.

## Characterization of nanostructures formation in black-silicon obtained by CF4/H2 plasma process

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Nanostructured silicon (black silicon, BS) was prepared by means of a mask-less plasma process (Reactive Ion Etching) employing CF4 and 10 % of H2 as reaction gases. A full texturing effect was achieved supplying 250W RF power, for a 20 minute process time. These process parameters were previously found as the optimal ones to fabricate silicon surfaces with an ultra-low reflectance. In this work samples obtained with different process time (30 sec-20 min) were studied to investigate in detail the resulting morphological and chemical changes with the aim to identify a growth mechanism of the nanostructures constituting the black silicon. They were characterized via Secondary Electron Microscopy (SEM), 3D mechanical profilometry, X-ray Photoelectron Spectroscopy (XPS), Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and Atomic Force Microscopy (AFM) while the plasma phase was investigated using Optical Emission Spectroscopy (OES). In order to discern from the effect of the morphological features, two different experimental procedures were followed to study the effects of the plasma chemistry on the nanostructures growth. The first was to treat the Si surface with the plasma continuously at different exposure times (0.5, 1, 2, 5, 15, 20 minutes). The second was to expose the Si surface to the plasma for a net total time of 20 minutes but cycling between 1 minute of plasma treatment and 1 minute of pumping of the exhaust mixture. In this way the reactive species formed in the plasma phase were removed before the plasma was regenerated.

The results showed that the net process is an etching process. However the etching rate decreases with the exposure time. The two procedures and OES spectra showed that the chemistry of the plasma phase does not change and therefore is not responsible for such decrease. SEM, AFM, XPS and ToF-SIMS results suggested that such decrease is related to a continuous change of the chemistry and the morphology at the surface. A rationale is given via a proposed grow mechanism of the nanostructures. Finally the reflectance of the full nanostructured BS was simulated with a simple model.

# A capacitance diaphragm gauge with a 1.3Pa full scale

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Etching of semiconductors chips is a complex process and there are critical process steps that tend to go to lower pressures. At lower pressures scattering at the residual gas is reduced which allows obtaining narrower and deeper vias, important for threedimensional chip structures. Many etch process pressures today are around 1 Pa and use a 13.3 Pa full scale CDG in the second measurement decade where accuracy is already lower.

We have developed a heated capacitance diaphragm gauge with 1.33 Pa (10 mTorr) full scale. The low full scale is achieved by the deflection of a thinner membrane together with focus on noise reduction and not by electronic amplification. We will present performance parameters, especially calibration data against 13.3 Pa CDG and stability over 4 years as measured by the SE2 static expansion system of PTB.

# A Gate-Free Monolayer WSe2 pn Diode

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Monolayer transition-metal dichalcogenides (TMDs) are known to be one of the most promising candidates for future nanoelectronic and nanooptoelectronic devices owing to their outstanding electrical and optical properties [1-3]. Interest in bringing p- and n-type monolayer semiconducting TMD into contact to form rectifying pn diode has thrived since it is crucial to control the electrical properties in two-dimensional (2D) electronic and optoelectronic devices. Usually this involves vertically stacking different TMDs with pn heterojunction or, laterally manipulating carrier density by gate biasing [4-6]. Here, by utilizing a locally reversed ferroelectric polarization, we laterally manipulate the carrier density and created a WSe2 pn homojunction on the supporting ferroelectron BiFeO3 substrate. This non-volatile WSe2 pn homojunction is demonstrated with optical and scanning probe methods, scanning photoelectron micro-spectroscopy (SPEM), and transport measurement. A homo-interface is a direct manifestation of our WSe2 pn diode, which can be quantitatively understood as a clear rectifying behavior. The non-volatile confinement of carriers and associated gate-free pn homojunction can be an addition to the 2D electron-photon toolbox and pave the way to develop laterally 2D electronics and photonics.

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# Nanoscale mapping of carrier collection in single nanowire solar cells using X-ray beam induced current

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We demonstrate how nanofocused X-rays can be used to investigate the carrier collection in single nanowire solar cells with nanoscale resolution with the technique called X-ray beam induced current (XBIC). The spectrally resolved XBIC qualitatively agreed well with the XAFS measured simultaneously by X-ray fluorescence (XRF) signal. In another study of nanowire solar cells, the amplitude of the XBIC is saturated over the middle segment of the nanowire at reverse bias, which indicates that most carriers are collected in this region. At forward bias, which is the relevant condition for solar cells, the carrier collection is only efficient in a small region of the middle segment. Comparison with finite element modeling suggests that this is due to non-intentional p-doping in the middle segment. The results are in line with a nano-XRF study of similar nanowires (A. Troian et al., 2018), that showed unintentional Zn-doping of about 5x10^17 cm^-3. The result of these XBIC measurements provide a better understanding of nanowire solar cells, and we anticipate that nanofocused XBIC could be used to investigate carrier collection in a wide range of nanostructured devices.

# CSI: The development of a new space instrument calibration facility at TNO

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Early 2018 TNO started the conceptual design for a new facility for the characterization and calibration of Space Instruments.

This facility will be called Calibration Space Instruments (CSI) and will be operational from 2021.

At the end of 2018 the suppliers for both the Thermal Vacuum Chamber (TVC) and the Mechanical Ground Support Equipment (MGSE) were selected.

The TVC will be a vertically placed stainless steel cylinder with a diameter of 2.75 meter and a height of 2.5 meter. The chamber and thermal shrouds are sliced diagonally, resulting in a wedge shaped bottom half and top half which reduces the room height needed for loading a space instrument.

The thermal shroud of the TVC will be able to create an environment between 193K and 353K. Two thermal plates will be present to cool part(s) of the instrument up to 100K if required.

During the calibration of a space instrument, its position relative to the optical stimuli unit (Optical Ground Support Equipment or OGSE) has to be changed with a high accuracy and reproducibility.

To achieve this, TNO has selected a vacuum compatible hexapod on a rotation table that meets the stringent accuracy and stability requirements. TNO has designed an active thermal system around the hexapod in order to locally create a thermal stable environment for the hexapod.

During the oral we will briefly discuss the overall CSI facility and in more detail the design, and the current manufacturing status of both the TVC and the MGSE.

# Fast I-V Measurements on Single-Molecule Junctions

Electronic structure of single-molecule junctions has a significant impact on their transport properties and performance of electronic devices using the molecular junctions. On the single-molecule scale, the junction structure and related electronic structure are subject to thermal fluctuation. To comprehend the transport properties towards their possible application to electronic devices, understanding the electronic structure of single-molecule junctions in the structural fluctuations is necessary. Here we developed a fast I-V measurement approach to obtain time dependent change in the electronic structure of single-molecule junctions in the structural fluctuations. Single-molecule junctions of 1,4-bezenedithiol (BDT) sandwiched by two Au electrodes was fabricated by STM-based break junction technique that was combined with the field programmable gate array (FPGA) technology. Time dependent I-Vs of the single-BDT junctions were measured during the self-breaking process of the junctions at room temperature. Temporal resolution of the I-V measurement was 100 µs, which is two order of magnitudes faster than that in our previous study. [1] By analyzing the measured I-Vs, time dependent change in the electronic structure was captured. We found that, in a 1 ms time window just before the breakage of the BDT junctions, the molecular orbital energy decreased and the electronic couplings to the two Au electrodes became asymmetric. This study provides new insight into the electronic fluctuation in the molecular junction that had been inaccessible by the standard molecular conductance measurement.

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# Growth of a nano-structured coating during plasma electrolytic oxidation of Al in "soft" regime conditions

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The Plasma Electrolytic Oxidation (PEO) process is an electrochemical process to produce multifunctional ceramic coatings on light-weight metals (AI, Mg). Growth of the oxide layer is assisted by the generation of micro-discharges (MDs) over the processed surface. It is well established that the use of a pulsed bipolar current to supply the electrodes is beneficial to the growth of the PEO coating. Especially when the positive to negative charge quantity ratio is less than one, a particular regime occurs, usually called "soft"-regime. Within this specific regime, the growth kinetic is significantly enhanced while drastic changes in the MDs behaviour are observed. In the literature, the possible proposed mechanisms that govern the "soft"-regime appearence remain rare and debateable mainly because the PEO oxide coating growth has not yet been observed and described at very local scales.

For this purpose, using a silicate-based electrolyte, aluminium was PEO-processed in "soft"-regime conditions and a multi-scale description of the coating was conducted mainly with XRD, SEM, TEM measurements. The main results show that the occurence of the "soft"-regime is concomitant with the formation of a stratified nanocomposite morphology, which gradually fills the cavity of the so-called "pancake"-structure. Nanoscale measurements evidence that this nanocomposite consists of Al2O3 lamellae (90 nm thick), depleted in elements from the electrolyte, which alternate periodically with a metastable 1Al2O3-1SiO2 mullite lamellae (30 nm thick). Combining these observations with the presence of a nanometre-size porosity network, a possible coating growth mechanism will be discussed when the PEO process runs within "soft"-regime conditions.

# Development of a Zero-Length Fin-Type NEG Pump Coated with Oxygen-Free Pd/Ti

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We developed a new zero-length fin-type non-evaporable getter (NEG) pump with a DN 160 conflat flange using a new NEG material, i.e., oxygen-free Pd/Ti thin film, for evacuating residual H2 and CO. After baking at 150 °C for 12 h, the pumping speeds of the NEG pump were measured with the orifice method. Initial pumping speeds of 2350–800, 2240–900, 2080–915, 1950–915 L/s were estimated for H2 after baking at 150 °C for 12, 6, 3, and 1.5 h respectively, in a pumped-quantity range of 0.01–30 Pa L. On the other hand, pumping speeds of 1560–20, 1560–20, 1560–20, and 1560–20 L/s were estimated for CO after baking at 150 °C for 12, 6, 3, and 1.5 h respectively, in a pumped-quantity range of 0.01–30 Pa L. On the other hand, pumping speeds of 1560–20, 1560–20, 1560–20, and 1560–20 L/s were estimated for CO after baking at 150 °C for 12, 6, 3, and 1.5 h respectively, in a pumped-quantity range of 0.01–30 Pa L. The advantages of the new NEG pump are as follows: 1) pumping speeds are not degraded even after repeated venting–activating cycles; 2) it can be activated by baking at 150 °C for 12–1.5 h; 3) no dedicated power supply and electric feedthroughs are required; 4) compact and light weighted. The new NEG pumps are a suitable alternative to conventional NEG pumps or titanium sublimation pumps.

# Ta:TiO2 ultrathin films with tunable electrical and optical properties for IR plasmonic applications

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Recently, transparent conductive oxides (TCO) have demonstrated plasmonic properties that can be tuned, by doping or engineering oxygen stoichiometry, from the visible to the mid-IR range [1], potentially overcoming issues typical of metal nanostructures in which the application range and tunability are limited; this can have an impact e.g. in the fields of photoconversion, sensing, optoelectronics.

Ta-doped TiO2 (Ta:TiO2) is a performing TCO, with the advantages of TiO2, such as photoactivity, low-cost, non-toxicity and stability [2]; Ta:TiO2 in form of ultrathin films or nanoparticles is thus a promising material for IR plasmonics, in particular for active electrical modulation of the plasmonic response.

In this work, Pulsed Laser Deposition (PLD) and vacuum annealing of Ta:TiO2 thin films enable a fine control of thickness and nanostructure, while permitting a systematic investigation of the effect of Ta content (5–10% at.) and O stoichiometry on the material electrical properties and optical/plasmonic behaviour in the UV/Vis/NIR range. We show that fine tuning of defect chemistry allows control of carrier density (or carrier density gradient) over one order of magnitude in polycrystalline transparent electrodes. The synthesis of Ta:TiO2 nanostructures and ultrathin films is then discussed together with their potential development as novel mid-IR, tunable plasmonic materials. In particular, conductive ultrathin films have been successfully obtained down to 10 nm, which represents an attractive size for the realization of plasmonic metamaterials or active-modulated TCO-based plasmonic devices.

[1] Naik et al, Adv Mater 25, 3264 (2013).

[2] Mazzolini et al, J Phys Chem C 119, 6988 (2015)

# Transport and reaction mechanisms in Li-sulfur batteries

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The lithium-sulfur battery is widely considered as one of the most perspective post lithium-ion systems. However, the high theoretical capacity of 1672 mAh g-1 is difficult to attain in practice. Moreover, the typical power capability lags behind that of the Li-ion rivals. An important reason for performance limitation of the Li-S system is the deposition of non-conductive solid products, in particular Li2S, on the active surface of the cathode. We will show, contrary to such expectations, that the solid products released during discharge of Li-S battery hardly block the main electrochemical reaction(s). This is due to their highly non-uniform morphology which is a result of the special growth mechanism as identified in the study. Based on experiements using carefully designed cells we will determine and comment on the values of the main transport-reaction parameters (rate constants, diffusion coefficients etc.). We will further show that, rather than solid deposits, the actual reason causing the performance limitation of Li-S system is the drastic drop of polysulfide concentration close to the active surface under different conditions of practical interest. The new results offer a new fundamental insight into the transport-reaction mechanism occurring in Li-S battery which will serve as important guidelines for further improvement of this system.

# Thermoelectric study of ZnO-based thin films: the effect of Bi dopant content

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This work reports on the attempt to optimize the thermoelectric properties of ZnO-based thin films for applications that envisage coatings as transparent thermoelectric electrodes in devices.

As several reports indicate, point defects are very effective in controlling the thermal conductivity on oxide-based thermoelectrics. The approach consists in introducing Bi ions, a higher mass element, into the ZnO metal-oxide matrix, in order to hinder phonon mediated heat conduction, whilst maintaining the Seebeck coefficient and high electrical conductivity.

Hence, the effect of Bi dopants on ZnO-based thin films has been investigated on two thickness series (500 nm and 70 nm thick films) and for three types of films: ZnO; ZnO:Ga and ZnO:Al; all produced by a custom-built d.c. magnetron sputtering setup in the confocal geometry. The films were characterized concerning their structural, electrical, thermal and optical features, which are influenced by dopant incorporation.

A comparison between undoped and doped ZnO films is made regarding their thermoelectric properties. Preliminary results show that undoped ZnO has an almost zero Seebeck coefficient, which is substantially enhanced for ZnO:Al,Bi (-44e-6 V·K-1) and ZnO: Ga,Bi (-45e-6 V·K-1) for optimized conditions. It was observed that Seebeck coefficient decreases with film thickness. In the best case scenario we attained a thermoelectric figure of merit of ~0.01 at room temperature.

# Modeling of time-dependent gas pumping systems in a wide range of the Knudsen number

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Gas pumping systems operating in a wide range of the Knudsen number may be found in many industrial processes and technological fields including semiconductor technologies, material deposition, vacuum metallurgy and food packaging, as well as in fusion reactors and accelerators. Since these systems operate from very low pressures up to the atmospheric pressure, mesoscale kinetic modeling, based on the Boltzmann equation or reliable kinetic model equations, is required. Recently, at the Transport Processes & Process Equipment Laboratory of the University of Thessaly, in Volos, Greece, an in-house code has been developed for modeling rarefied gas distribution systems under steady-state conditions and it has been successfully applied to model the ITER divertor pumping system [1]. In the present work, this code is extended to time-dependent gas pumping in vacuum systems using a hybrid methodology introduced in [2]. At each time step, based on kinetic modeling, a steady-state flow configuration is solved to estimate the amount of gas pumped out of the vacuum system. Then, the pressure of each evacuated (or filling) container connected to the distribution system is updated by applying mass conservation. This explicit-type coupling between the mesoscale kinetic solver and the macroscale pressure evolution is shown to be computationally efficient and accurate. The described methodology is implemented to simulate benchmark vacuum gas distribution systems, as well as the dwell phase pump-down of the ITER vacuum vessel.

[1] N. Vasileiadis, G. Tatsios, S. Misdanitis and D. Valougeorgis, Modeling of complex gas distribution systems operating under any vacuum conditions: Simulations of the ITER divertor pumping system, Fusion Engineering and Design, 103, 125, 2016.

[2] M. Vargas, S. Naris, D. Valougeorgis, S. Pantazis and K. Jousten, Hybrid modeling of time-dependent rarefied gas expansion, Journal of Vacuum Science and Technology A, 32 (2), 021602, 2014.

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# As-grown p-type doped GaN for high-efficiency green light-emitting-diodes

Son Phuong Le, Chih-Wei Hsu, Per-Olof Holtz

InGaN/GaN quantum wells and dots grown on the top of micro-sized GaN pyramids, fabricated by hot-wall metalorganic chemical vapor deposition (MOCVD), have been demonstrated to exhibit excellent optical emission properties, such as linearly polarized light without filtering. Although such structures are promising for development of light-emitting-diodes (LEDs) applications, neither p-type doped GaN nor demonstrated LEDs by hot-wall MOCVD have been reported so far. Towards the demonstration of LEDs by this technique, as-grown p-type doped GaN has been investigated in this work. The growth of a nucleation layer on a SiC substrate was followed by a GaN buffer layer and a Mg-doped GaN layer grown at 1030 oC . Subsequently, the reactor was cooled down in an ambiance of H2 and N2 gases. In this way, we have obtained as-grown p-type doped GaN with a resistivity of 5 ohm-cm and a hole concentration of up to 2x10\*\*17 /cm3 as evaluated by Hall-effect measurements, almost the same for the doped GaN films with the thicknesses of 200 nm and 700 nm. After additional thermal annealing in nitrogen gas at 750 oC in 5 min, the hole concentration was increased up to 5x10\*\*17 /cm3, while the resistivity was decreased to 1.5 ohm-cm, supporting the benefits of the hot-wall MOCVD for growth of nitride materials, especially for p-type doped structures. By employment of such structures for fabrication of InGaN/GaN LED devices, a bright green emission has been demonstrated at room temperatures, indicating the potential of the hot-wall MOCVD for high-efficiency green LEDs.

# Ge cluster formation on dielectric surfaces by decomposition of metastable (Al1-xGex)N coatings, studied by simultaneous in-situ hard X-ray photo electron spectroscopy and X-ray diffraction

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The thermal decomposition of a metastable solid solution wurzite (Al1-xGex)N phase in vacuum has been utilised to form metallic Ge clusters on the surface of the dielectric coating. This process has been studied in-situ using simultaneous hard X-ray photoelectron spectroscopy (HAXPES), and grazing incidence X-ray diffraction (XRD) between annealing steps. Additionally the release of gaseous species from the samples was followed by mass spectrometry. In-situ experiments were conducted at the Spanish beamline BM25B at the European Synchrotron Radiation Facility in Grenoble.

The decomposition of wurzite (AlGex)N1+x towards AlN + Gex + x/2N2 was observed at temperatures above 750 °C. Changes in the crystal structure were observed by XRD, where shifts indicates a decrease of Ge in the wurzite phase, coupled with the appearance of crystalline Ge. At the same time the electronic structure as observed by HAXPES changed and the Ge 2p peaks indicates the formation of metallic Ge. Mass spectroscopy confirms the decomposition process through observation of N2 during annealing. At temperatures above 850 °C, Ge was found to evaporate from the samples and the photoelectron signal from Ge decreased.

These observations were further confirmed by post-annealing ex-situ characterisation. Scanning electron microscopy (SEM) showed clusters (average diameter ~200 nm) on the surface and scanning transmission electron microscopy (STEM) X -ray spectroscopy (EDX) confirmed that the formed clusters were Ge. Further studies, varying annealing temperature and annealing time will enable controlled formation of Ge clusters of selected sizes on top of the dielectric wurzite phase.

## Local diffusion coefficient calculated from time dependence of permeated hydrogen distribution on a metal surface

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Hydrogen easily diffuses into the metal and causes deterioration called hydrogen embrittlement. When various kinds of diffusion in the local structural material (crystal structure, crystal grain boundary, crystal orientation, etc.) and/or the hydrogen behavior at the trap site become clear, the origin of hydrogen embrittlement and delayed fracture will be found. Hydrogen-resistant materials will be designed, too.

We have developed "operando hydrogen microscope" and measured local hydrogen permeation and its time dependence by observing hydrogen permeation into a vacuum chamber through a metal sample of a thin plate, 100 micron [1]. Hydrogen maps were measured by using electron stimulated desorption technique and the original equipment. The local structures of the metal were estimated from the SEM image and the diffusion coefficients were calculated for the areas of the austenitic structure (FCC-like structure) and the martensitic dislocation (BCC-like structure) which are the main structures of the SUS 304 steel.

[1] N. Miyauchi et al., Scripta Materialia 144 (2018) 69-73

# Systematic study of the outgassing behavior of different ceramic materials

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Ceramics show interesting mechanical, thermal and electrical properties and are supposed to have relatively low outgassing rates. Therefore, in vacuum applications they are often used, for example for feedthroughs. In literature, however, quantitative numbers on outgassing of most of the ceramic materials are hard to find.

In order to facilitate the estimation of outgassing rates and pumping times of vacuum systems, the outgassing rates of various ceramic samples were systematically investigated. For this purpose the Outgassing Measurement Apparatus (OMA), which uses the difference method, was applied. This method is a modified throughput method where a second chamber is used as a reference to allow a direct measurement of the pure outgassing of the sample. At OMA oxide ceramics like alumina, nitride ceramics like aluminum nitride, as well as carbide ceramics like silicon carbide were measured. All measurements were performed for 100 h at room temperature, 100 °C and 200 °C to investigate the time and temperature dependence of outgassing. Additionally, the outgassing species were determined by a quadrupole mass spectrometer.

The paper shows quite low outgassing rates for some of the examined ceramics. After 100 h at room temperature an outgassing rate of about 2·10^-8 (Pa·m^3)/(s·m^2) is for example achieved for alumina. However, there are relatively large differences between the ceramic materials, for the initial outgassing rates as well as for their behavior at elevated temperatures. The mass spectra show similar residual gas spectra as seen for metals, but some spectra also show high peaks for water.

# Ab initio modelling of rarefied gas flows

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## <sup>1</sup> Federal University of Parana

To model gas flows in vacuum systems, various methods of rarefied gas dynamics are applied. All kinds of calculation of rarefied gas flows use some potential of intermolecular interaction. The widely used phenomenological potentials such as hard spheres, Lennard-Jones, Stochmayer, variable hard spheres, variable sort spheres, contain several fitting parameters usually extracted from experimental data on transport coefficients (viscosity, thermal conductivity, diffusion) or from virial coefficients. Recently, the potentials for many gases and their mixtures have been calculated from main physical principals applying quantum-mechanical calculations. Some papers provide potentials for helium, neon and argon, respectively. These potentials can be implemented to solve the Boltzmann equation and to apply the direct simulation Monte Carlo method. These results showed that some phenomena like mass flow rate, shear stress and heat flux in a single gas with a small temperature variation are not sensitive to the potential so that the simplest potential like the hard sphere model can be successfully used if the molecular diameter is well adjusted. However, some phenomena in gaseous mixtures like diffusion and thermodiffusion are strongly sensitive to the potential and should be modeled applying ab initio potentials when available. In the presentation, recent results on rarefied gas flows based on ab initio potentials will be reviewed. A comparison of results based on ab initio with those obtained using phenomenological potentials will be performed.

# Magnetic field-assisted chain formation of aerosol nanoparticles

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- <sup>3</sup> NanoLund

We will present the formation of nanoparticle chains by deposit magnetic iron oxide aerosol nanoparticles in a combined electric and magnetic field. Aerosol methods, in particular spark ablation, provides a good means to produce magnetic nanoparticles with a controllable size and concentration in a broad size range without agglomeration. These aerosol nanoparticles are usually deposited using an electrostatic precipitator (ESP) where a large voltage attracts the charged particles towards the substrate where they are collected. As the concentration of the particles on the substrate increases, large clusters are formed due to the interaction between the particles on the substrate and the particles in the gas.

In this study, we have added a magnetic field to the conventional ESP to modify the cluster formation. As the particles approaches the surface, the magnetic interaction between the deposited particles and the particles in the gas becomes more dominant. The particles will have a higher tendency of colliding and forming free-standing chains. With increased concentration these chains will collapse into bundles. The added magnetic field enables the formation of nanoparticle structures not achievable with an ESP alone. The nanoparticles are deposited with low concentration, making it possible to study the growth of the chains by off-line analysis using electron microscopy and correlate these results to simulations. We will demonstrate how the chains and bundles are influenced by the strength of the magnetic field and the electric field as well as the size and concentration of the particles.

# Deciphering the origin of our solar system by mass spectrometry

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<sup>1</sup> University of Bern

Although the Rosetta stone, found by the troops of Napoleon in Egypt near the city of Rosetta (Rashid) contains only a small amount of text in three languages it was key in deciphering Hieroglyphs. The Rosetta mission tried to achieve something similar: by looking at a tiny body its goal was to decipher the origin of the solar system, planets including Earth and life. After more than 12 years the Rosetta spacecraft softly crash-landed on comet Churyumov-Gerasimenko on September 30, 2016. It has traveled billions of kilometers, just to study a small (4 km diameter), black boulder named 67P/Churyumov-Gerasimenko. The results of this mission now seem to fully justify the time and money spent in the last decades on this endeavor.

High resolution mass spectrometry in the tenuous atmosphere of a comet for more than two years revealed a huge amount of organics up to amino acids. The ROSINA (Rosetta Orbiter Sensor for Ion and Neutral Analysis) was able to identify many molecules and isotoplogues, which let us reconstruct where these molecules have formed and under which conditions. Almost three years after end of mission we now have a good overview on the chemical composition of the nucleus, although data analysis is still ongoing and will need several more years to be completed.

In this talk I will show how our perception changed on how the solar system formed thanks to Rosetta and especially ROSINA measurements.

# Mechanism of monolayer MoS2 pattern growth by deep learning

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#### <sup>1</sup> National Chung Cheng University

In this study, we used chemical vapor deposition (CVD) to grow a single layer of MoS2 two-dimensional material on a 300 nm SiO2/Si and sapphire substrate. Since the growth mechanism of MoS2 crystals has been a part of extensive research, growth methods have resulted in roughly adjustable control parameters, including powder/vapor materials, gas flow rates, substrate materials and locations, and temperature control, from previous studies. Two-dimensional materials with different shapes. However, in the experiment, subtle changes in these parameters can also lead to significant differences in the growth quality of MOS2, and it is known that changes in growth parameters are particularly sensitive to the growth process. We have initially found that the morphological change of MOS2 is highly dependent on the spatial position on the substrate. The change from triangular to hexagonal geometry is mostly due to the concentration ratio of the powder reactants, and the coupling change between gas flow, diffusion and heat conduction. So that its local variation or dynamics affect the edge growth. Therefore, we hope to use the deep learning model to assist in the understanding of MOS2 structure growth and shape evolution. First, some parameter features will be explored and observed. After learning through neural networks, many MOS2 forms will be obtained, for example: Shapes such as triangles, hexagons, truncated triangles, three-pointed stars, butterfly shapes, and fishbone shapes. In the future, it is hoped that the synthesis results will be pre-simulated by parameter setting before the CVD growth, and used to predict and control the morphology and characteristics of the synthesized two-dimensional materials to save experimental time and material cost.

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# From 2D to 1D - Tb silicide nanowires on Si(hhk)

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The deposition of about one monolayer Tb on Si(111) and annealing leads to the formation of the metallic Tb disilicide monolayer, which pins the Fermi level near the Si conduction band minimum making it interesting for ohmic contacts on n-type Si. Its electronic structure near the Fermi level is characterized by sharp bands forming a hole pocket at the center of the Brillouin zone and strongly anisotropic electron pockets at the M points.

Here, the growth and the electronic structure of Tb disilicide on Si(hhk) surfaces, which are vicinal to Si(111), was studied with scanning tunneling microscopy and angle resolved photoemission spectroscopy (ARPES). In general, narrower Tb disilicide structures are observed for larger offcut angles, but the morphology of these structures strongly depends on the offcut direction. For Si(hhk) surfaces with h < k, the silicide forms well defined nanowires with sharp edges while only irregular stripes are formed for h > k. Nevertheless, the characteristic two-dimensional electronic structure of the disilicide monolayer is observed with ARPES on all vicinal surfaces. Thereby, the bands, which were sharp for the extended monolayer on planar Si(111), broaden in the direction perpendicular to the step edges due to the confinement of the silicide structures to finite widths. This effect is quantified for nanowire samples by an analysis of the electron pockets. Furthermore, electronically purely one-dimensional bands emerge for low Tb coverage on Si(335). Tb silicide structures possibly corresponding to these bands are discussed.

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#### Simulation of He leaks in the cryogenic accelerator vacuum system of SIS100

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Vacuum systems of accelerators with superconducting beam guiding components are commonly designed as cryo-pumped low-temperature vacuum systems. Although cryo-pumping is extremely efficient in terms of achievable ultimate pressures, it makes the detectability of potential He leaks in cryo-pumped vacuum systems highly difficult. If He leaks into a vacuum system held at LHe temperatures, it is steadily cryosorbed in the immediate vicinity of the leak position leading to the time-delayed built up of a localized He pressure gradient whose fronts spread out slowly throughout the cold beam pipe. Helium leak-triggered pressure gradients may not only cause premature beam losses, but also quenches of superconducting magnets. Small He leaks even remain commonly undetected for a long time since pressure monitoring in cryogenic systems is technologically challenging and frequently not applied. The necessity to predict pressure profiles in cryogenic beam tubes in the presence of localized He inflows is obvious.

A novel simulation code, originally developed at GSI for the calculation of dynamic hydrogen density profiles in longitudinal non-isothermal vacuum systems, was successfully extended for the computation of helium density profiles. Using this code, we investigated the time-dependent propagation behavior of helium density gradients in the cryo-pumped beam vacuum system of the SIS100 at FAIR (Darmstadt, Germany). We introduce the basics of the code, provide theoretically derived He adsorption isotherms for the temperature range between 5...10K, and present latest simulation results for different He leak scenarios. Finally, in order to demonstrate the performance of the code, an experiment of delayed helium propagation in the cryogenic sections of the LHC at CERN conducted by Wallén [1] over 20 years ago was simulated. His experimental results will be compared with simulation results.

[1] J E Wallén, J. Vac. Sci. Technol. A 15(6), Nov/Dec 1997, 2949

# Ultra Low Emittance Light Source Vacuum System

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The beam stability issues of an ultra low emittance light source are always treated at a high priority. The rf-impedance and gasdesorption rate are two key indices to the performance of the vacuum system of a low emittance synchrotron light source.

The vacuum system of the 3 GeV TPS storage ring showed superior performance in the rf-impedance and gas-desorption rate. With solutions to the rf-impedance issues, such as on the bellows, pumping ports, flanges, gate vales, BPM, the tapers etc., a small effective longitudinal impedance of |Z/n| eff = 0.12  $\Omega$  was achieved at TPS. An ethyl-alcohol machining followed by an ozonate water (30 ppm) cleaning process had been applied to fabricate the TPS aluminum bending chamber, where most of the photo-desorption generated. A low thermal outgassing rate of ~ 6.5×10-15 mbar-l/s-cm2 was achieved after a 24 hr in-situ bakeout at 150°C. Without coating the chamber with getter materials, a low photo-desorption rate of ~ 1.5×10-5 molec./ph. was quickly achieved at a dose of ~ 10 mA-h. The photo-desorption curve showed a declined slop of -1.06 in a log-log plot of the photo-desorption rate vs. the beam dose in the range of 10 to 1000 A-h. A photo-desorption rate of ~1x10-13 mbar/mA was achieved at a beam dose of ~ 4,930 A-h when operating with 500mA beam current. Due to the quick reduction of the photo-desorption rate, the thermal outgas has become the dominant residual gas in the TPS vacuum system.

# GaN-based VCSELs with AllnN/GaN distributed Bragg reflectors

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GaN-based VCSELs are expected to be superior to LEDs as light sources for retinal scanning displays, adaptive headlights, highspeed visible light communication systems, and in-vehicle LAN systems. Since a fabrication of GaN-based distributed Bragg reflectors (DBRs) is not straightforward, like GaAs-based DBRs (AIAs/GaAs), there have been two approaches to form a cavity of the GaN-based VCSELs: one is to use double dielectric DBRs and the other is to use a combination of a top dielectric DBR and a bottom AlInN/GaN DBR. The two approaches contain contrasting pros and cons. It is straightforward to form a dielectric DBR itself, but very complicated and costly to form an entire VCSEL structure with the DBRs. On the contrary, it is an issue to epitaxially grow a GaN-based DBR, but now straightforward to process a VCSEL structure once the bottom GaN-based DBR is included in a device wafer. We have developed lattice-matched AlInN/GaN DBRs. After developing MOVPE growths of AlInN and AlInN/GaN heterostructure, we have successfully obtained high-reflectivity (99.9%) AlInN/GaN DBRs for a 410 nm wavelength region. We demonstrated a GaN-based VCSEL emitting a 4.2 mW light output power of 410 nm emission. In addition, we developed n-type conducting AlInN/GaN DBRs with modulation doping of Si and graded interfaces. Our VCSEL with the conducting AlInN/GaN DBR now shows a 1.8 mW light output power. The device resistance is also reduced from 150 Ω to 90 Ω. Such a conducting DBR will be a key for further developments and a commercialization of GaN-based VCSELs.

# Growth, reduction and re-oxidation of sub-nm thin ceria islands on oxidized Cu(111)

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The exploitation of sustainable energy sources requires the development of new effective low-temperature catalysts for various applications, e.g., for the conversion of surplus renewable energy into effective energy carriers. A promising candidate for the methanol production are Cu nanoparticles on ceria supports. In order to study how the reactivity of the system depends on the crystalline orientation of its constituents, we have prepared the inverse model catalyst system of ceria on Cu(111) and performed an extensive in-situ study employing low-energy electron microscopy (LEEM) and spectroscopic photoemission electron microscopy (PEEM) at the nanospectroscopy beamline at ELETTRA. Depending on the surface oxygen concentration, on Cu(111) ceria islands can be grown in (100) and (111) orientation [1]. Furthermore, oxidized Cu(111) was prepared as substrate by exposing Cu(111) to molecular oxygen at 475°C and 2x10-6 mbar. The deposition temperature of ceria was kept at 475°C while adjusting the oxygen background pressure in the range of 2x10-6mbar and 3x10-6mbar. A detailed micro-diffraction and LEEM-I (V) analysis shows that the lower pressure gives rise to the formation of equal shares of CeOx(100) and CeOx(111) while the higher pressure results in a majority of (100)-oriented islands. This surface represents a perfect nano-laboratory for reactivity tests on the different surface orientations under identical conditions. Initial experiments show that annealing at 425°C leads to a significant reduction of the ceria islands, subsequent O2 exposure to re-oxidation, as confirmed by X-ray absorption spectroscopy (XAS) and resonant photoelectron spectroscopy (RPES), respectively.

# Functional thin polymer films deposited from the vapor phase and their application for drug delivery and stimuli recognition

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Functional thin films offer innovative solutions for many technological applications: organic electronics, smart devices for biotechnology, microfluidics, membrane technology, sensors and drug delivery systems. The development of functional thin films, engineered to achieve all the desired properties, requires advanced growth techniques. The development of dry growth methods - based on vacuum- aims to complement and enlarge the applicability of functional thin films to fields where the presence of solvent is detrimental.

Successful results in terms of rationally designed micro- and nanoengineered materials will be demonstrated using as a case of study the growth of functional polymers by initiated CVD (iCVD). The high versatility of iCVD in driving application-specific properties into the material, creating a platform for the implementation of polymeric coatings into device fabrication will be discussed.

A case study will be presented in the field of stimuli-responsive materials, in particular, hydrogels whose size and shape change when stimulated by light, humidity, temperature and aqueous environments. A chemical functionalization of the hydrogel surface was performed to add multiple stimuli-responsive functionalities and obtain a smart material that responds to two stimuli at the same time. Modifying the hydrogel surface with solution-based methods is often problematic because of the damages caused by the permeation of solvents in the hydrogel. This issue is completely bypassed by the use of solvent-free techniques, like iCVD. It will be also demonstrated how the stimuli-responsiveness can be used to control the delivery of some drugs.

#### Pulsed laser deposition and nanoscale investigation of two-dimensional nanocrystals on metal substrates

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The future application of 2D materials and heterostructures in novel electronic and optoelectronic nanoscale devices poses important research challenges, such as the large-scale bottom-up synthesis of atomically thin crystals and the nanoscale characterization of their fundamental structural and electronic properties. To address these tasks, we explored a non-conventional experimental approach based on Pulsed Laser Deposition (PLD) combined with in situ Scanning Tunneling Microscopy (STM). Although STM investigations traditionally rely on conventional synthesis techniques, e.g. Molecular Beam Epitaxy, PLD offers, in principle, an alternative, versatile and potentially scalable approach to the growth of high-quality 2D crystals and heterostructures, thus ideally bridging the gap between model systems and device-oriented ones.

We focused our work on the PLD growth of 2D ZnO and MoS2 on metal surfaces, such as Au(111) and Ag(111). We observed the formation of well-ordered ZnO and MoS2 nanostructures of high surface quality, whose local structural properties were investigated by high-resolution STM measurements [1-2]. By tuning the PLD process, we could study the growth of the synthesized nanocrystals, being also able to achieve large-area single-layer (SL) MoS2 on both Au and Ag substrates. The interaction with the metal support influences the electronic, vibrational and optical properties of SL MoS2, as revealed by scanning tunneling spectroscopy, Raman and photoluminescence measurements.

Our approach will allow us to study the growth of novel 2D semiconductors, e.g. GaAs, as well as 2D heterostructures, e.g. ZnO/MoS2, MoS2/WS2 or pentacene/MoS2.

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# Structure-function relationship for CO2 methanation over supported Rh catalysts

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CO2 methanation offers a promising solution to the use of CO2 as a renewable and environmentally friendly carbon source. It is effective for the development of a long-term fossil-free carbon industry and can minimize the CO2 emissions. Ruthenium and Rhodium on various supports have been shown to be active catalysts for CO2 hydrogenation and the most selective towards methane. We recently showed that Rh-based catalysts are active for methane production from CO2 hydrogenation at atmospheric pressure conditions and relatively low temperatures (<625K). Several other studies, including our previous work, have shown a support-dependent reaction mechanism towards CO2 methanation via either a CO-route (for catalysts supported on non-reducible oxides) or a formate route (for catalysts supported on reducible oxides). In this work, in situ structural and chemical state characterization of Rh-based catalysts during atmospheric pressure CO2 methanation was performed by a combined array of time-resolved analytical tools including AP-XPS, XAS, HE-XRD and DRIFTS.

The results show that, for Rh/Al2O3, the linearly adsorbed CO species on metallic Rh is a more active precursor during the CO2 methanation as compared to the bridge-bonded CO species, which is attributed to smaller particle sizes. For the ceria supported catalyst, the strong metal-support interaction between Rh and ceria leads to increased activity and methane selectivity. Furthermore, the results provide evidence that an active state of the ceria-based catalysts is rich in Ce3+ sites which can be associated with oxygen vacancies on reduced ceria activating the CO2 molecule forming formate, an important species of the reaction mechanism.

## Development of porous conductance element for high vacuum gauge calibration

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The gas flow through the low permeable porous media have a great interest, especially in vacuum technology for filtering, separation process, protection and flow control. It can combine a high mass flow rate and a high level of rarefaction. The transient experimental technique, developed previously for the mass flow rate measurements through the microchannels [1], is generalized to obtain the permeability and conductance directly from the pressure variation measurements. The present experimental methodology, allowing for step by step data verification, leads for higher accuracy than the similar and commonly used method such as "pulse-decay" techniques [2].

The microporous medium having a characteristic pore size of 1.5 micrometers is placed between two reservoirs and the pressure variations with time, generated by the gas flowing through the medium, are measured for different gases.

These experimental data are fitted according to the exponential function with the pressure relaxation time as a single fitting parameter. The new expression for the permeability is proposed involving besides the geometrical parameters the ratio between the gas and pressure relaxation times. The free molecular flow regime, characterized by the constant conductance, is achieved below 30 mbar for helium. This property makes the microporous medium particularly suitable as a leak element, for example for calibration of ionization gauges or mass spectrometer [3].

References:

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# Quantum State-Resolved Studies of Methane Chemisorption by Vibrational Spectroscopies

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Methane dissociation is the rate limiting step in the steam reforming process used by the chemical industry to convert natural gas into a mixture of H2 and CO known as synthesis gas. To better understand the microscopic mechanism and reaction dynamics of methane chemisorption, we use vibrational spectroscopies and infrared lasers for quantum state-resolved studies of methane dissociation and state-to-state scattering on Ni and Pt surfaces. Our experiments prepare surface incident methane molecules in specific ro-vibrational quantum states by infrared laser pumping in a molecular beam. The state prepared molecules then collide with a clean single crystal transition metal surface in ultrahigh vacuum and both reactive and non-reactive processes are monitored by infrared spectroscopic techniques. Surface bound methyl species as products of the dissociative chemisorption of methane are detected by Reflection Absorption Infrared Spectroscopy (RAIRS). RAIRS allows for in-situ monitoring of the uptake of chemisorbed methyl species enabling quantum state-resolved measurements of reactive sticking coefficients. RAIRS detection yields surface site specific sticking coefficient for methane on step and terrace sites. Non-reactive, inelastic energy transfer is probed by combining infrared laser tagging with bolometric detection of surface scattered methane molecules. The detailed reactivity and state-to-state scattering data from our measurements are used as stringent tests in the development of a predictive understanding by first principles theory of these industrially important gas/surface reactions.

# The Influence of the Working Parameters on the Precision of Spinning Rotor Gauges

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Spinning rotor gauges (SRGs) measure the pressure in a vacuum system using a magnetically levitated steel ball. This rotating ball induces a voltage signal in pick-up coils. The time decay of the frequency of this small AC voltage is then accurately measured and used to calculate the gas pressure.

SRGs use a special algorithm to reduce the statistical scatter of the measured frequency decay. The standard deviation can be significantly decreased by increasing the sampling interval for the frequency-decay measurement. For ultimate precision the sampling interval can be extended up to 60 s in commercial SRG instruments. In this investigation we study the influence and correlation of the working parameters, such as the amplitude of the voltage signal, the sampling interval and the rotor frequency, on the measurement noise and the SRG offset. A long sampling interval could be undesirable when measuring the changing pressures. By optimizing some of the working parameters, the precision of the measurement can be increased, or the same standard deviations can be achieved with a reduced sampling interval.

By increasing the frequency from 400 Hz to 800 Hz, a decrease in the standard deviation was observed, even by a factor of 10. By increasing the measurement interval by a factor of 2, the standard deviation can be reduced by a factor of 5. A disadvantage of operating a SRG in a higher frequency range is the higher offset value and its frequency dependence.

## Plasma for cancer treatment: Modeling for a better understanding of the underlying mechanisms

Annemie Bogaerts, Pepijn Heirman, Wilma Van Boxem, Maksudbek Yusupov, Jamollidin Razzokov, Jonas Van Der Paal

Cold atmospheric plasmas are gaining increasing interest for cancer treatment and other medical applications, but the underlying mechanisms are far from understood. Reactive oxygen and nitrogen species (RONS) generated by plasma are believed to play an important role. For instance, a noticeable rise of intracellular ROS upon plasma treatment was reported in cancer cells vs. normal cells, which might lead to oxidative damage of biomolecules inside the cells.

I will give an overview of our recent simulations for plasma medicine, for a better understanding of the underlying mechanisms, at two different levels. First I will focus on modeling of the plasma chemistry and plasma-liquid interaction, to obtain more information on the stability and chemical reactivity of biomedically important species (RONS). Subsequently, I will show molecular level modeling of the interaction of RONS with biomolecules, e.g., how can these RONS affect the cell membrane and create pores. Specifically, I will show the effect of cholesterol (often present in higher concentrations in the cell membrane of normal cells than cancer cells). Our calculations reveal that it causes a drop in the probability of pore formation and in the RONS penetration ability. Likewise, I will show the higher permeability of H2O2 through aquaporins (which is more expressed in cancer cells) than through the cell membrane. This might both explain the selectivity of plasma therapy towards cancer cells vs normal cells. Moreover, I will discuss the synergistic effect of the electric field and lipid oxidation (both induced by plasma) on the cell membrane permeability.

# **Reduction and Oxidation of Zirconia Thin Films**

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Zirconia (ZrO2) is a catalyst support and solid-state electrolyte (when chemically doped with yttria). For these applications, it is essential to understand its interaction with oxygen. Furthermore, the oxidation state of zirconia is important for its structure, as it is known that the tetragonal phase can be stabilized by oxygen vacancies. We have investigated ZrO2 films [1] grown on Pt(111) and Rh(111) by experimental methods (XPS, STM) as well as DFT calculations.

Oxygen vacancies in the films are positively charged; this leads to a downshift of the bands detectable via XPS core level energies. We show that oxidation of reduced films occurs via spillover from metals, where oxygen can dissociate. While bare zirconia is essentially non-reducible, at highly reducing conditions, it is possible to fully reduce ZrO2 in contact with a noble metal, aided by the high enthalpy of Zr dissolution in these metals. DFT indicates another mechanism for partial reduction: a substantial decrease of the oxygen vacancy formation energy for ZrO2 in contact with a metal [2,3]. Our calculations rationalize this in terms of the electronic structure of oxygen vacancies, their electrostatic interaction, and lattice distortions. DFT also shows that the difference between bare ZrO2 and ZrO2 in contact with metals is especially large for surface vacancies; this can be understood from their geometric and electronic structure.

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# Fe3O4 integration on silicon using ultra-thin oxide barriers

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The integration of Fe3O4 films on silicon is of huge interest for semiconductor spintronics. However, the functionality of the system is strongly influenced by the structural properties of the system, especially regarding the interface quality. Because of this is fundamental to understand the interaction between the silicon surface and the deposited films and to develop new strategies for the preparation of high quality heterostructures without formation of mixed layers (Silicates or Silicides) at the interfaces that modify the desired behavior of the system.

We report on Fe3O4-based heterostructures prepared through different ultra-thin oxide buffer layers, concretely Fe3O4/SiO2/Si and Fe3O4/SrTiO3/Si. The synthesis parameters were optimized in order to obtain single phase magnetite films. Strong efforts were made to characterize the buried interfaces and understand the interaction between magnetite, silicon and the oxide buffer layer.

# Electrically active defects in n-type 4H-SiC introduced by neutron irradiation

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Silicon carbide (SiC) is a radiation-hard wide band gap semiconductor suitable for high temperature, high-frequency and highpower applications. Due to the high and isotropic mobility of carriers, SiC is becoming the preferred material for radiation detector applications. Deep level defects that act as charge carrier traps have high importance in semiconductor industry and applications of semiconductor devices. These defects are mainly created during i) semiconductor material growth, ii) processing by ion implantation or iii) operation under harsh ionizing radiation conditions.

We present a study of neutron radiation introduced defects in n-type 4H-SiC Schottky barrier diodes by means of capacitance transient techniques. The well-known electrically active defect related to the carbon vacancy (Vc) has been observed in as-grown material. The Vc acts as a strong minority carrier recombination center in n-type material, and it is called "lifetime killer" due to its strong influence on 4H-SiC device properties. The epithermal and fast neutron irradiation introduced two additional intrinsic defects, with energies of 0.4 and 0.7 eV, and with introduction rates of 0.1 and 0.9, respectively.

#### Controlling chemical reactions on silicon surfaces by means of electronic, vibrational, and thermal excitation

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The search for new, functional molecular architectures on surfaces calls for new strategies in controlling surface reactions. Here we show for ether cleavage on Si(001), the surface analogue of an SN2 reaction, that electronic and vibrational excitation open reaction channels beyond thermally activated reaction schemes: tip-induced excitation of the system in an STM leads to new final products and the type of final products is controlled by selectively addressing different excitation channels [1]: Above a threshold voltage of 2.5 V, direct electron transfer into the antibonding C-O orbital of tetrahydrofuran (THF) induces ether cleavage of the datively-bonded intermediate of THF on Si(001). Below the threshold, ether cleavage is induced by multiple excitation of vibrational modes. In both modes of excitation, additional final configurations are observed when compared to the thermally activated reaction. Furthermore, the distributions of final products significantly differ for these two excitation mechanisms. The results thus demonstrate how the steric constraints of the thermally activated reaction can be overcome both by electronic and vibrational excitation. What is more, they show how the final reaction products can be controlled by means of the different excitation mechanisms which in turn can be selectively addressed by the tunneling voltage. In particular in combination with on-surface reactions of organic building blocks, this can lead to new molecular architectures. The results are furthermore compared to the means and limitations of controlling reactions on silicon in the thermally activated regime.

[1] Mette, et. al., Angew. Chem. Int. Ed., DOI: 10.1002/anie.201806777 (in print).

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# Ultra-soft analysis of organic samples by means of cluster induced desorption/ionization mass spectrometry – high depth resolution and low matrix effect

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For the investigation of organic molecules in organic samples (surface and bulk), standard surface science methods such as XPS typically lack chemical information due to the complexity of the molecules. On the other hand, cluster-SIMS has been successfully employed; however, the following challenges remain: (1) Substantial fragmentation is still observed in biomolecular samples. (2) Depth resolution in organic material is limited. (3) For mixed samples, interaction between the different chemical components can lead to a change in ionization efficiency by up to several orders of magnitude (the so-called matrix effect). Thus, quantitative and even qualitative data interpretation can be most difficult.

In this contribution, we show that desorption/ionization induced by neutral SO2 clusters (DINeC) can be applied for very soft analysis and depth-profiling of biomolecular samples with high depth resolution and low matrix effect. We used mixed peptide/lipid samples which are known to exhibit a pronounced matrix effect in SIMS. In contrast, the relative amounts of substance of peptide and lipid as derived for the mixed samples by means of DINeC-MS were found to be close to the nominal values indicating a very low matrix effect.

Throughout the depth profiles, only intact molecular ions [M+H]+ as well as dimers of peptides and lipids were detectable, indicating the extremely soft nature of the DINeC process even when used for depth profiling of biomolecular samples. We observed intensity oscillations due to alternating bi-layers of peptide and lipid molecules indicating a depth resolution on the molecular scale. Sensitivity was < 0.001 ML.

# A New orifice flow system for vacuum calibration in NIM

Jinku Wang, Hongyan Yu

A new vacuum calibration standard for UHV pressure range has been been completed at National Institute of Metrology(NIM). This system is based on the continuous expansion method (also called the "dynamic" or "orifice-flow" method). The measurement range of this system is from 1E-7Pa to 5E-3Pa with uncertainty 5%(k=2). A residual pressure of 4E-9 Pa has been obtained in the calibration chamber. A new constant pressure flow meter has been developed to measure the conductance value of sintered stainless steel filter, and then use it to provide flow rate with known value. The uncertainty of the conductance measurement is 0.4%. The pressure in the front of sintered stainless steel filter is measured by capacitance diaphragm gauges. The orifice between the calibration chamber and evacuation chamber is an knife-edge hole with diameter 22.3mm, and the conductance value of it is been calculate by the dimension measurement result.

## Comparative outgassing studies of common vacuum chamber materials

James Fedchak, Julia Scherschligt, Dan Barker, Steve Eckel

Obtaining UHV and XHV pressures usually requires vacuum chambers with outgassing rates much less than 10-9 Pa L s-1 cm-2. Because the ultimate pressure of a vacuum system is proportional to the outgassing rate divided by the pumping speed, chambers with ultra-low outgassing rates also help reduce the cost of large vacuum systems by requiring fewer pumps (with the associated cost of operation and maintenance) to obtain the desired ultimate pressure. Low H2 outgassing rates are usually obtained by careful selection of metals, such as aluminum or titanium, or by special heat treatments of stainless steel. We have measured and compared the H2 and water outgassing rates for 7 identical vacuum chambers constructed of common vacuum chamber materials and heat treatments: 304L, 316LN-ESR (electro-slag remelt), titanium, aluminum vacuum-fired 316L, and vacuum-fired 316LN-ESR. These chambers are of identical geometry and are from the same manufacturer. In general, the outgassing rate of these chambers is dominated by H2 dissolved in the bulk after water has been removed by a short bake (a few days) at a temperature of 100 °C to 150 °C. However, the time-dependent water outgassing rate, determined before the short bake, can be critical in the design and operation of large vacuum systems, where the time it take to remove the water translates into time and cost of construction. Moreover, if the system is vented for maintenance, subsequent re-baking may not be feasible in many large vacuum systems. We will present the results of these studies and, if time allows, additional comparative studies possibly including 400 °C heat treatments of 304L under vacuum and in air, will also be presented.

# Fabrication of chromium carbide/a-C:H thin films by high power impulse magnetron sputtering: role of target poisoning and substrate bias

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The chromium carbide thin film has attracted lots of attention from academia and industry due to its outstanding chemical stability, low coefficient of friction, adequate hardness and wear resistance. In this work, the chromium carbide/a-C:H thin films were grown through a single high power impulse magneton sputtering (HiPIMS) and a superimposed HiPIMS-middle frequency (MF) deposition system, respectively. The Cr target poisoning status was controlled using a plasma emission monitoring (PEM) system by adjusting the gas flow ratios of Ar and acetylene (C2H2). Different Cr target poisoning status and different substrate bias were selected during deposition. The evolution of microstructure, crystalline phase, binding status, electrical conductivity, corrosion resistance, and mechanical properties were investigated. We can conclude that the Cr3C2 and CrC nanocrystallites were embedded in the amorphous CrCx/a-C:H substrate. The maximum hardness of ~27.5 GPa was obtained for the film deposited at the target poisoning degree of 70% and -600V substrate bias due to the Hall-Petch strengthening effect.

# First-stage of a defect reaction around Ga vacancy in GaN

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<sup>2</sup> Wakayama University

GaN is one of the most important materials in light-emitting diodes (LEDs), laser diodes, and also power devices. Although many studies have been carried out to characterize the mechanics of light emission and carrier transport, the mechanism of device degradation remains unclear. Defect reactions in GaN can cause degradation in the active regions of GaN-based devices; however, the microscopic mechanism of such defect reactions remain unclear. It is necessary to clarify the microscopic mechanisms of fabricate more efficient LEDs and transistors with longer lifetimes.

In the previous work, we have shown that a possibility of a defect reaction from VGa to NGa-VN complex in GaN occur under high carrier dope condition using the density functional theory[1]. However, quantitative reaction rate has not been determined yet. In this study, we construct a configuration coordinate oscillation model for the defect reaction. Using the model, we simulate the defect reaction with several conditions of carrier capture rate. It is revealed that an amplitude of a localized phonon mode is enhanced with the carrier capture rate above 0.6. We discuss the microscopic mechanism and the reaction rate minutely in the presentation.

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# Kinetic competition in MoS2 nanotube growth by catalytic CVD using FeO nanoparticles

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MoS2 and other layered materials are gathering much attention as ideal two dimensional materials platform for semiconductor or surface science applications. Although graphene has carbon nanotubes as its rolled one dimensional structures, there are only a few reports on nanotubes of MoS2 or related materials. Synthetic strategies so far have drawbacks of low yield, not scalable, and long time reactions. Here, we have developed a catalytic CVD route to make MoS2 nanotubes using catalytic metal nanoparticles. We found particles of Fe compound facilitate the growth of MoS2 nanowires among various transition metals[1]. We developed protocols to control the size and the shape of the FeO nanoparticles in the nanoscale by solution chemistry. The nanoparticles were dispersed on SiO2/Si substrate and CVD growth was performed by separate flows of MoO3 and S[2]. When FeO nanoparticles were octahedral with sharp apexes, MoS2 nanotubes were formed via VS mechanism. They were multiwall crystalline nanotubes of MoS2 with zigzag chirality. When spherical FeO particles were used, the product was SiO2 nanowires grown by VLS mechanism. It was found that Si came from quartz tube of the reactor. This MoS2/SiO2 product switching occurs because of the competition of the growth kinetics controlled by the size of the metal catalysts[3].

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#### Phase-engineered two-dimensional materials toward 2D/3D hybrid heterostructures

Yu-Lun Chueh

2D materials have attracted much attention because of frontier electronic materials due to its superior electronic transport properties and mechanical flexibility in the future, making it a potential material for high performance and wearable electronics. Graphene is a typical 2D materials with high carrier mobility; however, it still cannot be applied in transistor due to the lack of bandgap. A new type of 2D semiconducting materials called transition metal dichalcogenides (TMDCs), which are layered structure with the strong in-plane bonding and weak out-of-plane interactions similar to graphite, have been intensively studied. Recent studies have predicted exceptional physical properties upon reduced dimensionality attracting lots of attention due to the versatile physical chemical behaviors. Nevertheless, the synthesis and the study of the fundamental physical properties of TMDs are still in early stages. The lack of a large-area and reliable synthesis method restrict exploring all the potential applications of the TMDs. Chemical vapor deposition (CVD) is a traditional approach for the growth of TMDs; nevertheless, the high growth temperature is a major drawback for its to be applied in flexible electronics. In this talk, an inductively coupled plasma (ICP) was used to synthesize Transition Metal Dichalcogenides (TMDs) through a plasma-assisted selenization process of metal oxide (MOx) at a low temperature, as low as 250 °C. Compared to other CVD processes the use of ICP facilitates the decomposition of the precursors at lower temperatures; therefore, the temperature required for the formation of TMDs can be drastically reduced. WSe2 was chosen as a model material system due to its technological importance as a p-type inorganic semiconductor with an excellent hole mobility. Large-area synthesis of WSe2 on polyimide (30 x 40 cm2) flexible substrates and 8-inch silicon wafers with good uniformity was demonstrated at the formation temperature of 250 °C as confirmed by Raman and X-ray Photoelectron (XPS) spectroscopy. Furthermore, by controlling different H2/N2 ratios, hybrid WOx/WSe2 films can be formed at the formation temperature of 250 °C as shown by TEM and confirmed by XPS. The applications o including (1) water splitting, (2) gas sensors, (3) photodetectors, (3) anode materials in secondary ion battery will be reported.

# Atom Probe Tomography characterization of materials for electronic devices

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For more than ten years, the implementation of ultra-fast laser pulses in the atom probe tomography (APT) technique enabled the study of semiconducting materials. APT is an impressive technique since it has the ability to image in 3D at the atomic scale and measure composition in a semiconductor device with high sensitivity. This presentation aims at addressing the current state of the art of electronic device analysis by APT, including the advantages and drawbacks of the tehnique, by selecting striking exemples. Finally the improvements necessary in terms of sample preparations or reconstruction procedures, and the future evolutions of the technique are discussed.

# Monte Carlo study of a metal foil pump with normal and energetic deuterium gas molecules

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It will be a challenging task to reduce the tritium inventory in the next generation nuclear fusion reactor. This can be done by a smart fuel cycle architecture based on the idea of Direct Internal Recycling. An essential part of this concept requires a hydrogen separation stage at low operation pressures. This is planned to be performed by a Metal Foil Pump (MFP), which can separate the unburned hydrogen isotopes from the fusion exhaust by exploiting the effect of superpermeation. The MFPs will be placed very close to the torus and separated hydrogen can be directly recycled as fuel back to the reactor.

In gaseous form hydrogen is present as a molecule, but dissolves in atomic form in metal foils. Superpermeation assists the dissociation by an energy source such as a cold plasma or incandescent filament in combination with certain surface conditions of the metal foil. The performance of such a pump is governed by the parameters of the energy source and metal foil, such as the dissociation rate, the recombination rate, capture coefficient of the foil and by the pump geometry and internal vacuum flow.

The current design of a MFP employs a coaxial design with a linear plasma source as central core and a surrounding cylindrical metal foil. In this study we present the Monte Carlo simulation of this pump and derive the most important characteristics, such as the pumping speed and the separation efficiency. Meanwhile, intensive parametric studies will give the insight for further pump development.

# A comprehensive study of AIN nucleation layers grown onto on-axis and 4 degree off-axis SiC (000-1) substrates and its influence on GaN growth

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Group-III nitrides have been intensively investigated and widely employed in optoelectronic and electronic devices. Recently, nitrogen(N)-polar group-III nitrides have drawn much attention due to their unique characteristics compared with gallium(Ga)-polar nitrides in the application of high electron mobility transistors (HEMTs), such as the feasibility to fabricate low ohmic contacts, an enhanced carrier confinement with a natural back barrier, as well as high device scalability. The growth of N-polar group-III nitrides layers are expected on C-face SiC substrates. According to previous studies, the initial AIN nucleation step is critical to the polarity control of AIN and GaN layers on SiC substrates.

In this work, we study in a comparative manner epitaxial GaN layers grown onto on-axis and 40 off-axis SiC (000-1) substrates by hot-wall MOCVD. GaN epilayers are grown simultaneously on both substrates employing N-polar AlN nucleation layers (AIN-NLs). We investigate the difference in surface morphology and crystal quality of the GaN epilayers on the two substrates. Growth mechanisms leading to different polarities on the two types of substrates are discussed based on transition electron microscopy (TEM) findings. 'V' shape inversion domain boundaries are observed between N-polar and Al-polar at AIN-NLs at on-axis substrate while metal-rich Al-Al bonding layers are observed on off-axis substrates. The nature of AIN-NLs and its interfaces with the substrates and GaN epilayer is discussed. Atomic arrangement at the interface and possible bonding configurations are also analyzed. Furthermore, the stain and free charge carriers of GaN layers are investigated by infrared spectroscopic ellipsometry.

# Temperature-dependent physical properties of a spin crossover complex [Fe(tdap)2(NCS)2] thin film

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Spin crossover (SCO) is a phenomenon where the spin state of metal ions changes from a low-spin (LS) state to a high-spin (HS) one or vice versa by external stimuli. So far, the transition in spin states were studied either directly by magnetic susceptibility measurement or indirectly by X-ray diffraction measurement, vibrational spectroscopy, or absorption spectroscopy. Most of these studies were performed for SCO materials in crystal phase, and there are only few studies on SCO materials in thin film phase. Furthermore, there is no experimental study on the electronic states of SCO materials till now, though these information are indispensable to have a comprehensive understanding of their physical properties. In this paper, we will present the physical properties of a SCO complex [Fe(tdap)2(NCS)2] thin film grown on HOPG. [Fe(tdap)2(NCS)2] crystal is known to show SCO phenomenon with its LS state at below 180 K and HS one at above 400 K. By measuring the magnetic susceptibility, we found that the LS state of [Fe(tdap)2(NCS)2] thin film is below 100 K and its HS state is above 400 K. We also measured the temperature-dependent structure of the film, the absorption spectra, and the valence band electronic states. Based on the obtained results, we will discuss the SCO mechanism of the [Fe(tdap)2(NCS)2] thin film in details.

# Teaching vacuum science and the Professor Vacuum show

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Vacuum courses were given at a wide range of levels from engineers and general audience to beginning and advanced level university courses. They include laboratory exercises, demonstrations and visits to vacuum-based research laboratories. A web-based distance course used the study platform PingPong and had two meetings in Uppsala. One of the goals was to provide tools to simulate the performance of a more complex vacuum system, e.g. a system in student's laboratory or company. The Professor Vacuum show is given for 10-12 year old school children at SciFest, a science festival in Uppsala, since 2018 also as a part of SciCruise, a Swedish - Finnish cruise Stockholm - Turku with workshops and demonstrations for school children and accompanying teachers/parents reaching a wider range of ages. In the show we discuss pressure, the number of molecules/volume in air, in a vacuum system, on the moon and in space. We demonstrate Gallileo's experiment with falling feather and metal, water in a vacuum system and discuss why it is not possible to boil potatoes on high mountains. The most popular experiment is expansion of soft bakery products in a bell jar. In another experiment a lit match is dropped inside a bottle and an egg is paced on top of the opening, which is not large enough for the egg to pass through. We discuss gas laws, to what extent our daily surrounding depends on vacuum technology, and how this in the future can give rise to new environmentally friendly transport systems.

# Magneto-Seebeck tunneling on the atomic scale

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The tunneling of spin-polarized electrons in a magnetic tunnel junction driven by a temperature gradient is a fundamental process for the thermal control of electron spin transport. As we have shown recently, scanning Seebeck tunneling microscopy is a technique that enables spin-averaged thermopower measurements in a metal-vacuum-metal tunnel junction with atomic-scale lateral resolution [1]. Using a magnetic tip and sample allows for the experimental investigation of the details of the magneto-Seebeck tunneling, with vacuum serving as the tunneling barrier. Heating the tip with a laser and measuring the thermopower of the junction while scanning across the spin texture of the sample leads to spin-resolved Seebeck coefficients that can be determined and mapped with atomic-scale lateral resolution [2].

The experiments on Fe/W(110) and Fe/Ir(111) will be presented and discussed in terms of spin-averaged, magneto-Seebeck and anisotropic magneto-Seebeck thermopower in an ideal single atom tunnel junction. Based on the experimental findings we propose a spin detector for spintronics applications that is solely driven by waste heat, utilizing magneto-Seebeck tunneling to convert spin information into a voltage that can be used for further data processing.

[1] C. Friesen, H. Osterhage, J. Friedlein, A. Schlenhoff, R. Wiesendanger, and S. Krause,

"Scanning Seebeck tunneling microscopy", J. Phys. D: Appl. Phys. 51, 324001 (2018).

[2] C. Friesen, H. Osterhage, J. Friedlein, A. Schlenhoff, R. Wiesendanger, and S. Krause,

"Magneto-Seebeck tunneling on the atomic scale", Science (accepted).

# Towards a standard for ionisation gauges

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The EURAMET EMPIR project "16NRM5-ion gauge" is an EU-funded project between European National Metrological Institutes (NMI), Nova University of Lisbon, CERN, and the two vacuum gauge manufacturers VACOM and INFICON (LI) aiming to develop a standard for ionisation vacuum gauges. The objective is to provide recommendations for the construction and operation of such gauges, in order to allow reducing the relative high uncertainties and providing reliable relative gas sensitivity factors of ionisation gauges. Such relative gas sensitivity factors are needed to calibrate quadrupole mass spectrometers in situ. The considered pressure range is 10-4 to 10-8 mbar. The project has well advanced and is now in the prototyping phase. Laboratory gauges have been constructed based on prior simulations. These gauges are being tested and the results are compared with the simulations and stability expectations. We present the status of this project and the results obtained so far.

#### Energy and momentum driven growth of CuO by reactive magnetron sputtering

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Structure zone models give an overview of the microstructure as a function of the deposition conditions. It has been shown by our research team that these overviews can be interpreted in a quantitative way by studying the ratio between the diffusivity (D) and the deposition flux (F) [1-3]. The deposition flux can easily be derived from the deposition rate. To calculate the diffusivity the available energy per deposited atom (EPA) needs to be quantified which becomes possible by measuring the total energy flux with a passive calorimetric probe. In this paper, this approach is applied to understand the phase formation during reactive sputtering of CuO in an argon/mixture. The influence of the total pressure, and the discharge current was investigated. Within the experimental range hardly any changes in the EPA could be noticed, illustrating that the phase formation in the case of copper oxide thin films is solely defined by the oxygen partial pressure in the system. In the case of pure tenorite (CuO) thin films deposited at relative high oxygen partial pressures, the EPA could by increased, and it is shown that this leads to less crystalline films. The origin of this behaviour is further investigated by energy-resolved mass spectrometry to determine the influence of negative oxygen bombardment.

[1] Review paper : S. Mahieu, D. Depla, Journal of Physics D: Applied Physics 42 (2009) 053002

[2] Critical review paper : D. Depla, B. Braeckman, Thin Solid Films, (2016) 90-93

[3] J. Xia, W. Liang, Q. Miao, D. Depla, Applied Surface Science 439 (2018) 545-551

# Potential dependent diffusion behavior of Mg2+ ions at interfacial ionic liquid on Au electrode analyzed by electrochemical XPS

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lonic liquids (ILs) are promising electrolytes for electrochemical devices such as secondary battery, capacitor, electric double layer (EDL)-FET, due to their high chemical stability with negligible vaporization. However, it is known that diffusion of solutes in IL sometimes does not follow the Stokes-Einstein relation, where the diffusion is inversely proportional to the viscosity. The Mg2+ ion, which is a candidate for the secondary battery source instead of Li+, was recently found to be deviated from the relation.

The negligibly low vapor pressure of ILs at room temperature enables their analysis using various surface science techniques such as X-ray photoelectron spectroscopy (XPS) which essentially demand high vacuum conditions. Negligible vapor pressure also enables the electrochemical measurements themselves to be conducted under high vacuum. Thus, XPS, as an elemental analysis method, can potentially combine nicely with the electrochemical processes of ILs.

In this presentation, we will discuss the diffusion behavior of Mg2+ ions in an IL (BMIM-TFSI) in the vicinity to the Au(111) electrode analyzed by electrochemical XPS(EC-XPS) for the response to the electrode potential change.

In the EC-XPS experiment, the Mg2+-contained IL / Au(111) electrode interface was analyzed at thin IL area as a function of the solution thickness and the electrode potential in the three-electrodes cell. It was clearly demonstrated that concentration of Mg2+ was reversibly changed according to the electrode potential, which accompanied the change of cation and anion ratio of the IL.

[1] K. Fukui, Y. Yokota, A. Imanishi, Chem. Rec. 14, 964 (2014).

# III-V nanowire MOSFETs for high-frequency applications

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III-V materials have for long been used in high-electron-mobility-transistors (HEMTs) with a high performance. However, to improve the performance of the transistors, the scaling of the gate length and the barrier thickness is required, however, it also leads to increased short channel effects and increased gate leakage. One way to improve these characteristics is to use nanowire MOSFETs, where the nanowire geometry enables improved electrostatic control of the channel, and the oxide separating the gate contact from the channel reduces the gate leakage. MOSFETs. Nanowire MOSFETs is also one promising candidate for the very scaled CMOS nodes at 5nm and below.

In earlier work, we have demonstrated InGaAs nanowires grown with selective area growth in tri-gate geometry, with excellent performance. The devices demonstrate good DC performance with low SS and low Ron together with a high transconductance. In order to compete also in the RF domain, device architectures with low capacitance and maintained good RF performance is required. This is however challenging due to that many efforts to decrease the capacitances also increases the resistances, affecting the DC properties negatively.

In this work, we would like to present our techniques for growing high-quality lateral InGaAs nanowires, together with highly doped contact areas and spacers, all designed for the high-frequency domain.

#### Nanoscale heterogeneity of nucleating surface oxide on austenitic stainless steel

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Stainless steels (SS) are widely used because of their high corrosion resistance provided by the passive film of a few nanometers thick and strongly enriched in Cr(III) (hydr)oxide species. Recent surface analytical studies speculate that passivity breakdown, leading to local failure of the corrosion resistance, would originate from the surface heterogeneity of the Cr(III) oxide enrichment at microscopic level. Yet, despite decades of research, the mechanisms distributing the chromium oxide enrichment at small space scale remain poorly understood.

In this work, we applied Scanning Tunneling Microscopy to investigate in situ at small time and space scales the nucleation mechanisms of the surface oxide on a (100)-oriented model 304 austenitic stainless steel single crystalline surface. The experiments were performed by exposing an oxide-free Fe-18Cr-13Ni(100) surface, to gaseous oxygen at 250°C for exposure up to 3 L.

The results show how the local oxidation of chromium governs the nanoscale heterogeneity of the nucleating surface oxide. The initial oxide-free surface was reconstructed with self-organized vacancy lines in the topmost plane. After very first oxidation stage at 1 L exposure, chromium oxide islands nucleated preferentially at the step edges, forming nanometric square structures and causing a non-uniform distribution of chromium in the surface oxide layer. The heterogeneity resulted from diffusion of metallic chromium in the topmost layer to feed nucleation at the surface defects (step edges) leaving behind new vacancies on the terraces. Then Cr(III) oxide nucleated on the terraces after exposure of 3 L, forming square patterns of nanometric square structures.

## Outgassing of dynamic vacuum components

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Outgassing rate measurements have been utilized for the qualification of the vacuum suitability of materials and vacuum components for long time. At VACOM these measurements are fully integrated in the process chain of the production and cleaning of vacuum components for applications e.g. at particle accelerators, in aerospace industry and in the semiconductor industry. By this means, outgassing rate measurements are routinely performed with residual gas analysis (RGA) systems (utilizing either the throughput or the box-in-box method) in order to verify the cleanliness and vacuum suitability of the parts, components and assemblies. Whereas desorption rate and outgassing rate of unbaked and baked "static" vacuum components are straightforward to access by conventional outgassing rate measurements, the behaviour of "dynamic" vacuum components is more difficult to study.

In this talk, we present some results of outgassing rate qualification measurements of dynamic vacuum components. We characterized the outgassing behaviour of linear and rotary motion feedthroughs in unbaked and baked condition as well as in stationary and dynamic operation. The measurement setups are presented, the experimental findings will be discussed in detail and conclusions are drawn to the design, the vacuum suitability, and the application of dynamic vacuum components.

## Leakage in refrigeration compressor valves: an application of rarefied gas dynamics

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According to the International Institute of Refrigeration, the refrigeration sector (including air conditioning) is responsible for approximately 17% of the global electrical energy consumption. Therefore, any effort to improve the performance of refrigeration systems can have a great impact on global-warming reduction. In these systems, the compressor consumes most of the energy and, even though its efficiency has been improved considerably in the last decades, many irreversibilities take place in this component. Recently, leakage through compressor valves has become an important issue in terms of compressor efficiency. These leakages occur through very narrow gaps between the valves and their seats formed by surface irregularities on the order of few micrometers, where rarefied conditions generally take place. During the last few years, research on leakage through household refrigeration compressor valves has been conducted at the Federal University of Santa Catarina. A one-dimensional compressible flow model based on the Navier-Stokes equation with slip boundary conditions was developed to estimate valve leakage. In addition, an experimental setup was built to measure leakage through compressor valves. The comparison between numerical and experimental results allowed the estimation of the edge gap, a geometric parameter characterizing the sealing performance of compressor valves. Another experimental setup was developed to measure the mass flow rate of gases through microchannels and the tangential momentum accommodation coefficients of gases used in the refrigeration industry were determined. This presentation shows the application of rarefied gas dynamics to refrigeration compressors and the developments achieved at the Federal University of Santa Catarina.

# Integration of InSb on Si by Rapid Melt Growth

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Monolithic integration of III-V semiconductors with Silicon technology has instigated a wide range of new possibilities in the semiconductor industry, such as combination of digital circuits with optical sensing and high-frequency communication. Dissimilarities in the crystal structure symmetry and large lattice mismatch between III-V's and Si are the challenges that prevent direct epitaxial growth of III-V on Si. A promising method is Rapid Melt Growth (RMG) which integrates high-quality single crystalline III-V microstructures at low cost and in a process that is CMOS compatible[1]. In this growth, amorphous source material is deposited inside a micro-crucible with a nano-scale opening (seed) to the Si substrate. When the material is annealed above its melting point, the crucible contains the liquid. On cooling, epitaxial growth occurs from the seed to the end of the structure, resulting in a high quality crystal as strain-induced misfit dislocations are confined to the region near the seed. RMG of Ge on insulator, GaAs[2], GaSb[2] and InAs[3] has been reported. In this work we have developed for the first time the RMG process for integrating InSb nano and microstructures on Si. Such InSb materials are promising for integrated optoelectronics (mid-infrared) and topological quantum devices. We will here describe the process development and characterization of the resulting InSb material using x-ray diffraction, electron backscatter diffraction, atomic force microscopy, and electrical measurements.

- 1. Liu et al. APL. 84, 2563 (2004).
- 2. Chen et al. Electron Dev Lett. 31, 11 (2010).
- 3. Yuan et al. Symp VLSI Tech Dig. T54-5 (2013)
### Surface characterization of structural alloys

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Structural alloys like steels and aluminum alloys have in common that their surface oxides determine the material's properties with respect to e.g. corrosion, wear, joining, and coating. Therefore, a surface science approach was employed to study the chemical composition, thickness, and distribution of phases and particles. In an attempt to bridge the pressure gap, the different samples were studied in classical UHV environments as well as in experimental conditions mimicking their industrial applications. This contribution shows how different methods, mainly AP-, XPS, XPEEM, and XRR, can be applied to complex industrial systems.

In the case of aluminum brazing sheets, the breakup of the surface oxide is a crucial process for the joining of workpieces as it impacts the wetting of the faying surface and strength of the formed joint. Here, we found that especially the diffusion of Mg to the surface facilitates the decomposition of the oxide. The second example is heat-treatable aluminum alloy 6063 where the impact of the oxygen partial pressure on the surface oxide composition was studied. The influence is most visible at high temperatures and ambient conditions where the oxide composition changes from mostly Al-based to mostly Mg-based which is in stark contrast to the UHV conditions. Super duplex stainless steels as the here studied SAF 2507 introduce extra challenges to their surface characterization as they contain multiple phases. A range of cathode lens microscopy techniques was used to follow the phase transitions and partitioning of alloying elements throughout heat treatment.

# Decomposition of methanol on vanadium nanoclusters supported on thin film Al2O3/NiAl(100)

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The catalytic decomposition of methanol is extensively investigated because the principal reaction is applied in direct methanol fuel cells (DMFC) and also serves as a source of hydrogen. As the performance of DMFC or the production of hydrogen is governed largely by the catalyzed reaction, a knowledge of the detailed reaction kinetics and a correlation between reactivity and structure of the catalysts are desirable. To respond to the demand, we investigated adsorption and reaction of methanol on vanadium nanocluster supported on a Al2O3 thin film grown on NiAl(100), a realistic model system, under ultrahigh vacuum conditions and with various surface probe techniques. Vanadium was chosen as supported vanadium oxides are important industrial catalysts, particularly for oxidative dehydrogenation of methanol decomposed through dehydrogenation and C-O bond scission; hydrogen and methane were evidently produced whereas no CO was observed. The production of hydrogen and methane depends significantly on the vanadium cluster size: the hydrogen produced per surface vanadium site increased monotonically with the cluster diameter, but the methane attained a maximum at cluster diameter about 1.9 nm and decreased with further increased diameter. The presentation will discuss the origin of the size-dependent reactivity.

## Formic acid induced near surface restructuring of magnetite

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Magnetite (Fe3O4) nanoparticles can be applied, e.g., in catalysis, for water decontamination, or linked by oleic acid in hierarchical hybrid materials. The interaction of their surfaces with organic acids in general plays an important role in many applications. Particularly, formic acid is of interest since it is an intermediate, e.g., in the water-gas shift reaction and a probe molecule representing the anchoring group of larger molecules interacting with magnetite nanoparticles.

Previously, the reconstruction of the (001) surface of magnetite was found to be lifted upon formic acid adsorption [1]. But it remained unclear which adsorption site is preferred and how the underlying surface structure changes. This implies that the termination and reconstruction of the other major surface of magnetite, the (111) surface, which was debated over for a long time anyway, may also change upon formic acid adsorption.

Here, the results from studying the interaction of formic acid with the major surfaces of magnetite using multiple techniques are presented. Calculations based on density functional theory (DFT) allow us to understand the energetics of the adsorption. Changes in the reconstruction and termination of the surfaces are reviewed from a thermodynamics point of view. The predicted structural changes are also seen in surface X-ray diffraction (SXRD) data. Finally, calculated vibrational spectra are compared to infrared spectroscopy data to get further insight in the adsorption mode and even the underlying surface structure.

[1] Gamba et al., J. Phys. Chem. C 119, 20459 (2015)

# Strain mapping in nanowire devices using nanofocusing XRD

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Hard X-rays can be used to investigate electronic and optoelectronic devices in more or less realistic operational conditions, and modern X-ray optics reach the relevant length scales for nanoelectronic devices. Here, we demonstrate how nanofocusing X-ray diffraction (nano-XRD) can be used to reveal new phenomena in strained core-shell nanowires and nanowire transistors.

First, we in investigated strained GaAs–GaInP core-shell nanowires. Nominally identical growth conditions for each sample were achieved by using nanoimprint lithography, but we observed large individual differences, with neighboring nanowires showing either straight, bent, or twisted morphology. Using scanning X-ray diffraction with a 100 nm beam, we reconstructed and quantified the bending and twisting of the nanowires in three dimensions (Fig. 1). In one nanowire, we found that the shell lattice was tilted with respect to the core lattice, with an angle that increases from 2° at the base to 5° at the top. Furthermore, the azimuthal orientation of the tilt changed by 30° along the nanowire axis.

Second, nanofocused hard X-rays were used to quantitatively probe both strain and bending in a single nanowire device under electric bias. We measured and quantified the bending of the as-processed nanowire in the gap between the contacts. The device was then exposed to increasing bias voltages until breakdown, while simultaneously measuring the electrical current and performing scanning X-ray diffraction. The 3D shape of the nanowire was reconstructed from the XRD data. We observed that the nanowire changed shape, correlated with a reduction in electrical conductance.

# Electronic properties and device performance of organic donor/acceptor materials upon their environment effects

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The emerging of new polymer donor, acceptor, especially non-fullerene acceptors (NFAs), and interfacial materials as well as developments in device architecture such as ternary and tandem solar cells have pushed the power conversion efficiencies (PCE) of organic solar cells (OPV) in a high level [1-2]. Besides PCE, the stability is another important issue needed to be addressed for OPV on the way to large scale commercialization, which is less studied compared to PCE topic due to complicated processed in the materials degradation under different environments.

Here we present our recent studies of the stability of different fullerene and NFAs acceptors and their derivatives as model molecules to explore the stability of high performance in OPV [3]. To overcome the complicated pathways in degradation of organic films in ambient, we perform in-situ exposure of oxygen and water vapor separately in a controlled manner to organic films and vacuum annealing to simulate thermal effects on them. The modifications of the chemical or electronic structure and the interface properties, and the resistance to thermal stress and illumination here are probed by x-ray spectroscopy. For instance, our studies show that the NFAs show higher resistance to water vapor and thermal stress than fullerenes. Furthermore, the origins of the measured effects on the degradation will be discussed with density-function-theory calculations upon the possible change of molecular packing structure probed by diffraction, and the expected effects on device performance are commented upon.

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### Comparison and minimization of stimulated outgassing in particle accelerators

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Particle accelerators require excellent vacuum conditions for intensive beams of sufficient life time. Next generation facilities force up the beam intensities, resulting in loss levels that are in the order of the primary beam intensity of nowadays machines. This leads to increased stimulated desorption and limits the intensity or life time of the beam, regardless if it is an electron, proton or heavy ion accelerator. In all cases, high distributed pumping speed is favorable but on the other hand the stimulated outgassing has to be reduced to operate these accelerators reasonably.

We have compared thermal desorption with electron-induced and heavy ion-induced desorption and found some similarities that hint to a complex interaction of these stimuli in any particle-induced kind of desorption. However, a simple cure was found to generally minimize the amount of released gas significantly.

In the talk, we will discuss the interaction of different outgassing channels within particle-induced desorption. Some experimental and theoretical results will confirm the new model and explain the effect of the proposed method to reduce the induced outgassing in particle accelerators.

# **Quantum Based Cold-Atom Vacuum Standard**

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The National Institute of Standards and Technology (NIST) has a long history of laser cooling and trapping of neutral atoms, largely motivated by building better time standards or clocks, and has recently begun a program to extend the metrological capabilities of cold trapped atoms to measurement of vacuum. This will align vacuum metrology to the emergent "Quantum SI" paradigm, in which a measurement has intrinsic traceability and the line between sensor and standard is blurred. Since the earliest days of neutral atom trapping it has been known that the background gas in the vacuum limits the lifetime of atoms in the trap. Because the measured loss-rate of ultra-cold atoms from a trap depends on a fundamental atomic property (the loss-rate coefficient or thermalized cross section) such atoms can be used as an absolute sensor and primary vacuum standard. While researchers have often observed that the relationship between the trap lifetime and background gas can be an indication of the vacuum level, but a true absolute sensor of vacuum has not yet been realized. This is because there are many technical challenges that must be overcome to create a device that's truly absolute and primary. We will discuss our progress toward meeting these challenges, including a very brief review of the ab initio theory, systematic uncertainty analysis, and apparatus design and operation. We will also discuss how the Cold Atom Vacuum Standard fits into the broader picture of the NIST dissemination of the Quantum SI.

# Electron heating mechanisms in magnetron sputtering discharges

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According to the established view, magnetron discharges are sustained by secondary electrons. These electrons emerge from the target and obtain high energies from the sheath. In collisions with the surrounding gas they crate new ion-electron pairs and thus sustain the discharge. This paradigm needs to be re-evaluated with recent findings that magnetron plasma is not azimuthally homogenous rather it is concentrated in several dense regions, called spokes. Spokes, which are regions of enhanced ionization, usually form periodic patterns and rotate above the magnetron in the azimuthal direction. Their number and dynamics depend on the gas pressure and discharge current. Spokes were observed in continuous and pulsed discharges and appear to be an essential feature of magnetron plasmas [1, 2].

Measurements of the plasma potential demonstrated that spokes are locations of high electric potential relative to the surrounding region with the largest potential gradient near the spoke's edge [3]. Electric field distribution associated with the spokes suggests that another mechanism provides energy to electrons. Namely, when electrons drift from the low to the high potential side of the spoke they can gain more than 50 eV of energy, which exceeds the ionization thresholds of atoms and ions. In this talk, we will present our latest understanding of electron heating mechanisms in the magnetron discharges.

Acknowledgment: The experimental work reported here was done at Lawrence Berkeley National Laboratory in USA.

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# Radio-frequency STM for mechanical resonance spectroscopy at the single-molecule level

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While single-molecule imaging is routine since the advent of the scanning tunneling microscope (STM), their chemical identification by STM remains a challenge. Recent advances of conductance spectroscopy utilizing low-temperature STM combined with radio-frequency modulation of the tunneling voltage [1-4] promise to turn the STM into an identification tool with sub-molecular spatial resolution. Our method, denoted as radio frequency scanning tunneling spectroscopy (RFSTS), is based on a spectroscopic STM system operating at GHz frequencies and combines the excellent spatial resolution (< 1 µeV) of microwave resonance techniques. After introducing our RFSTS experimental setup, I report on the resonant detection of mechanical degrees of freedom in individual surface-adsorbed molecules. I will end my presentation, discussing future directions of RFSTS for chemical identification at the single-molecule level. [1] Phys. Rev. Lett. 112, 117201 (2014). [2] Nanotechnology 25, 135705 (2014). [3] Phys. Rev. Lett. 113, 133001 (2014). [4] Sci. Rep. 7, 9708 (2017).

# Cross-Sectional X-ray Nanodiffraction Analysis of Microstructure-Stress-Property Relationships in Thin Films

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Nanocrystalline thin films possess complex gradients of microstructure and residual stresses, which originate (i) from selforganized film growth, (ii) from intentionally varying deposition conditions and/or (iii) from inhomogeneous thermal and/or mechanical loads applied during film service. In order to optimize functional properties of the thin films, it is necessary to assess both types of gradients at the nanoscale.

Cross-sectional synchrotron X-ray nanodiffraction (CSnanoXRD) [1] using monochromatic X-ray beams with a diameter down to ~30 nm provides representative depth-resolved data on the evolution of phases, crystallographic texture, grain morphology and strains/stresses across thin film cross-sections. The aim of this contribution is to discuss methodological and instrumental aspects of the approach as well as to present recent achievements from experiments at the beamlines ID13 of ESRF and P03 of PETRA III. By the examples of hard nitride, diamond and metallic thin films, it will be demonstrated that the new approach can serve as an effective tool to characterize the inhomogeneous properties of as-deposited and thermally cycled thin films. The observed gradients can be correlated with the varying film deposition conditions, providing an opportunity to optimize the time-dependent synthesis process. Additionally, results from strain and microstructure characterization in in-situ loaded monolithic and multilayered thin films will be presented. Finally, an outlook, especially on in-situ experiments as well as an analysis of complex depth gradients of structure-property relationships in nanocrystalline thin films, performed with even smaller X-ray beams, will be shortly discussed.

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# Nanostructured silicon with bi-metallic filling - a self-organized magnetic nanocomposite

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The purpose of this work is to fabricate nanostructured silicon by self-organization with two different materials of embedded magnetic nanostructures to exploit the magnetic properties of both metals and gain control of the exchange coupling between the two metals especially with respect to their volume ratio. Furthermore a variation of the structure size and the proximity of the metal deposits modify the exchange coupling and thus the energy product. The final goal is to achieve nanocomposits with an energy product as high as possible to give rise to on-chip applications using nanoscopic permanent magnets, especially arranged in arrays.

Two different templates, porous silicon in the mesoporous regime and porous silicon nanotubes are utilized to achieve such nanocomposites. The morphology (pore diameter, tube diameter) of the two systems is comparable. In the case of the utilization of mesoporous silicon templates the oriented and separated pores are filled with two different metals, namely Ni and Co which are deposited alternatingly by electrodeposition resulting in exchange coupled bi-metal structures. A further approach is the chemical growth of Co nanoparticles within porous silicon nanotubes (SiNTs) and the additional deposition of a Ni layer on the outer surface of the tubes. Since the silicon wall of the tubes offers a porous structure the Co particles, which are localized near the surface on the wall of a given nanotube, can touch the Ni layer and thus exchange coupling between them is enabled.

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# Technologies and Concepts of the UHV System for the MAIUS-2/3 Sounding Rocket Missions

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<sup>4</sup> The MAIUS project is a collaboration of LU Hannover, HU Berlin, FBH Berlin, JGU Mainz and ZARM at U Bremen. It is supported by the German Space Agency DLR with funds provided by the Federal Ministry of Economics and Technology (BMWi) under grant number DLR 50WP1435.

During the two sounding rocket missions MAIUS-2 and MAIUS-3, it is planned to perform sequential and simultaneous dualspecies atom interferometry with Bose-Einstein condensates of Potassium-41 and Rubidium-87. The scientific payload of the MAIUS missions will be launched on-board a VSB-30 sounding rocket launched from Esrange in Sweden. The flights of these rockets allows for approximately 360s of microgravity conditions.

The microgravity environment offers experiments on timescales that are not possible on ground based experiments. To perform long lifetimes of the BEC, a pressure  $\leq 5 \cdot 10-10$  mbar needs to be reached and maintained in the vacuum chamber. During ascent of the rocket, vibrational loads of 1.8 g RMS in the frequency range of 20-2000 Hz and accelerations of up to 13 g are applied to the vacuum system and the payload. During re-entry and landing static loads can reach a level of up to 50 g. The ultra-high vacuum system presented in this talk is designed to withstand these loads while maintaining the vacuum quality.

Therefore, the sealing technologies and pumping concepts which are used under this challenging requirements, needed to be tested and qualified. This talk presents the ultra-high vacuum system of the MAIUS-2/3 payload in detail, as well as its vibration and qualification tests at the shaker test facility at the Center of Applied Space Technology and Microgravity (ZARM) in Bremen.

# Can atomic-buckling control chemical reaction? The case of dehydrogenation of phthalocyanine molecules on a GdAu2/Au(111)

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The efficiency of chemical reactions on surfaces is traditionally related to their lattice structure. The periodic out-of-plane lattice distortions of supported 2D layers offer an alternative strategy to surface functionalization, scarcely investigated so far. Here, we show that the variable buckling geometry of a GdAu2 Moiré overlayer supported on the Au(111) surface exposes specific singleatom sites that control the dehydrogenation process of phthalocyanine (H2-PC) molecules. Thus, at most 1/3 of the adsorbed H2-PC molecules, corresponding to the ones adsorbed on the most reactive sites, undergo the dehydrogenation reaction. The outward displacement of distinct Gd sites is a spontaneous consequence of the lattice mismatch between the substrate and the alloy as previously reported. We show that these atomic sites promote the selective dehydrogenation of H2-PC molecules.

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## Ion induced secondary electron yield from surfaces exposed to environments of ionisation gauges

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The intensity of ion current in ionisation gauges is affected by ion induced secondary electron emission from the collector. Since namely this current is used to determine pressure, the pressure reading is influenced by the Ion Induced Secondary Electron Yield (IISEY). In the case of ions with energies up to 300 eV, secondary electron emission is a consequence of ion interaction with outermost surface layer. Therefore, changing collector surface properties, which can occur during the ionisation gauge operation, will contribute to pressure reading instabilities.

An ionisation gauge simulator was built in order to create environment typical for ionisation gauges. The exposures were performed for different gases, such as argon, H2 or water vapour. Several materials (Mo, Au, graphite) of potential interest as ion collectors were studied. Surfaces were characterized using XPS, IISEY and by following work function change.

The results show that IISEY, which is initially about 10-15 %, decreases with the exposure to about 7 %. The result of the exposure by different gases is always hydrocarbon contamination, which is strongly enhanced when samples are bombarded by ions created inside the simulator. Work function of different materials apparently converges to the same value due to the exposure. The smallest impact of the exposure on IISEY and overall surface properties was found in the case of graphite.

# On-surface synthesis of ethynylene bridged anthracene polymers

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The design of low bandgap  $\pi$ -conjugated polymers has received great attention during the last decades. These materials show unique properties due to the delocalized  $\pi$ -electrons and therefore are useful in many different application including LEDs, solar cells, organic field-effect transistors and biosensors. However, to date and despite the potential of such oligoacene compounds for plastic optoelectronics, the design of high quality  $\pi$  conjugated polymers exclusively based on oligoacene building units has been elusive.

Here, we present a comprehensive SPM and DFT study of the on-surface synthesis of poly(p-anthracene ethynylene) molecular wires on Au(111) in UHV conditions. A quinoid anthracene precursor functionalized with =CBr2 was sublimated and adsorbed on Au(111). By annealing polymeric wires consisting of anthracene moieties linked through ethynylene bridges form on the Au(111) (Fig.1). The reaction occurs in 3 different steps: dehalogenation, homocoupling and aromatization of the quinoid center.

The theoretical study of the reaction pathways, complemented with high resolution NC-AFM with Co-tip, illustrates that the homocoupling process is based on an efficient dehalogenation of the molecular precursors and diffusion of the surface-stabilized carbenes, finally leading to homocoupling and aromatization of the polymeric molecular chain. STM reveals the shape and the energy location of the frontiers orbitals, resulting in a gap of 1.4 eV.

Our results herald novel pathways to engineer  $\pi$  conjugated polymers on surfaces, addressing the relevant family of acenes, and thus contribute to develop the field of on-surface chemistry and to steer the design of modern low bandgap polymers.

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# Gas flows through porous media based on deterministic kinetic modeling on unstructured meshes

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Gas flows through porous media are encountered in industrial and technological applications including shale gas extraction, gas chromatography and microscale vacuum pumps without moving parts. Based on the local pore size the flow may be in a wide range of the Knudsen number and proper modeling is based on kinetic theory via the Boltzmann equation. Unstructured meshes are needed to properly recover the complicated geometry of porous media and the typical finite volume differencing results to the computationally expensive solution of large systems of algebraic equations. The so-called marching schemes do not require the solution of such systems and offer an alternative more efficient approach [1]. They are limited however, due to the peculiarities of their implementation, to structured meshes. In the present work a methodology is introduced extending the application of marching schemes solving kinetic equations in unstructured meshes and its computational effectiveness and efficiency is demonstrated by solving pressure driven rarefied gas flows through porous media. Prototype geometries are considered consisting of porous media with fractal cross-sections. The fractal cross-sections are discretized using unstructured meshes with triangular elements and the kinetic equations are solved providing the flow characteristics.

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# Spin State Manipulation of Nickel Quinonoid by Chemisorbed to a Co(001) Substrate

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We studied the structural, electronic and magnetic properties of recently synthesized Ni(II)-Quinonoid molecule adsorb on magnetic Co(001) substrate by means of density functional theory (DFT)+U calculations. A strong covalent interaction at the interface increases the Ni-O(N) bond lengths in the chemisorbed molecule leads to a spin state switching in the molecule from S = 0 state (in the gas phase) to S  $\approx$  1 state upon adsorption on the Co(001) substrate. Our DFT+U calculations shows that the molecule is ferromagnetically coupled with substrate. The exchange mechanism between the Co surface and metal centre in the molecule (Ni atom) was carefully investigated. It has been found that an indirect exchange interaction via quinonid ligands of the molecule, stabilizes the spin moment in the molecule in ferromagnetic alignment with the Co surface magnetization.

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# Charge transfer effects in sp-carbon atomic wires

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Carbon-atom wires are the ultimate 1D systems comprising ideally an infinite chain of sp-hybridized carbon atoms (i.e. carbyne) with two possible structures: semiconductive polyyne with an alternated single-triple bond sequence and metallic cumulene with equalized double bonds. In a finite system the wire length and the terminations can affect the overall structure of the wire thus ideally allowing to tune the electronic and optical properties from semiconductor to metal behaviour [1,2].

Here we discuss structure-property relationships in carbon-atom wires by means of a combined experimental and computational approach, based on Raman, surface enhanced Raman scattering (SERS) and density functional theory (DFT) calculations. The effect of chain length, termination and conjugation on wire structure is investigated. A charge transfer between wires and the metal nanoparticles used for SERS is observed and interpreted as a polyyne-to-cumulene transition (i.e. from semiconductor to metal-like). The effect of different sp2 endgroups of increasing size in driving this transition is investigated, highlighting how a wide range tunability can be obtained by controlling charge transfer effects or by proper chemical design [3]. In addition, we show how the molecular design of the wire can tune the charge distribution and the charge transfer direction from a donor to an acceptor behaviour [4].

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# Non-magnetic UHV chambers for optical applications: A challenge for vacuum, optics and mechanics.

Klaus Bergner<sup>1</sup>, Maximilian Biethahn<sup>1</sup>, Andreas Trützschler<sup>1</sup>, Michael Flämmich<sup>1</sup>, Ute Bergner<sup>1</sup>

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Vacuum-optical experiments in basic science as well as in the industrial environment are becoming more and more demanding. In particular, the interplay between vacuum technology, mechanical and optical requirements must be taken into account. Vacua in the UHV/XHV range have to be achieved, several optical access ports for different optical tools have to be positioned in the range of a few µm to each other and the optical glasses used, have to be matched with regard to their material, quality, and coating.

In order to fulfill all this demands efficiently, aluminum CF components offer the possibility of providing customized solutions with high geometrical accuracy, reduced weight, outgassing rates of 1E-14 mbar\*l/s/cm<sup>2</sup> as well as non-magnetic properties.

The talk covers the design of non-monolithic and monolithic CF vacuum chambers made from aluminum by using AluVaC®technology. By discussing customized chamber designs, the talk shows that a monolithic design leads to a paradigm shift, since a monolithic chamber can be designed much more compactly, manufactured faster and without welding seams.

In combination with the rapidly developing technology of adhesive bonding, the talk addresses the UHV compatibility of AluVaC®viewports. This technology enables a cost-efficient non-magnetic viewport solution, independent of the glass material. Thorough tests prove the UHV suitability with low outgassing rates. Impact investigations like mechanical or thermal stress test shine light on product-relevant changes under extreme conditions.

### Metallic biomaterials, surface microstructure of retrieved hip endoprostheses components

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The endoprosthetics of hip joint replacements is currently the most common and successful method in advanced surgery to treat degenerative joint disease, for relieving pain and for correcting deformities.

The surface chemistry and microstructure of Ti and CoCr Mo alloys of (retrieved and new) hip endoprostheses components were studied in details using advanced electron spectroscopy techniques FE-SEM, FIB, EDS, EBSD, AES and XPS. We will present the findings from clinical point and from materials science point of view. All X-ray images of implants in the patients are stored in the data base of the UMC.

The surface chemistry results showed that thin oxide films on (a) Ti6Al4V are primarily a mixture of TiO2 with a small amount of Al2O3, while the V is depleted, (b) Ti6Al7Nb is primarily a mixture of TiO2 with a small amount of Al2O3 and Nb2O5, and (c) the CoCrMo alloy is primarily a mixture of Cr2O3 with small amounts of Co and Mo oxides. The thin oxide film on the CoCrMo alloy should prevent intergranular corrosion and improve the biocompatibility. The thin oxide films on the Ti alloys prevent further corrosion, improve the biocompatibility, and affect the osseointegration.

# Visualizing On-surface Intramolecular and Intermolecular Chemistry of Porphyrins: Planarization, Gold Self-metalation and Coupling

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The development of synthetic protocols on surfaces and hereby the control of intramolecular versus intermolecular chemical reactions is crucial for the development of surface-confined novel compounds and nanostructures with tunable properties.

Here we report an experimental and computational study on the self-assembly, conformational changes, electronic structure, and thermally-induced chemical transformations of a fluorinated free-base porphyrin, 2H-4FTPP, on an Au(111) surface. An initial annealing step at 500 K produces planarization of the adsorbed free base via dehydrogenation and ring-closing reactions that preserve the integrity of the C-F bonds. The planarized species (2H-4FPP) establish C-F···H-C interactions that drive their self-assembly into supramolecular linear polymers. A second annealing step at 575 K induces metalation, producing unprecedented surface-supported gold-coordinated planarized porphyrins (Au-4FPP). One last annealing step at 625 K induces C-F and C-H activation, leading to intermolecular C-C coupling between phenyl termini to form planarized porphyrin oligomers in which the constituent porphyrin units keep their monomeric precursors' planar conformation.

These results show that the chemical reactions of surface-confined porphyrins can be controlled by using porphyrin precursors with appropriate molecular designs, and that it is possible to selectively trigger stepwise intra- or inter-molecular reactions by manipulating the annealing temperature. Such on-surface syntheses can enable the creation of unprecedented structures and oligomers, as demonstrated here for gold porphyrin nanoarchitectures. We anticipate that these findings will further the development of the emerging field of on-surface synthesis.

# Defects in Monolayer Films with the Honeycomb Structure: Ti2O3 and Nb2O3 on Au (111)

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Defects in monolayer oxide films can lead to novel properties such as enhanced chemical reactivity. By a combination of scanning tunneling microscopy (STM) and density functional theory (DFT), we compare the structures and properties of defects in monolayer films of Ti2O3 and Nb2O3 supported on Au(111). The Ti2O3 and Nb2O3 films have an epitaxial (2 × 2) honeycomb structure that can act as a suitable template for metal atom adsorption.1 For both systems, a rich variety of defects including atomic vacancies, local structural defects,2 island edges and domain boundaries are observed. Characteristic domain boundaries consist of 4, 5, 7 and 8-membered rings. Interestingly, the same domain boundary structures have different stabilities in Ti2O3 and Nb2O3. For the Nb2O3 monolayer films, a larger variety of structures within domain boundaries have been observed. Furthermore, the edge structures for both systems have been studied. While the Ti2O3 forms disordered edges containing nonhexagonal rings, the Nb2O3 forms armchair and zigzag edges containing only hexagonal rings. It is surprising that although both Ti2O3 and Nb2O3 form the same structure, the defects in these systems are distinctly different.

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# One-dimensional sp1-sp2 hybrid carbon systems on Au(111): atomic-scale structure, electronic and vibrational properties.

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Low-dimensional materials based on linear sp1-hybrid carbon, e.g. carbon atom wires (CAWs) and two-dimensional (2D) crystals graphyne and graphdiyne, have attracted huge interest in the last ten years owing to their outstanding predicted properties [1]. Recently, one-dimensional (1D) sp1-sp2 carbon structures have been synthesized on metallic surfaces, under ultra-high vacuum (UHV) conditions, and investigated by means of Scanning Tunneling Microscopy (STM).

Focus of our work is the synthesis of 1D carbon structures, investigation of their structural and electronic properties and characterization of their vibrational properties by means of Raman spectroscopy.

1D sp1-sp2 carbon nanostructures have been synthesized on Au(111), under UHV conditions, as the result of dehalogenative homocoupling reaction [2] of molecular precursors supported by the surface. The structural and electronic properties have been investigated at the nanoscale level by means of in-situ STM/STS measurements, whose interpretation has been supported by theoretical calculations based on density functional theory. In addition, ex-situ Raman spectroscopy revealed the sp1-carbon fingerprint and elucidated the vibrational properties of linear carbon structures with the help of numerical simulations.

Within the context of low-dimensional materials with tunable functional properties, current efforts are dedicated to the synthesis and investigation of heterostructures of sp1-carbon systems and 2D materials, e.g. graphene and MoS2.

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# Vacuum system design and modeling for the Jefferson Lab Electron Ion Collider Interaction Region

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Jefferson Lab and Brookhaven National Lab are both pursuing designs to build an electron ion collider in the United States following the 2015 US Nuclear Science Advisory Committee recommendations for such a facility. The design of the Jefferson Lab Electron Ion Collider (JLEIC) interaction region (IR) requires vacuum in the UHV regime to reduce background rates sufficiently in the detectors. Additionally, though the final bending magnets are far upstream from the IR in the electron line, the interaction between residual gas and the electron beam will produce synchrotron radiation and subsequent elevated gas load in the interaction region. Preliminary designs of the vacuum system for the JLEIC interaction region and the cryogenic final focusing quadrupoles will be presented using the Molflow+ software. Synchrotron radiation due to the finite beam envelope traveling through the quadrupoles will be also modelled using Molflow's complementary program SynRad. However, since the primary synchrotron radiation in this system may be from the beam-gas interactions in the long straight section upstream of the IR, synchrotron radiation distributions and their effect on the gas load will also be studied using an existing 2D radiation prediction code and GEANT4 beam-gas interaction cross section calculations.

# TiO2-Fe2O3 binary thin films prepared by magnetron sputtering for photocatalytic applications

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The preparation and characterization of TiO2-Fe2O3 binary thin films is reported. Films were deposited by magnetron sputtering using a configuration of multiple targets. It was investigated the effect of the iron content in the films on the composition, structure, optical properties and morphology. The composition was determined by Energy Dispersive Spectrometry, X-ray Photoelectron Spectroscopy and Elastic Forward Analysis; the crystalline phases formed were identified by X-ray diffraction and micro-Raman spectroscopy; surface morphology was observed by atomic force microscopy whereas optical properties were determined from UV-Vis and Photoluminescence measurements. To test their photocatalytic response, the deposited films were evaluated in the degradation of the malachite green dye. It was found that by using this experimental configuration the iron content was incorporated in a controlled way, from 0 up to 23.5 at. %, by varying the ratio of sputtered areas of Fe to Ti. X-ray diffraction and Raman results suggest that at low iron contents the obtained material consists of a mixture of the anatase and rutile phases of TiO2, whereas at higher iron concentrations nanocomposites formed by the rutile and hematite phases are obtained. The prepared films showed enhanced photocatalytic response for the dye degradation under irradiation with visible light compared with TiO2 films being in some cases even better than Degussa P-25 powders.

## Antimonene and Bismuthene: growth and electronic properties

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Recently a new group of elemental 2D materials has been discovered in 15th group of periodic table and include bismuthene and antimonene in alpha and beta crystallographic forms. Interestingly bismuthene supports topologically protected surface states.

Our recent LEEM/PEEM experiments allowed us for the first time to observe growth of bismuthene. Surprisingly, we discovered that growth of Bi islands is characterized by their anomalous diffusion with islands jump length distribution described by truncated Levy statistics. Moreover, for the first time we were able to investigate electronic structure of single 2  $\mu$ m wide bismuthene island using  $\mu$ ARPES. These experiments allowed us to understand both crystallographic and electronic structure of bismuthene.

We decided to use bismuthene islands as a support for antimony films in order to engineer antimonene on bismuthene heterostructure. Surprisingly we fabricated two Van der Waals heterostructure systems: alpha- and beta-antimonene grown on top of bismuthene. It is worth pointing out here that alpha-antimonene was never synthetized before. Crystallographic structure of both Van der Waals heterostructres is investigated using STM and is further confirmed by moiré pattern simulations. Their electronic structure is probed experimentally using STS and theoretically using DFT. In particular DFT results suggest that alpha-Sb is 2D topological insulator while beta-Sb is topologically trivial semiconductor. We note that the α-phases of Bi and Sb have a black phosphorus-like structure which has not previously been employed in van der Waals heterostructures.

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# Nanostructural tailoring in thermoelectric Ca3Co4O9 thin films by employing different sputtering deposition scheme

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The development of high performance thin film thermoelectric materials is crucial for emerging miniaturized thermoelectric applications, e.g., on-chip Peltier cooling and wearable thermoelectric applications. The misfit layered Ca3Co4O9, because of its high Seebeck coefficient and good electrical conductivity, can be a good alternative to the conventional BiTe-based materials, containing toxic and scarce element tellurium. Due to the inherent layered structure, the growth of good-quality Ca3Co4O9 thin films and achieving control over its microstructure is quite challenging. Here, we report an interesting sputtering/annealing method to grow preferentially nanostructured Ca3Co4O9 thin films. In this method, first CaO-CoO films are deposited by rf-magnetron reactive cosputtering from elemental targets of Ca and Co. The final phase of Ca3Co4O9 is obtained by thermally induced phase transformation from CaO-CoO films. The nanostructure of the films is tuneable by tuning relative arrangements of CaO and CoO phases in as-deposited films by employing different sputtering deposition scheme. For example, the flexible Ca3Co4O9 film on mica substrate is obtained from cosputtered CaO-CoO film, whereas the nanoporous transferable film is obtained from sequentially sputtered CaO/CoO films. The flexible film can sustain bending stress until the bending radius of 14 mm, while providing power factor of 0.1 mWm-1K-2 near room temperature, which is comparable to the values reported for bulk polycrystalline Ca3Co4O9. On the other hand, transferable nanoporous film provides power factor above 0.2 mWm-1K-2 in a wide temperature range. With such high power factors and tuneable properties nanostructured Ca3Co4O9 thin films open a new area of flexible thermoelectrics.

# Metal-support interaction in the 2D Fischer-Tropsch catalysts

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Fischer-Tropsch synthesis (FTS), which produces long chain hydrocarbons via the use of biomass or coal derived synthetic gas, is currently of great interest due to unpredictable crude oil prices and global energy challenges.[1,2] FTS proceeds via a hydrogenation reaction:  $nCO + (2n+1)H2 \rightarrow CnH2n+2 + nH2O$ , where water is a by-product. Catalysts consisting of metallic Co nanoparticles (NPs) supported on high–surface area refractory oxides, such as SiO2, Al2O3, or TiO2 are currently used in the commercial plants worldwide. The metal-support interface (MSI) plays an important role in the FTS catalysts reactivity and stability since it defines the Co NPs' structure (crystallinity/polymorphism) and morphology (size/shape). Previous efforts to understand interaction of the Co NPs with the support were performed using the bulk samples (powders and pellets) where the signal was averaged over a large number of NPs of different size.[1,2] Also taking into account that the metal active site loading in the catalyst is often only a few percent, the measured signal mainly originates from the bulk volume and not from the surface where the reaction takes place. Considering that the Co NPs undergo structural transformation during reduction and in the early stages of catalytic activity, it is of particular interest to perform in operando surface characterisation on the planar two-dimensional (2D) FTS catalysts.

# real-space evidence of base-pairing on Au(111)

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DNA and RNA are both essential building blocks for life, which play pivotal roles in biological processes with their abilities to store and reproduce genetic information. DNA-quadruplexes, as a kind of non-canonical DNA structure, normally formed by stacked guanine(G)-quartets with unusual tetrads like GCGC (guanine and cytosine tetrad) located at the end. RNA duplexes are built up on the principle of complementary base-pairing sets of guanine(G)/cytosine(C) and adenine(A)/uracil(U). These specific bindings are responsible for the stabilization of DNA and RNA. Thus, the principle of complementary base-pairing is fundamentally important in vivo. From the interplay of high-resolution scanning tunneling microscopy (STM) imaging and density functional theory (DFT) calculations, we show the real-space evidence of the formation of GCGC tetrad on the Au(111) surface, and further investigate its competition with the well-known G-quartet under ultrahigh vacuum (UHV) conditions. Besides, Watson-crick and Hoogsteen AU base pairs are also achieved on the Au(111) surface with the employment of base derivatives, while the relative stability of the two types of AU base pairs are further explored. Such studies may provide the model system to unravel some biologically relevant issues in DNA quadruplexes and RNA duplexes. Furthermore, bulk water can be introduced into the model system, which may allow us to gain fundamental insight into the hydration process in the base pair stacking systems.

# Graphene-mediated tailoring of oxide-metal interfaces

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Subnanometric oxide films stabilized on metallic substrates are intensively investigated in modern surface science [1,2]. The atomic scale control of the oxide/metal interfaces is a crucial step for tuning the physical and chemical properties of the oxide layers [3]. Here we show that graphene can be used as buffer layer for the epitaxial growth of Cr oxide (CrxOy) and Fe oxide (FexOy) on the Ni(111) surface. The structural, chemical and electronic properties of oxide films deposited on the native and on the graphene-covered Ni(111) surface are compared. X-ray photoemission spectroscopy reveals that graphene promotes the development of a chemically sharp interface by hindering the redox reactions occurring when the films are deposited on the clean substrate. Scanning tunneling microscopy (STM) shows that CrxOy grows layer-by-layer on the graphene/Ni(111) surface, while FexOy forms three dimensional islands. Atomically-resolved STM images indicate that the Cr oxide surface is characterized by an h-BN like structure in which Cr and O atoms are threefold coordinated, forming a honeycomb lattice with the same lattice parameter of graphene. On the other hand, the images acquired on the FexOy surface display a hexagonal lattice with a larger lattice constant, suggesting a weak interaction between the islands and the substrate.

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[3] Picone, A.; Riva, M.; Brambilla, A.; Calloni, A.; Bussetti, G.; Finazzi, M.; Ciccacci, F.;Duò, L. Reactive metal–oxide interfaces: A microscopic view. Surf. Sci. Rep. 2016, 71, 32–76.

# A Quantum-Based Pressure Standard for a New SI Realization of the Pascal

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Moving forward, the next generation of pressure standards will provide a new route of SI traceability for the pascal. By taking advantage of both the properties of light interacting with a gas and that the pressure dependent refractive index of helium can be precisely predicted from fundamental, first-principles quantum-chemistry calculations, a new route of realizing the pascal has been demonstrated. This talk will briefly cover the classical methods of realizing pressure that have served the metrology community well for the past 375 years. And then will take a deeper dive into the next generation of light-based pressure standards that will enable the elimination of mercury manometers. The new standard is a fixed length optical cavity (FLOC) and is smaller, lighter, faster, and higher precision than the classical mercury manometer. From a metrology stand point, the new quantum-based SI pascal will move us from the classical force/area definition, to an energy density (joules per unit volume) definition. Should the technique be further miniaturized, it will lead to a revolution in pressure metrology, enabling a photonics-based device that serves both a gas pressure sensor and a portable gas pressure standard all in one. That talk will also briefly highlight recent advances of photonics-based techniques for measuring temperature, and XHV using cold atoms traps.

# Neutron Scattering Investigations of Molecular Interactions with Surfaces of Nanomaterials

Many of the technological challenges currently faced by society involve understanding and modifying the interaction of molecules with the surfaces of nanomaterials. Often times these issues involve familiar topics such as gas separation, lubrication and energy conversion, storage or generation. Although neutron scattering is widely viewed as a highly penetrative probe of bulk materials, both elastic and inelastic scattering methods can be effectively employed to examine the structure and dynamics of molecular interactions with nanometer scale materials. In this presentation we will demonstrate that by employing a research regime that includes novel material synthesis, adsorption thermodynamics, and computational modeling an attractive opportunity exists for observing and understanding the behavior of single and multilayer molecular adsorption on pure and metal decorated surfaces. Selected examples of investigations that encompass topics of both fundamental and commercial relevance will be discussed. These include: [1] the structure and wetting properties of normal alkanes films on MgO, graphite and h-BN, [2] the structure and dynamics of methane and hydrogen adsorbed on MgO [3] hydrogen interaction with Pd decorated ZnO to illustrate the "hydrogen spillover" process and [4] the interaction of ethanol with alumina (time permitting). The advent of new, high-intensity, pulsed sources such as SNS in the US and ESS in Lund presents exciting possibilities for new discoveries in molecule-surface interactions and advanced energy materials.

# Visualizing geometric structures of small molecules coordinated to metallo-porphyrin on Au(111) using scanning tunneling microscopy

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The coordination reaction between small molecules and metallo-porphyrins play crucial roles in functional processes such as biooxidation and catalytic activation. Their geometrical structures such as tilted binding of NO to metallo-porphyrin have been recently studied by high-resolution scanning tunneling microscopy (STM) images at the single molecule level. Here, we present STM images of further systems, di, tri, and quadra-atomic small molecules, coordinated to metallo-porphyrin on Au(111). We observed square ring, rectangular ring, and center-bright structures for three different small molecules. With the help of density functional theory (DFT) calculations, we reproduce the experimental STM images in the simulated images. Thus, our study shows that geometric structures of small molecules coordinated to metallo-porphyrins can be probed with STM combined with DFT methods.

# Oxygen-Free Palladium/Titanium Coating, a New Long-Life Non-Evaporable Getter Coating with an Activation Temperature of 133 °C

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We developed a new non-evaporable getter (NEG) coating with an activation temperature as low as 133 °C, that is, a palladium/titanium coating with extremely low oxygen concentration (oxygen-free Pd/Ti coating). The substrate was coated with Ti, and then overcoated with Pd using sublimation under the pressure range of 10-7-10-8 Pa. The morphology and surface elemental composition of the Pd/Ti thin film were investigated with electron microscopes and X-ray photoelectron spectroscopy, respectively. The thicknesses of Ti and Pd films were approximately 1.3 µm and 50 nm, and the Ti film was completely overcoated by the Pd film. Ti and oxygen were found to be negligible on the oxygen-free Pd/Ti surface. The oxygen-free Pd/Ti coating was applied to formed bellows. The bellows was successively baked at 133 °C for 12 h, 176 °C for 3.5 h, and 200 °C for 3.5 h. After sealing off a turbomolecular pump from the vacuum system containing the bellows, the pressure reached values of  $4.6 \times 10-6$  Pa,  $1.7 \times 10-7$  Pa, and  $6.1 \times 10-8$  Pa, respectively. The pumping speeds of the bellows were estimated to be 0.028, 0.23, and 0.23 L s-1, respectively. Oxygen-free-Pd/Ti deposition can be used as a new NEG coating for vacuum systems with a baking temperature of 133 °C or higher. Oxygen-free Pd/Ti coating was applied for a NEG pump that can be activated by baking at 150 °C for 12 h. The pumping speeds for H2 and CO do not be degraded even after repeated venting–activating cycles.

# Tunneling-induced luminescence on organic photovoltaic molecular heterodimers

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Organic photovoltaic devices rely on acceptor-donor interfaces to efficiently separate the optically excited excitons—bound electron-hole pairs. These heterojunctions provide the energetic driving force for separation and movement of charge away from the interface, thus holding the key to increasing power conversion efficiency and reducing recombination losses. To study the optical and electronic properties of acceptor-donor interfaces, heterodimers of organic semiconductors on insulating NaCl layers on a metallic substrate were examined using scanning tunneling spectroscopy and tunnelling induced luminescence. In tunnelling induced luminescence, tunnelling electrons decay inelastically emitting photons that can be spectrally resolved. Concurrent pixel-by-pixel scanning tunneling spectroscopy energetically resolves molecular orbitals, giving energy level alignments between the dimerized acceptor and donor molecules vital to charge separation. Together these give a unique sub-nm view of the excited states involved in photogeneration of charge. Understanding the factors that drive charge transfer between acceptor and donor materials will illuminate pathways for organic semiconductor device development.

# Development of operando PTRF-XAFS technique for elucidating 3D structure-activity relationship in heterogeneous catalysis

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Polarization-dependent total reflection fluorescence (PTRF)-XAFS is a powerful technique which can determine 3D structure of highly dispersed metal species on a single-crystal surface by measuring polarization-dependence of XAFS of the metal species. To obtain atomic-level understanding of metal/oxide-support interaction in heterogeneous catalysis, we have determined the precise 3D structures of single metal atoms and metal clusters deposited on single-crystal oxide surfaces such as TiO2(110) and Al2O3(0001) by UHV PTRF-XAFS apparatus.[1]

Recently we have constructed a new apparatus which enables us to measure PTRF-XAFS of active metal species dispersed on a single-crystal oxide surface under working condition. We call this method "operando PTRF-XAFS" technique. The apparatus consists of a compact vacuum chamber connected to a gas inlet line for reactant gases and an outlet line for products analysis by a quadrupole mass spectrometer (QMS), and this chamber works both as PTRF-XAFS cell and batch-type reactor. The sample can be transferred from another UHV chamber where the sample preparation (ion sputtering, annealing and metal deposition) and its surface characterization (LEED, XPS) are carried out. The sample in the PTRF-XAFS cell can be heated at high temperatures (< 700 degC) in the presence of reactant gases (typically 1~100 Pa), which makes the operando PTRF-XAFS measurements possible. Thus 3D structure-activity relationship of the active metal species on a single-crystal oxide surface can be obtained. We will show the details of the operando PTRF-XAFS technique and its application to CO oxidation on a Pt/Al2O3(0001) surface.

[1] S. Takakusagi et al., Chem. Rec. 18 (2018) 1, J. Phys. Chem. C 120 (2016) 15785, Top. Catal. 56 (2013) 1477, Phys. Chem. Chem. Phys. 15 (2013) 14080.
# Interplay between charge balance and surface structure on superconducting properties of Ca10(Pt4As8)(Fe2As2)5

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Ca10(Pt4As8)(Fe2As2)5 contains both superconducting building blocks (Fe2As2 layers) and conducting spacers (Pt4As8 layers), unlike the insulating spacers in other Fe-based superconductors. Prior work using scanning tunneling microscopy and spectroscopy (STM/STS) showed the important role played by the charge environment and surface structures in this material's superconducting properties: evidence for superconductivity is absent in the bare Pt4As8 surface but recovers when Ca atoms are atop, while different surface reconstructions also lead different superconducting features [1]. I will describe our recent scanning tunneling microscopy and spectroscopy (STM/S) results confirming the role of charge balance and surface structures on superconductivity in this compound. Cleaving provides large areas of bare Pt4As8 layer, which originally does not show superconducting features. Deposition of additional Ca atoms on the bare Pt4As8 surface, while the sample is on the STM scanning stage, results in changes in spectral features allowing us to probe the role of charge balance and structure. I will discuss the relationship between surface structures and superconducting features based on the Ca structures formed by controlling the deposition temperature.

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## The Scanning Laue Diffraction Microscopy at Taiwan Photon Source

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The X-ray Nanodiffraction Beamline (XND) is one of the phase-I projects for Taiwan Photon Source (TPS) in NSRRC. The endstation called "FORMOSA" (FOcusing x-Ray for MicrO-Structural Analysis) is dedicated to the use of white/mono-beam Laue diffraction for structural analysis. For instance, users could obtain the 2D and 3D distribution of crystal phases, orientations, residual stain/stress, and dislocations for materials in a complex form without annoying specimen preparation and distorting the sample during measurement. The current spatial resolution is better than 80 x 80 nm at lateral plane. Furthermore, FORMOSA also provides many complementary tools other than x-ray. The Tetra-probes could deploy several scanning probe methods such as atomic force microscopy, scanning tunneling microscopy and scanning near-field optical microscopy to collect surface, electrical, and optical properties of specimen together with structural information from Laue simultaneously; the projection x-ray detector for absorption contrast imaging; the x-ray fluorescence detector providing elemental information; the integrated hexapod scanner providing nanometer resolution in 6-degree of freedom to carry on user's own sample holder for precision measurement, and the cryogenic stage integrated with heater for temperature dependence experiments. Particularly, FORMOSA is equipped with high-resolution field emission scanning electron microscopy (FESEM) inside the end-station to obtain real-time imaging of specimen. This SEM sophisticated aligned with focusing x-ray beam at the same position on the sample surface, enables users to find out the regions of interest on the screen and obtain the corresponding diffraction pattern instantly. All these equipment were meticulous arranged in a tiny space inside the analysis chamber of FORMOSA as shown in figure 1. In summary, XND beamline and FORMOSA end-station provide not only 2D/3D-Laue Microscopy but also nano-XRF, nano-XAS, nano-XEOL/CL, SPM and SEM information for diverse research programs.

In this presentation, we will briefly introduce to you the design and commissioning results for XND and FORMOSA. In addition, the presenter also will cover some very preliminary and exciting results from users research projects in the areas of ultra-thin films, emergent materials and nanostructures to demonstrate the capabilities of FORMOSA.

# Reliability Tests for Water Vapor Transmission Measurements by Using Standard Gas Barrier Films with Clay-Polyimide Nanocomposite Material

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Gas barrier films to prevent water vapor permeation are widely used to elongate the shelf and/or life time of products such as foods, medicines, solar cells, and electronic devices. About ten types of methods/devices are used to measure the water vapor transmission rate (WVTR) to accommodate the wide measurement range from over 10 to 10-6 g m-2 day-1. Standard gas barrier films to characterize the methods/devices are, however, only available in the limited range. We have developed standard gas barrier films (SGB films) by directly adhering a clay polyimide nanocomposite (CPI) film on a stainless-steel sheet with an aperture. SGB films having WVTR from 10-2 to 5×10-6 g m-2 day-1 were fabricated by changing the inner diameter of the aperture from 20 to 0.6 mm. The reproducibility of the WVTR of SGB films was examined by differential-pressure throughput method with a quadrupole mass spectrometer as a detector (QMS method)[1]. The comparison among MOCOM method, a differential-pressure accumulation method, an atmospheric pressure ionization mass spectrometer (API-MS) method, and QMS method is reported.

[1] H. Yoshida, et al., Review of Scientific Instruments 88, 043301 (2017).

#### Atmospheric pressure plasma for surface modifications and coatings

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A microwave-powered atmospheric-pressure plasma torch has been developed which has the capability to inject material directly through the antenna at the center of the torch, or into the surrounding area. This material can be gaseous, such as a volatile chemical precursor; liquid, such as an organic precursor; or even solid, such as a wire or a powder. There is also a gas curtain surrounding the torch so air/oxygen can be kept from interacting with the material process. These capabilities give the torch a wide range of operating conditions and uses. The torch can operate without the use of helium or other noble gasses. Stable operation is possible in compressed room air. In addition the shape of the output of the torch can be cylindrical, made into a line, or miniaturized. This makes operation economical and suitable for a wide array of commercial applications.

This presentation will cover the most recent results for three industrial applications. First, is the use of the torch to replace chemical-based surface preparations in advance of priming and painting aluminum and steel. In particular, the conversion coating of hexavalent chrome can be replaced by depositing ZrO2 from a gas phase precursor. The second application is to prepare surfaces for bonding. In this use dissimilar materials can be fastened together with a bond strength that even exceeds the strength of the aluminum. The third is the application of nanoparticle coatings where the nanoparticles can be decorated with activated species in the application process.

# On-surface synthesis of single molecular magnets by contacting magnetic atoms to $\pi$ -conjugated molecules using STM manipulation

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Single organic molecular magnets are one of promising building blocks for architecting 1-nm-size high functional spintronics device. Tuning of quantum spin states in the single molecules are important key issue. Although chemical syntheses in liquid solutions have produced several molecular magnets, here we demonstrated on-surface synthesis of single organic molecular magnets. On atomically-flat noble metal surfaces, Fe and Co single atoms were gently adsorbed and manipulated by using a scanning tunneling microscopy (STM) tip to make contact with phthalocyanine and porphyrin single molecules [1-3] simultaneously adsorbed on the same surface. All experiments were performed in ultra-high vacuum (UHV) at 4.6 and 78 K using home-built UHV-STM setups [1-3]. Scanning tunneling spectroscopy dl/dV measurements directly showed how the contacting magnetic atoms affected the local density of states (LDOS) inside the molecule. For example, single Fe atoms have two preferable adsorption sites in one phthalocyanine molecule. Owing to different local ligand fields, the adsorbed Fe atoms at different sites form independent spin configurations. These experimentally obtained LDOS peaks were deeply investigated by theoretical DFT calculations. We also demonstrated a deposition of magnetic atoms on porphyrin monolayer array. Surprisingly, depending on atom species, generated molecule-atom complexes formed different structures. Details will be shown.

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# Chemistry atom-by-atom: Probing reactivity of a surface-bound molecular catalyst by STM and AFM

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Heterogeneous catalysts play a vital role in numerous industrial chemical processes, yet their complexity – involving interfaces and a distribution of reactive sites – can hamper understanding and efforts towards rational design. Surface-bound molecular catalysts offer the potential to create identical reactive sites – especially by exploiting high fidelity self-assembly methods – bringing molecular design to heterogeneous catalysis. Scanning tunneling microscopy (STM), spectroscopy (STS) and non-contact atomic force microscopy (ncAFM) provide unique atomistic views of surface structures and the frontier molecular orbitals that give rise to reactivity. I will describe our recent work investigating the reactivity of self-assembled surface-bound Fe-terpyridine (tpy) species with small-molecule gaseous reagents using STM, STS, and ncAFM at low temperatures (4-40K) in ultrahigh vacuum. STM and ncAFM images indicate that both CO and ethylene react with the undercoordinated Fe-tpy sites via a surface-bound intermediate step prior to forming a chemical bond with the Fe site. STS of the nascent and bonded species shows a distinctive signature for each reactant, indicative of changes in the frontier orbitals responsible for further reactivity. Statistical analyses show that subsequent annealing steps up to 40K lead to ensemble progression through these reaction stages and towards higher-order structures, indicating that reactivity can be induced at low-temperature through minimal heating, and revealing the reaction pathway. The ability to probe individual components of the distribution while also building ensemble data allows us to identify and characterize intermediate reaction steps, providing detailed reaction pathway information about this novel well-defined surface-bound reactive site.

# Electronic structure of Bi(110) ultra-thin films grown on a Si(111) $\sqrt{3}\times\sqrt{3}$ -B substrate

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Recently, Bi(110) ultra-thin films with black-phosphorus-like (BP-like) structure have attracted much interest as a candidate of twodimensional topological insulator depending on the buckling angle of Bi atoms and the charge doping[1]. From our scanning tunneling microscopy (STM) study of Bi(110) ultra-thin films on a Si(111) $\sqrt{3} \times \sqrt{3}$ -B surface, the growth of Bi was revealed to follow the SK mode and the areal ratio of even-layer height islands to odd-layer ones is 3:1 below 10 mono-layer (ML) of Bi on average [2]. In the present study, the electronic structures of these ultra-thin films were investigated by angle-resolved photoelectron spectroscopy (ARPES).

Previous theoretical calculation for free-standing Bi(110) films predicted that the band structure of odd-layer height film with bulklike structure has a metallic band with Dirac-cone-like dispersion around the M point[3]. However, all the examined ultra-thin films in the present ARPES study showed no indication of such a band and the dispersion relations are rather similar to those of BP-like structure calculated for even-layer height films. This suggests that the even-layer height islands in our previous STM study has BPlike structure. The present results also imply that the structure of odd-layer height islands is different from the bulk-like structure.

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- [2] K. Nagase et al., Phys. Rev. B 97, 195418 (2018).
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## Metallic Glass Coating: A Superb and Promising Material for Metallic Nanotube Arrays and Beyond

Jinn P. Chu

Metallic-glass coating have received increasing attention in recent years because these coatings with the amorphous structure could be obtained readily using PVD techniques such as magnetron sputter deposition. Metallic-glass coatings are thus now available not only in monolayer and multilayer forms but also in nanotube arrays with sizes up to tens of mm. With the advent of these materials exhibiting unique physical and mechanical properties, the metallic-glass coating materials are also of great importance for scientific research and engineering application. In this presentation, we will present the first-ever metallic glass nanotube (MGNT) arrays on Si which are successfully fabricated by a simple process of lithography and sputter deposition of metallic glass coating for very large-scale integration. Some important properties of MGNT arrays are reviewed, with focuses on the high strength, excellent ductility and controllable surface properties such as hydrophobicity. Then, the MGNT array-based applications in the field of biosensors are introduced.

# The Electronic and Vibrational Structure of Lanthanide Zirconates

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The lanthanide zirconates are of interest for their use in inert matrix fuels and as nuclear wasteform containment material. For use in these applications, the material's structure must be as resistant as possible to radiation damage, and, therefore, at a basic level, present an electronic and vibrational structure with thermodynamic and mechanical properties that are favourable to long term structural stability under harsh radiation environments. The rare earth zirconates are interesting model systems to explore such problems. This study finds that in these materials the f-electrons play a localized-valence decisive role in determining their thermomechanical properties making them an intriguing model for the interplay between the localised and delocalised valence nature of such oxide materials, the full understanding of which may also lead to novel material development. The f-electronic structure has historically proved rather difficult to model, however.

The full series of lanthanide zirconates was synthesised using solid state techniques and a variety of neutron and synchrotron experiments performed to study the electronic and vibrational structure of this series In conjunction with a density functional theory (DFT) model, the electronic and vibrational structure is determined and the role of the 4f electrons to the stability of these interesting materials studied. Unlike the lanthanide titanate series, the interplay between electronic and vibrational character plays the decisive role in determining the fate of the materials stability.

# Identifying 3D Conformation of Adsorbed Molecules using Atomic Force Microscopy with Simultaneous Tunneling Feedback

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Functionalizing the tip of a low temperature atomic force microscope (AFM) with a single CO molecule facilitates imaging of single adsorbed molecules with submolecular resolution, this is often denoted as bond imaging AFM. Therewith identification of adsorption structures, reaction pathways, etc. becomes feasible. In the standard bond imaging technique, the sensor scans the samples in constant height mode. While this scanning mode is, in particular, suitable for types of molecules that adsorb planar on the substrate, it is incapable of imaging 3D adsorption structures. To solve this problem, we utilize a scanning mode that achieves submolecular resolution while it tracks the topography by applying a constant current. Constant height and constant current scanning modes are systematically compared and advantages and disadvantages are presented.

# ToF-SIMS and XPS analyses of thermal stability of thin films of organic corrosion inhibitors

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Using surface sensitive techniques SIMS, XPS and AFM we studied adsorption of two corrosion inhibitors, propargyl alcohol (PA) and cinnamaldehyde (CIN) on a steel surface. These compounds are known in acidising oilfield applications. In our work we confirmed and explained cinnamaldehyde and to be effective corrosion inhibitors for lower-grade steel materials propargyl alcohol molecules adsorption on steel surface. The direct evidence of the adsorption of CIN and PA molecules was possible due to the low detection limit and selectivity of the ToF SIMS method, even for very thin layers in the nm range. In the SIMS analysis of CIN corrosion inhibitor molecules an (M-H)+ signal was identified at 131.04 Da, corresponding to C9H7O+. The adsorption of PA molecules was also confirmed by a molecular (M-H)+ signal at 55.02 Da (C3H3O+) in the positive SIMS spectrum. The possibility of spatially resolved ToF-SIMS analyses with high mass resolution allowed us to follow the lateral distribution of the adsorbed corrosion inhibitors. In this way we identified the non-homogenous distribution of CIN molecules on the steel surface. In the case of PA a more homogenous distribution of PA molecules on the steel surface with some PA agglomerates was detected. We also showed that using SIMS method it is possible to study the temperature stability of the CIN corrosion inhibitor to be  $(150 \pm 10)$  °C, from which the desorption energy for the CIN layer on the C15 steel was calculated to be  $(122 \pm 5)$  kJ/mol. For the PA corrosion inhibitor, desorption energy for the PA corrosion inhibitor to be in the range of 107–167 kJ/mol. Obtained data will be used during design of corrosion protection of metallic tubes for the oilfield application.

# Production of non-oxidized Ge quantum dot lattices in amorphous Al2O3, Si3N4 and SiC matrices

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Production of non-oxidized Ge quantum dot lattices embedded in Al2O3, Si3N4, SiC matrices by self-assembled growth was studied. The materials are produced by magnetron sputtering deposition, using different substrate temperatures. Deposition regimes leading to self-assembled growth type and formation three-dimensionally ordered Ge quantum dot lattices in different matrices were investigated and determined. Oxidation of Ge quantum dots in different matrices were monitored and the best conditions for production of non-oxidized Ge quantum dot s were found. Optical properties of Ge quantum dot lattices in different matrices show strong dependence on Ge oxidation.

# CO oxidation over ultra-thin FeO(111) films studied by APXPS using transient gas supply

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Ultra-thin FeO(111) grown on Pt(111) is one of the most studied ultra-thin metal oxide films. It is highly active for CO oxidation and this activity has both been explained by a FeO2 trilayer formed at oxygen rich conditions [1] or by coordinatively unsaturated ferrous sites formed at the edge of the FeO islands [2]. The different explanations for the high activity has until now only based on reactivity experiments on FeO films characterized by UHV techniques before and after the reactivity experiments, and very limited in-situ work has so far been performed [3].

In this contribution, we will demonstrate how transient gas supply and ambient pressure x-ray photoelectron spectroscopy (APXPS) can be used to study activity and phase changes simultaneously for Pt(111) with and without an ultra-thin FeO overlayer. By exposing clean and FeO covered Pt(111) to CO pulse trains in the mbar regime we will show that Pt(111) quickly gets poisoned by CO, while the FeO covered Pt(111) maintains its reactivity throughout the entire pulse train. Furthermore, we will characterize the active FeO2 like phase present at reaction condition in detail and show that this phase co-exist with bare Pt(111) patches formed during the reaction.

On a more general level our study also demonstrates how transient gas supply coupled to APXPS can be used to probe the transition region where the catalyst surface change from one phase to another as a response to changes in gas composition with sub-second time resolution – something which until now is essentially unexplored.

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- [3] Johansson et al., Top. Cat. 59, 506 (2016)

# Spin-polarized surface states of a Sn atomic layer at graphene/SiC(0001) interface

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Symmetry at the crystal surface plays a crucial role in determining the nature of the spin splitting of the band. Especially, a K point of the surface with three-fold symmetry is of interest due to the emergence of peculiar spin-polarized bands. For example, Zeeman-type spin splitting was found at the K point of a monolayer TI-adsorbed Si(111) surface that belongs to the plane group of p3m1 and thus the K point has C3 symmetry. In contrast, Rashba-type band crossing for a monolayer Bi-adsorbed Si(111) surface that belongs to the plane group of p31m was revealed at the K point having C3v symmetry. In the present study, we show spin-polarized bands of a Sn triangular lattice atomic layer (Sn-TLAL) formed by intercalation into the interface between graphene and the SiC(0001) substrate. We find both Zeeman-type and Rashba-type spin-polarized bands at the K point by spin- and angle-resolved photoelectron spectroscopy. Here, the K point of Sn-TLAL has C3 symmetry with taking the crystal structure into account. Thus, the Zeeman type is consistent with the lattice symmetry while the Rashba type is inconsistent. Our density functional calculations reveal that the charge density distribution of the Rashba-type (Zeeman-type) band has C3v (C3) symmetry at the K point. Therefore, the symmetry of the charge density distribution clearly explains the nature of the spin-polarized bands. We conclude that the symmetry of the charge density distribution is important to understand the nature of the spin splitting

# Single step process for creating complex nanoparticles, nanowires and nanotrusses: an insight in the diversity in the hollow cathode sputtering technique

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High-power pulsed hollow cathode sputtering is used to grow a variety of different nanoparticles and therefrom assembled nanostructures in a single step process. Large flexibility is obtained using several hollow cathodes which are operated with a variation of smart pulsing sequences and different collection techniques. A wide diversity of particles and structures can be obtained, and the approach on how to utilize this for different applications is discussed. Some of the areas covered are listed here. How to achieve different cathodes. How to use reactive gas to form compound nanoparticles to alloys, through changing the pulsing sequence of the different cathodes. How to use reactive gas to form compound nanoparticles. How to use electric fields to steer nanoparticles to desired areas. How magnetic fields can be used to grow 3D structures of nanowires and nanotrusses with huge surface areas, and why these are interesting for electrocatalytic applications. The hollow cathode source used is an in-house design, and we demonstrate why we think this can be a competitor to established nanoparticle sources based on e.g. magnetron sputtering.

# Gas permeability of thin films for food packaging

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Advances in food processing and food packaging play a primary role in keeping safe food supply. Modified Atmosphere Packaging (MAP) is the most appropriate technology for packaging fresh and fresh-cut produces [1] and consists in controlling or modifying the atmosphere surrounding the product within a package made of various types of films. Usually the thickness of the films is on the order of micrometers.

Packaging materials can be metals or plastics. Plastic materials are composed by different polymers, while the most popular metal is aluminum. However, nowadays technology efforts are focused to find advanced solutions in terms of new materials to guarantee more value to the packaging market [2].

In this work we measure the permeability P of the package to several gases (O2 and CO2, primarily). An accurate measurement of P is not easy [3], above all for ultra-thin films [4]. For this reason, it is important to make a good characterization of packaging with respect to this quantity.

For the scope we employ an experimental set-up for P and diffusivity D measurements. It consists in a High Vacuum Chamber (HVC) equipped with pressure gauges with high accuracy. It can work in two modes: dynamic and static (constant-volume/variable-pressure) allowing measurement of P and D in a range of more of four order of magnitude.

Thanks to this equipment we investigate the gas transport properties of the previous cited materials in commercial form. Results of these test are compared with data supplied by the manufacturers, when are available.

# Attempt to precise leak rate measurement of weld defect by pressure rise method

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A precise measurement of a leak rate through a weld defect will give a useful information. Properties of the defect, e.g. the pressure dependence of the leak rate, will have a different feature from a crimped capillary due to their different structures and origins. A leak rate through the defect, however, is not well studied due to the difficulty to obtain such a defect. Recently, we obtained two samples with a weld defect by chance. In this study, the leak rate through the defect was precisely investigated and compared with others. The samples were a blank-flanged 1/4" pipe welded on a CF34 flange. The weld defect was confirmed by a He leak detector by a spray method. A test sample was covered with an outer chamber to change the applied pressure to the defect. The CF34 flange side was connected to a flow meter by a pressure rise method [1]. The test gas was nitrogen. The applied pressure to the defect was changed from 10 kPa to 100 kPa, while the pressure at the CF34 side was kept at about 100 kPa. The measured leak rate was changed from 1.4x10-4 Pa m3/s to 1.8x10-3 Pa m3/s. At the same time, a hysteresis-like feature in the leak rate between the ascending and the descending pressure was observed. Its maximum was about 10 % at the applied pressure of about 60 kPa, which was much larger than the uncertainty of the leak rate of about 1.7 % (k=2). Although another sample showed similar hysteresis, the crimped capillary did not show such a hysteresis.

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# Understanding the interaction of nanoparticles and cells - what we know and where to go from here

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Engineered nanoparticles (NPs) possess unique properties for numerous applications and heightened research has been performed to determine if the potential benefits of nanotechnology could be utilized without any adverse effects to humans. Thus, a better knowledge of cellular consequences upon the direct exposure of (human) cells to these NPs is prerequisite for their safe-by-design and successful use in any applications including biomedicine where targeting efficacy and low side effect is relevant. In order to understand such interactions the detection, localisation and quantification of NPs within cells is important to understand how physico-chemical parameters might play a significant role [1,2]. Once inside the cells the particles initially are localized in early and late endosomes, which then fuse with lysosomes, complex digestive organelles that have a low pH (~4.5) and a salt rich environment filled with hydrolytic enzymes [3]. Such an environment also might strongly impact the stability and aggregation behavior of NPs and needs to be studied by a combination of different techniques to gain some indications as to their potential biological impact, as well as how to design NPs for a specific cell response to take advantage of nanotechnology applications in biotechnology and in medicine.

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# Cross-sectional stress distributions within scratch track areas of a multi-layered CrN-Cr thin film on steel revealed by 50 nm focusing X-ray diffraction

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In order to assess the microscale response of thin films to scratch tests, it is necessary to elucidate local stress fields and microstructural changes in the scratch track area. In this study, cross-sectional 50 nm focusing X-ray nanodiffraction has been applied to characterize multiaxial residual stress gradients in a multi-layered brittle-ductile thin film consisting of 1.2 and 2 µm thick CrN and Cr sublayers on a high-speed-steel substrate. Two scratch traces were formed at loads of 200 and 400 mN, respectively, and afterwards analysed ex-situ by scanning experiments at the ID13 beamline of the European Synchrotron Radiation Facility in Grenoble, France. Focused-ion-beam milling and scanning electron microscopy were used to characterize crack patterns in the sublayers, which were pronounced especially at higher loads. In the as-deposited multilayer, average stress magnitudes of ~-3 and -1 GPa in the CrN and Cr sublayers, respectively, were found. On the contrary, complex variations of in-plane stress concentrations in the deformed volume were observed in the CrN sublayer reaching magnitudes up to -6 GPa in the near CrN/Cr interface region. The film volume close to the film surface was almost stress free indicating full stress relaxation of the deformed zone. Within the Cr sublayer, tensile in-plane stress near the CrN/Cr interface regions and compressive stress of ~-1.5 GPa near the film-substrate-interface were detected. In summary, the experiments revealed that the ductile Cr sublayers served as a stabilizing component for the CrN-Cr-laminate microstructure upon mechanical loading, effectively suppressing catastrophic failure of the otherwise brittle CrN system.

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# Tuning the ion-energy distribution in HiPIMS and its effect on properties of titanium nitride thin films

Rommel Paulo Viloan, Jiabin Gu

High power impulse magnetron sputtering (HiPIMS) is known to produce energetic ions of the sputtered material illustrated by a broader ion energy distribution function (IEDF). Despite the presence of these energetic ions, the IEDF is still dominated by lowenergy ions. In a typical deposition set-up these low-energy ions are accelerated by introducing a negative substrate bias (Us). Recently, a mode of operation known as bipolar HiPIMS, wherein the conventional negative voltage pulse is followed by a positive/reversed voltage (Urev) pulse, has attracted much attention. [1] In this mode of operation it is possible to tune the IEDF and accelerate the ions, without applying any Us.

In this study, we operate HiPIMS discharge both in conventional and bipolar modes to deposit TiN thin films. The magnitude of Urev was varied from 0 to 150 V and time-averaged ion mass spectroscopy measurements show that a large portion of the ion species are accelerated to an energy corresponding to Urev. The energetic ion bombardment results in densification of the film as observed by transmission electron micrographs and both compressive stress and hardness are increased dramatically.

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# Cross-sectional X-ray Nanodiffraction Reveals Structural Evolution and Mechanical Response of Nanocrystalline NiTi During Micro-Cantilever Bending

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Nanostructured materials and small structures, e.g. in modern microelectronic devices, often display properties that are difficult to infer from the well-known properties of classical bulk materials. Since especially the mechanical characteristics, such as elasticity, strength and toughness, play a crucial role for the lifetime of components on all length scales, it is important to properly characterize and understand them. Cross-sectional X-ray nanodiffraction at a synchrotron light source, with beam diameters down to the sub-30nm range, offers the possibility to assess individual microstructural features and their composition, texture and strains state with very high spatial resolution [1].

This contribution aims to present the current possibilities of the method and features the implementation of an in-situ testing apparatus for micromechanical loading of samples. A piece of nano-crystalline NiTi shape memory alloy wire was chosen as a demonstrator sample, from which a notched micro-cantilever beam was milled using a focused ion beam workstation. A comparison of the states before, during and after bending of the cantilever reveals various highly localized stress concentrations in the region around the notch, as well as partial austenite-martensite transformation and re-transformation. Briefly, also texture and effects observable by peak broadening will be addressed, showing the evolution of a combination of grain size, microstrains and macrostrain gradients. Finally, a short outlook on future developments of the experimental setup and further analyses of the investigated sample will be presented.

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## Improvement of optical pressure measurement system by stabilizing temperature inside chamber at 1 mK level

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National metrology institutes have been developing optical pressure measurement systems as the next generation pressure standard. Those systems are mainly based on refractive index measurements. NMIJ has been also developing an optical pressure measurement system. An aluminum chamber with thick wall was adopted in order to reduce the temperature distribution and the short-term temperature fluctuation inside the chamber. A laser frequency of about 473 THz is locked to the resonant line of a Fabry-Perot resonator in the chamber. The refractive index of nitrogen gas is measured from the ratio of the resonant frequency under a vacuum condition and under an arbitrary gas density condition. The repeatability of the pressure measurement is influenced by the resonator length change. To improve the repeatability of the series of measurements, long-term temperature stability is required.

The vacuum chamber is surrounded by plates with flow paths for constant temperature water. Then they are covered by a heat insulating box. The temperatures at 4 positions inside the chamber were measured using 4 thermistors. In order to reduce the effect of self-heating, the current and the resistance were set to 1  $\mu$ A and 10 k $\Omega$ , respectively. As the result, the temperature fluctuations at each position were kept at 1 mK level for one day. Furthermore, the resonator length change due to 1 mK temperature fluctuation was compensated using the thermal expansion coefficient of its material.

The repeatability of the pressure measurement in the range of 1 Pa to 100 kPa with the improved system is reported.

# Nanocluster-Based Metal Oxide Films for Hydrogen Gas Sensing Prepared by Advanced Magnetron

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Metal oxide semiconductors (MOSs) are well established as active materials in gas sensor assemblies. Especially nanostructured MOSs attract the attention because of the unique electronic properties of nanomaterials and a high reactive area.

Here, we present the study of various architectures based on MOS nanoclusters and thin films. The nanoclusters were prepared by use of a gas aggregation cluster source (GAS). The thin MOS thin films were prepared by a conventional reactive dc magnetron sputtering and/or by reactive High Power Impulse Magnetron Sputtering (HiPIMS) technique.

The optimization of the architecture (combination of materials, thickness of layers, amount of nanoclusters) enhanced the sensorial response and allowed us to form gas sensitive nanostructured materials without the need of use of any wet technique. Sputtering conditions were tuned to vary the chemical composition (stoichiometry) and structure (crystallinity) of the prepared films.

Various combinations of thin films and nanoclusters of tungsten trioxide (WO3) and cupric oxide (CuO) were prepared and tested.

The specimens were tested for the response to a time-varied hydrogen concentration in synthetic air at various temperatures. The sensitivity and the response time were evaluated. The optimum combination is presented.

Both the magnetron sputtering and GAS deposition of clusters are techniques compatible with industrial microelectronic procedures which is of key importance for further expansion of hydrogen-based technologies for mobile technologies.

[1] S. Haviar, J. Čapek, Š. Batková, et al., Int. J. Hydrogen Energy 3 (2018) 2-10.

# Catalytic promotion effects of Fe heteroatoms in CoO nanoislands on Au(111)

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Iron heteroatoms act as a catalytic promoter when mixed cobalt-iron oxides/(oxy)hydroxides are used in the electrochemical oxygen evolution reaction[1,2]. Understanding the nature of the iron as the promoter in the catalytic process is a key finding, but a missing structural model means that the mechanism of such promotion effects, especially the link between the atomic-scale structures and their interesting chemical properties, is poorly understood.

Here, aiming to associate the catalytic promotion effects with the structural properties, we have synthesized a range of catalytically active Fe doped CoO nanoislands on Au(111) substrate. Using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and cyclic voltammetry (CV) on such atomically defined Fe-doped cobalt-iron oxides/Au(111) system, we investigate the link between Fe content in the Co oxide and the resulting atomic structure, the hydroxylation behavior and, ultimately, the electrochemical performance.

Our findings show that the reactivity of the model system on Au(111) correlates well with an optimum reactivity for low concentration of Fe and illustrate that the positioning, as well as the aggregation of the Fe species within the CoO nanoislands may be possible ways to engineer the catalytic promotion effects.

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# Vacuum systems for cold atom sensors on microgravity platforms

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Cooling atoms to Nano-Kelvin requires an ultra-high vacuum system with complex features, such as coated optical accesses, paramagnetic materials, or differential pumping stages. Furthermore, the sensitivity of atom interferometers, one promising application of ultra-cold atoms, scales with the free evolution time (T) of the cold ensembles. In order to increase T, microgravity becomes necessary. Hence, the development of reliable, miniaturized UHV systems with the capability to withstand the rough environment of microgravity platforms is a key task to pave the way for high performance cold atom instruments.

In order to minimize such complex vacuum systems various tests have to be performed. For instance the measurement of outgassing rates for critical components inside the chamber and leakage rates of metal sealed windows allow a more detailed dimensioning of the vacuum pumps.

In addition to the challenge of miniaturization, most of the microgravity platforms are linked to a rough thermal and mechanical environment. Vacuum pumps and seals are supposed to endure vibrations and loads of rocket launches or drop tower impacts. In the case of the sounding rocket mission MAIUS, the motors induced loads to the payload of up to 13 g.

This talk presents the challenges for vacuum systems on microgravity platforms. Test beds for outgassing rate measurement, window sealing technologies and loaded CF flanges are shown and first results for the tests are given.

# A Robust, Lightweight and Transparent Anti-icing Coating Based on Functionalized Graphene

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Ice formation on surfaces has very big societal consequences in the modern world with a major impact on a broad range of applications including airplanes, ships, wind turbines, power transmission lines, solar panels, buildings and roads. The search for an anti-icing strategy preventing ice formation and accumulation on surfaces in harsh environmental conditions without an additional chemical or heat treatments has been intensified over the last one decade. However, most surfaces investigated so far have not been very robust or transparent. Hence, practical anti-icing strategies remain conventional thermal, chemical, and mechanical approaches, which are expensive and inefficient.

Here we present the first experimental study of the anti-icing properties of graphene and functionalized graphene. We demonstrate a completely new approach to anti-icing surfaces, defining a new class of materials, where anti-icing is achieved solely by structuring on the atomic level. The results showed excellent anti-icing performance with freezing delays up to several hours in a high humidity environment [1]. It presents a realistic anti-icing solution that can be implemented in practice. Furthermore this research introduces graphene as a new model-system for understanding ice nucleation mechanism. Finally the results and further work with this new class of material may contribute to the improvement of climate models through the understanding of the role of ice formation in clouds via seeding materials.

[1] Akhtar N. et al. (January 2019) Fluorinated graphene provides long lasting ice inhibition in high humidity. Carbon 141: 451-456.

## Heterogeneous dynamics of perylene epitaxy on Ag(110).

Kirill Bobrov, Laurent Guillemot

We present a room temperature STM study of perylene epitaxy on Ag(110) at monolayer regime under coverage close to saturation. The dominating molecule-substrate interaction laid the molecules and compressed the monolayer beyond the limit implied by the molecule close packing. We observed that lateral displacement of the comprised molecules reduced their interlock, relaxed partially the strain and favored molecule diffusion. We found that the strain precluded the diffusing molecules to precipitate into a periodic 2D network whereas the substrate crystal field excluded eventual molecule frustration. Intrinsic perylene ability to recognize define adsorption sites of Ag(110) was not altered by the strain relaxation. We observed that the diffusing molecules still recognized substrate sites albeit locked into them transiently in a non-equal time manner. The transient locking alternated heterogeneously the molecule dynamics giving rise to "fast" unlocked molecules and "slow" locked molecules which interchange throughout the Ag(110) lattice under the molecule propagation. The dynamically binding molecules revealed a well-defined epitaxial monolayer fully compatible with the crystal field as well as its dynamics. The monolayer conformed its structure, energetics and dynamics to that of the underlying substrate and complied with the particular substrate morphology. The monolayer persisted the permanent substrate restructuring driven by silver adatom diffusion and spread over mono- and bi-atomic surface steps preserving all its qualities and following the (533-3) substrate site arrangement.

# Adhesion and growth of cells of soft and hard tissues on biomaterials with various surface modifications - a review.

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Artificial and nature-derived materials, such as synthetic and natural polymers, metals and their alloys, ceramics and carbon-based materials, are widely used for the construction of replacements of irreversibly damaged tissues, e.g. blood vessels, heart valves, skin, bone, joints, cartilage, etc. Physicochemical properties of the material surface, such as its wettability, electrical charge and conductivity, roughness and topography, and also rigidity or deformability, are decisive for the interaction of the materials with surrounding cells after they have been implanted in vivo or during the creation of tissue-engineered constructs in vitro. The adhesion, growth and differentiation of cells can be modulated by various modifications of the material surface, which can be realized by subtractive technologies, by additive technologies or by a combination of both technologies. Subtractive technologies degrade or reduce the surface layer of the material and include, for example, acid and alkali etching, plasma treatment, UV- and ion irradiation, grinding, polishing, machining, and shot peening. Additive technologies create additional structures on the surface of the material, e.g. carbon-based films (nanocrystalline diamond films, diamond-like carbon), ceramic films (electroactive BaTiO3 coatings, zeolite coatings) and organic films (amine rich coatings, hydrocarbon films functionalized with tropoelastin etc.). Additive and subtractive technologies can be combined, e.g. plasma-activated polymers can be further grafted with various biomolecules and nanoparticles, or nanoscale features can be superimposed on macroscale or microscale irregularities created by subtractive technologies, in order to mimic the hierarchically-organized architecture of the natural bone tissue. This review lecture summarizes our experience with the behaviour of bone, vascular, skin and stem cells on materials modified by various technologies mentioned here.

# The field enhancement effect in production of dimercaptoazobenzene induced by localized surface plasmon

Satoshi Kaneko<sup>1</sup>, Shuhei Watanabe<sup>1</sup>, Shinya Kasai<sup>2</sup>, Kazuhito Tsukagoshi<sup>2</sup>, Manabu Kiguchi<sup>1</sup>

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Plasmon induced reaction has attracted wide attention due to its potential ability to convert the solar energy into the chemical energy. The field enhancement effect takes decisive role in initiation of the reaction; however, the contribution of the field enhancement effect in the reaction rate of the plasmon induced reaction is still unclear because it is difficult to control the field enhancement effect. In this research, we investigated the contribution of the field enhancement effect to the plasmon-induced reaction. In order to control the field enhancement effect, we use structurally well-defined gold nanostructures fabricated by electron beam lithography technique. The arrays of gold nanodimers with different gap size were fabricated by electron beam lithography and lift-off process. The field enhancement effect was modified by changing the gap size of the gold nanodimers. The ethanol solution of nitrothiophenol was dropped onto the substrate. The Raman spectra were continuously monitored during the laser irradiation. The reaction rates of the reduction were evaluated at the different gap size. As a result, the reaction rate of the production of the demercaptoazobenzene was enhanced at the small nanogap. It is considered that the localized surface plasmon was effectively coupled at small nanogap, leading to large field enhancement effect. We observed contribution of the field enhancement effect to the reaction rate of the Plasmon induced photoreduction.

# Vicinal ZnO surfaces - structure, stability and reactivity

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Zinc oxide (ZnO) takes an active role in many catalytic reactions; however the role of under-coordinated atoms in the reactions is still poorly understood. As a base for future investigations of the influence of the under-coordinated atoms we have studied the structure and stability of vicinal ZnO surfaces using a combination of surface x-ray diffraction, scanning tunneling microscopy, photoelectron spectroscopy and density functional theory.

The low-index surfaces of wurtzite ZnO are polar, resulting in surface instability. Instead a higher-index surface, (10-14), has been suggested to be the most stable ZnO surface. The proposed model for this surface consist of Zn-terminated (0001) terraces and O-terminated steps, resulting in a charge neutral, high step-density, vicinal surface. However there are hitherto no studies of the single crystal ZnO(10-14) surface structure or stability. In general, the interaction between steps on vicinal surfaces plays a crucial role for the equilibrium structure and very little is still known about the equilibrium structure of vicinal oxide surfaces. Here we perform the first studies using a curved ZnO crystal, going from (0001) to (10-14), to investigate the stability of the vicinal facets. Further, we have studied the ZnO(10-14) surface in more detail and determined the atomic structure of this stable, high-step-density facet of ZnO. We will also discuss how the under-coordinated Zn- and O-atoms on the vicinal surface interact with water and methanol under UHV conditions.

# Electronic superlattice periodicity on the surface of highly--doped MoS2

Steven Schofield<sup>1</sup>, Mohammed Bin Subhan<sup>1</sup>, Asif Suleman<sup>1</sup>, Gareth Moore<sup>1</sup>, Peter Phu<sup>1</sup>, Hidekazu Kurebayashi<sup>1</sup>, Chris Howard<sup>1</sup>

#### <sup>1</sup> University College London

We have used low temperature (~5 K) scanning tunnelling microscopy (STM) and spatially- resolved tunnelling spectroscopy (STS/CITS) to investigate the surface of highly--doped molybdenum disulphide (MoS2). In agreement with previous STM investigations of intrinsic MoS2 we find the surface exhibits a large density of charged point defects [e.g., ACS Appl. Mater. Interfaces, 9, 19278 (2017)]. Fourier analysis of our atomic--resolution imaging and spectroscopy data from the doped MoS2 surface reveals two separate superlattice periodicities in addition to the 1x1 sulphur lattice, one of which is enhanced in the vicinity of the charged defects. We present an interpretation of the observed superlattices consistent with prior DFT and ARPES data.

# Effects of size and shape in reaction kinetics of metal nanoparticles

Henrik Grönbeck<sup>1</sup>, Mikkel Jorgensen<sup>1</sup>

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A key focus in heterogeneous catalysis is to understand the dominant reaction paths and isolate the character of the active site. This is challenging because of the dynamic character of the catalyst, which may undergo structural and phase changes as a response to the reaction conditions and stresses the importance to perform physical and chemical characterization of catalysts during operando conditions. These challenges apply also to computational work, aiming at establishing links between elementary steps and catalyst activity.

This contribution will discuss recent efforts to understand methane and CO oxidation over palladium and platinum using first principles calculations exemplifying different aspects of kinetic simulations based on theoretical data [1-4]. Special attention will be given the attempt to perform explicit simulations of reaction kinetics over metal nanoparticles. The simulations reveal that kinetic couplings between different sites on the particles largely determine the overall catalytic activity. Our results show that it is rather the site-assembly than a special site that determines the activity.

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# In-situ TEM mapping of transient events during nanowire growth

Axel R Persson<sup>1,2</sup>, Daniel Jacobsson<sup>1,2</sup>, Marcus Tornberg<sup>1,3</sup>, Robin Sjökvist<sup>1,2</sup>, Reine Wallenberg<sup>1,2</sup>

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Controlled and fine-tuned growth of nanowires are of importance for a number of applications, including photovoltaic devices. Insitu TEM has emerged as a useful tool for understanding this process, especially tracking of nucleation events, seed particle shape and seed particle composition during growth using EDS. The in-situ characterization can reveal transient processes associated with changes in conditions. While such analysis has started to emerge, no frame-by-frame quantitative mapping (XEDS) of a growing nanowire has been produced, due to the long acquisition time needed for a single map.

Here we demonstrate growth of Au-catalyzed GaAs and InAs nanowires in a Hitachi HF-3300 ETEM at varying temperatures and precursor-gas pressures (TMGa, TMIn and AsH3) which produce different growth events. These events include the "birth" of a nanowire from a droplet, interrupted and resumed growth. The imaging and XEDS were performed using scanning TEM at which analysis is performed for each pixel in the image. The processes were possible to follow spatially using our method of principal component analysis (PCA) filtered mapping, in which the noisy data of one frame is filtered by the PCA components obtained from the summed data. The resulting spectrum image (SI) frames are possible to quantify pixel-by-pixel and frame-by-frame.

This method of tracking nanowire growth by composition is a promising way for understanding the complex process of particleassisted epitaxial growth. With increasing sensitivity and collection efficiency of modern and future XEDS-detectors this method holds even higher promises of both spatial and temporal resolution.

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# In-situ growth study of NiFe2O4 thin films using surface sensitive high energy x-ray diffraction

Martin Hoppe<sup>1,2</sup>, Tobias Pohlmann<sup>1,2</sup>, Jannis Thien<sup>2</sup>, Kevin Ruwisch<sup>2</sup>, Jan Röh<sup>1</sup>, Florian Bertram<sup>1</sup>, Joachim Wollschläger<sup>2</sup>

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The (inverse-) spinel structure of ferrites displays a large variety of electronic and magnetic properties, making some of them interesting for potential applications in spintronics. The performance of such ferrites as thin film devices, however, is strongly coupled to the structure and interface of these materials, which are determined by the growth conditions.

With the help of surface sensitive time-resolved High Energy X-Ray Diffraction (tr-HEXRD) it was possible to record simultaneously the temporal evolution of several crystal truncation rods (CTRs) and Bragg peaks of the ultrathin films on a large area detector achieving a good time resolution within the few seconds range.

In this study, we investigated a temperature series of NiFe2O4 growth on SrTiO3(001) substrates. We found a small change in lattice constant for all temperatures during deposition. In the end the lattice constant of all samples goes towards the same final value. This final value of 8.63 Angström in-plane is larger than the expected nickel ferrite bulk value of 8.34 Angström. This is unexpected as the doubled lattice constant of the substrate is even smaller with 7.81 Angström. The final out-of-plane lattice constant with 8.225 Angström is smaller than the bulk value of nickel ferrite. This indicates a strain in the opposite direction regarding the substrate.

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## Real-time STED imaging of living cells during nanostraw-mediated electroporation

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The cellular membrane serves as a highly-selective barrier protecting the cell from potentially harmful exogenous agents. Yet, many state-of-the-art therapeutic interventions based on molecular biology require efficient delivery of molecules across the cell membrane while leaving the cellular integrity intact.

Such gentle delivery can be achieved by seeding cells on substrates of hollow metal-oxide nanotubes ("nanostraws") which provide a fluidic path across the membrane, and applying a low-magnitude external electric field across the nanostraws. Understanding the resulting changes of the permeability and geometry of the live-cell membrane is of particular interest for optimizing substance delivery across the cell membrane.

We used STimulated Emission Depletion (STED) superresolution microscopy to image A549 cells cultured on nanostraws and decorated with a fluorescent dye compound targeting the outer leaflet of the cellular membrane.

This allowed us to resolve the nanometric membrane topology: the membrane wraps tightly around the nanostraws. We observed disk structures and ring structures in cross section views of the nanostraw tip and shaft, respectively. The application of a low-magnitude electric field across the cell membrane resulted in the formation of a several nanometer sized gap between the nanostraw and the membrane. The nanostraws thus serve to focus the electric field and confine membrane openings to well-locatable, merely nanoscopic regions.

Using our approach of nanostraw-mediated local membrane perforation at low electric fields, we were successful at delivering large cargoes into living cells (e.g. fluorescent nanodiamonds) and could demonstrate their homogeneous distribution inside the cytosol.

# On the revision of the International System of Units (SI)

Micheal Krystek

Keywords: International System of Units, kilogram, base units

On 20 May 1875 the Metre Convention was signed in Paris by representatives of 17 nations, establishing the metric system. Based on it the International System of Units, the SI, was subsequently introduced in 1960. Since that time, several improvements of the SI have taken place. However, of the seven base units of the SI, only the kilogram is still defined in terms of a material artefact, namely, the International Prototype of the Kilogram (IPK). The fact that the current SI definitions of the ampere, mole and candela depend on the kilogram is little known, but has consequences, especially for precise electrical measurements.

During the last several decades the National Metrology Institutes (NMIs) as well as the BIPM made significant efforts to prepare for the possibility that SI base units can be defined in terms of fundamental physical constants. Consequently, in 2014 the CGPM encouraged the CIPM to develop a plan for a revision of the SI that links the definitions of the kilogram, ampere, kelvin, and mole to exact numerical values of the Planck constant h, elementary charge e, Boltzmann constant k, and Avogadro constant N\_A, respectively, and to complete all work necessary for the CGPM to adopt a resolution to replace the current SI with a revised SI. This decision has been made on November 2018 by the CGPM. The revised SI will become in force at the World Metrology Day on May 20th 2019.

The presentation will give an overview of the changes which will take place in the revised SI, its consequences, as well as some background information of its implementation.
# Magnetron sputtering coatings for erosion protection of epoxy based carbon fiber reinforced polymers

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Physical Vapour Deposition (PVD) coatings are well known as coatings for tribological applications, including erosion protection on different substrates. Although, PVD coatings can be applied on polymer based substrates to provide metallic aesthetics, there are critical issues to address in order to enable their use as protective coatings on soft substrates. While metallic aesthetic coatings on polymers are typically below 1 micron thick, tribological coatings on metallic substrates are in the range of 2-3 microns thick and temperature is typically applied during processing to increase adhesion. In the case of polymeric substrates low temperature processes are required to not damage the substrate. Additionally, to provide erosion protection on soft substrates it is necessary to grow thick coatings in order to avoid delamination of the coatings due to local deformation of the substrate under the impact of particles, but the thicker the coating the higher residual stresses, which are detrimental for adhesion.

In this work, magnetron sputtering Ti/TiN coating processes are investigated on epoxy based carbon reinforced polymers for erosion protection. Process parameters including substrate pretreatments have been analyzed in order to obtain thick coatings with good adhesion and low residual stresses. The coatings where tested on sand erosion conditions and mechanisms of failure were examined for different thicknesses. The results show how surface finishing of the substrate is a key issue and how an effective sand erosion protection can be achieved by using 12 microns thick Ti/TiN multilayers.

#### Oxygen-Mediated Self-Assembly of Porphyrins on Ferromagnetic Substrates

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Spinterfaces, i.e. interfaces between a ferromagnet and an organic semiconductor, are a topic of great interest since they can effectively combine the spin-polarized character of ferromagnets with the great responsivity to external stimuli of molecules, which makes them very appealing for spintronic appications[1]. Metallo-Tetra Phenyl Porphirins (M-TPP) are ideal candidates for building spinterfaces because of their flat morphology and the fact that their ion core can possess its own magnetic moment, which might lead to an enhancement of the spin-dependent properties of the system. However, ferromagnetic materials typically strongly interact with organic molecules, making it difficult to obtain well-ordered structures.

This contribution focuses on the growth and the magnetic character of a single layer of Zn-, Co- and Ni-TPP on either the oxygenfree or the oxygen-passivated Fe(001) surface, investigated by means of Scanneling Tunneling Microscopy (STM) and X-ray Magnetic Circular Dichroism (XMCD). Results highlight how the passivation of the metal surface can promote an ordered selfassembly of the molecules [2]. STM measurements also reveal that the arrangement of the molecules on the passivated substrate varies with the ion core species. Finally, the dichroic signal of the metallic core is reported for the different molecules.

References:

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## Tuning the coupling of an individual magnetic impurity to a superconductor: quantum phase transition and transport

Laëtitia Farinacci<sup>1</sup>, Gelavizh Ahmadi<sup>1</sup>, Gaël Reecht<sup>1</sup>, Michael Ruby<sup>1</sup>, Nils Bogdanoff<sup>1</sup>, Olof Peters<sup>1</sup>, Benjamin W. Heinrich<sup>1</sup>, Felix von Oppen<sup>1</sup>, Katharina J. Franke<sup>1</sup>

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Magnetic impurities on a superconductor induce an exchange scattering potential that perturbs the Cooper pairs of the latter. This leads to the presence of a bound state, so-called Yu-Shiba-Rusinov (YSR) state, within the gap of the superconductor whose energy depends on the coupling strength between the impurity and the Cooper pairs. At weak coupling, the bound state is unoccupied and the system is a free-spin ground state. Upon increase of the coupling strength, the system undergoes a quantum phase transition to a screened-spin ground state in which the YSR state is occupied.

Here, we investigate YSR states induced by Fe-porphin molecules on a Pb(111) surface with scanning tunneling spectroscopy. By approaching the tip toward the molecule, the flexibility of the latter allows for a controlled distortion that modifies the YSR state energy and enable us to drive the system through the quantum phase transition. Moreover, as the tip is brought closer to the molecule, the transport properties of the STM junction are modified so that we can investigate the YSR excitations by single-electron as well as by (multiple) Andreev reflections. [1]

[1] Farinacci et al., PRL 121, 196803 (2018)

## Recording real-time atomic resolution video of semiconductor growth in a CVD-TEM

Reine Wallenberg<sup>1,2</sup>, Axel R Persson<sup>1,2</sup>, Daniel Jacobsson<sup>1,2</sup>, Carina B Maliakkal<sup>1,3</sup>, Marcus Tornberg<sup>1,3</sup>, Jonas Johansson<sup>1,3</sup>, Lars Samuelson<sup>1,3</sup>, Kimberly A Dick<sup>1,2</sup>

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<sup>2</sup> nCHREM / Chemistry Institution

<sup>3</sup> Solid State Physics

Semiconductor nanowires (NWs) with group III-V combinations of elements holds great promise for application in high-speed electronics, LEDs and solar cells. Common growth techniques for NWs are for example metal-organic chemical vapor deposition (MOCVD), molecular beam epitaxy (MBE), and the recently developed Aerotaxy process.

To be able to understand the growth of the crystalline nanowires, usually with a metal seed particle, we have constructed a CVD-TEM, using the same type of precursors as in larger-scale production. The basic pressure of the microscope is < 2 10-9 Pa at the field emission electron gun, but differential pumping allows up to 2 Pa at the specimen of the metalorganic and hydride precursor, which is sufficient to grow various combinations of

III-V semiconductors. We have chosen to use an open sample holder to allow for simultaneous chemical analysis by XEDS and to maintain the point resolution (0.86 Å) of the aberration corrected transmission electron microscope. The CVD system supplies 9 different gases, and the gas composition inside the microscope is monitored by quadrupole mass spectrometers. The sample can be heated up to 700°C.

We will show video recordings from the Environmental TEM (ETEM) with atomic detail of the nucleation from seed particles, and controlled growth of nanowires, paired with XEDS analysis of the composition of the seed particle.

## STM patterned arsenic nanostructures in silicon

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Scanning tunnelling microscopy - hydrogen desorption lithography (STM-HDL) combined with a detailed understanding of phosphine (PH3) surface chemistry [1], and low temperature epitaxy (LTE) silicon growth, has been developed over the past two decades, such that atomic scale devices can be fabricated by positioning individual phosphorus (P) atoms in a silicon (Si) lattice with near atomic precision [2]. Expanding this fabrication technique to include multiple species of dopant impurity atoms could provide new possibilities for device structure and function. Working towards the broader goal of expanding the materials palette of atomically precise doping via STM lithography, we have investigated the compatibility of arsine (AsH3) and arsenic (As) with all stages of STM-HDL + LTE fabrication. We have used STM and density functional theory to study single molecules and saturated monolayers of AsH3 adsorbed on Si(001). In addition to the adsorption and dissociation behaviour of the AsH3 molecules on the Si surface, we also investigate the substitutional incorporation and encapsulation of STM patterned As layers within the Si lattice. Secondary ion mass spectrometry and magneto-transport measurements are used to study the confinement and electrical transport properties of As delta-layers buried beneath LTE Si over-layers. Finally, we demonstrate STM-HDL nano-scale device structure patterning in Si using two unique donor species (P and As) within a single Si plane.

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[2] M. Fuechsle et. al., Nature Nanotechnology, 7, 242-246 (2012)

## Structure of an ultrathin Fe3O4 nanosheet

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Experiments involving ultrathin iron oxide films grown on silver surfaces revealed the existence of a puzzling phase whose surface structure resembles that of FeO(111), but which evidently incorporates a substantial portion of Fe(III) [1,2]. It was proposed previously [2] that this phase corresponds to 3-monolayer-thick FeO(111) with oxygen termination at both the vacuum and metal interfaces. We have investigated this phase using grazing incidence X-ray diffraction and density functional theory calculations, and found that the structure differs markedly from FeO; the structure shows mixed coordination and distinct charge segregation: it is composed of one close-packed Fe(II) layer in octahedral coordination at the center of the slab and two close-packed Fe(III) layers in tetrahedral coordination at the exterior. The geometrical arrangement is distinct from any bulk iron oxide phase, and from the 'wurtzite' surface reconstruction observed for FeO(111) [3]. The formation of the structure is furthermore not driven by bonding at the interface, which is very weak. We propose, therefore, that the phase should be considered a distinct, metastable form of Fe3O4 with a thickness of about 1 nm, and a true two-dimensional material.

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## Investigating and influencing on-surface covalent-coupling reactions

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The on-surface synthesis of covalently bonded molecular frameworks offers a promising route towards custom 1D and 2D materials.[1] Such on-surface reactions, in which the substrate itself may be employed as a catalyst, potentially provide alternative reaction pathways to those available in solution-phase synthesis. In order to gain control over the efficiency and selectivity of these reactions an appreciation of the underlying mechanism is required: specifically with regards to the role of substrate chemistry and topography. These molecule-surface systems are readily studied by scanning probe microscopy (SPM) techniques, allowing identification of the covalently bonded products, as well as intermediate states, and additional chemical analysis can be provided by photoelectron spectroscopy measurements.

Here we present details from our recent studies, illustrating aspects of on-surface synthesis including; (i) the influence of surface topography on the reaction pathway,[2] (ii) the effect of utilising a porous self-assembled molecular overlayer as a template to confine reactions on a catalytic surface,[3] and (iii) details of surface adatoms participating in the formation of metal-organic intermediate structures. The reactions studied are based upon Ullmann-type on-surface coupling performed on metallic substrates held under ultra-high vacuum (UHV) conditions, and are characterised via scanning tunnelling microscopy (STM) and synchrotron based X-ray standing wave (XSW) measurements.

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- [2] Judd, C. J., et al. Sci. Rep. 2017, 7 (1), 14541.
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## ZnO/ZnMgO heterostructures on ZnO nanorods grown by a two-stage technique

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Semiconductor nanowires with axial or radial quantum heterostructures are considered as basic elements for future electronic or optoelectronic devices, like nano-LEDs or nano-lasers. For many semiconductors, such as III-V compounds (including nitrides), such quasi-1D objects can be fabricated in one technological process based on molecular beam epitaxy (MBE), a technique well-suited to growing quantum structures. Unfortunately, for ZnO, an important wide-band-gap semiconductor, such a convenient procedure cannot be applied. Although reports on preparation of pure ZnO nanostructures of various shapes are quite numerous in literature, only very few papers describe growth of ZnO nanowires with quantum structures. The MBE procedure for ZnO nanowire growth is still not well established. In this paper, we describe how to overcome that obstacle by growing nanowires with heterostructures in a two-stage procedure. The ZnO nanorods were prepared by a hydrothermal method, the axial heterostructures were grown on the top face of the nanorods by an MBE process. The morphology and optical properties of the obtained system were studied by cathodoluminescence (CL) spectromicroscopy and micro-photoluminescence. Those experimental techniques enabled us to confirm successful growth of 4 nm was discerned, with considerable intensity even at room temperature. The carrier diffusion length in ZnO was also estimated from the acquired CL data.

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#### Total Tomography of III-As Nanowire Emitters: Correlating Composition, Strain, Polytypes, and Properties

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Ternary III-As nanowires (NWs) offer high efficiency, tunable emission and allow for direct growth on current Si CMOS technology, making them ideal as nanoscale emitters and detectors for on-chip photonic communications. In particular, (In,Ga)As quantum well (QW) shells grown on GaAs NW cores can emit in the near-IR by tuning the QW composition and diameter. In this work, we characterize (In,Ga)As/GaAs QW heterostructures that exhibit a blue-shifted emission near the top of the NW measured by spatially resolved cathodoluminescence (CL). As we aim to produce efficient, uniform emitters, it is necessary to understand the nature of this emission variation.

Electron backscattering diffraction and nano-probe x-ray diffraction measurements reveal an extended segment of the polytypic wurtzite (WZ) structure embedded in the zincblende (ZB) NW. Direct correlation with CL shows an alignment between the blue-shifted region and the WZ segment. Additionally, strain measurements by nanodiffraction reveal minimal strain variations between the WZ and ZB regions. Atom probe tomography (APT) was used to map the composition of these structures in 3D. APT revealed a decrease in In mole fraction in the WZ region by about 4%. These measurements of morphology, composition, structure, and strain were combined as input for k-p calculations of the QW band structure that reveal an emission shift between the WZ and ZB of about 80 meV, matching well to the CL results. Ultimately, this correlative analysis allowed us to deconvolve the complex emission behavior of this NW QW heterostructure.

# Advanced Processing for All-III-V CMOS on Si

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Complementary metal-oxide-semiconductor (CMOS) circuits are the fundamental building blocks for performing logical computations. Thus, continuously improving the CMOS circuits are essential for increased power efficiency. In light of the traditional Dennard scaling coming to an end it is vital to implement technology boosters to further increase device performance in metal-oxide-semiconductor field-effect-transistors (MOSFETs). Suggestions have been made regarding a change of the active channel material from Si to various III-Vs inside the MOSFET due to their excellent transport properties. Specifically InAs and GaSb represent attractive III-V material options due to their high bulk mobility for electrons and holes respectively. Furthermore, for increased packing density as well as reduced short channel effects the International Roadmap for Devices and Systems (IRDS) are suggesting that a vertical transistor architecture with gate-all-around is essential for sub-6 nm nodes.

We have developed a process where vertical nanowire n-type (InAs) and p-type (GaSb) MOSFETs are simultaneously processed and co-integrated with a common gate-stack on top of Si substrates. Small critical dimensions have been achieved with gatelengths and diameters down to 40 and 10 nm respectively. The transistors are based on InAs-GaSb heterostructure nanowires, overgrown with a highly doped InAs shell. The overgrown shell protects the highly sensitive GaSb which allows the use of hydrogen silsesquioxane (HSQ) spacers, with adjustable thickness, crucial for implementation of a self-aligned gate-last process. In spite of increased complexity we are able to demonstrate state-of-art performance for both n- and p-type MOSFETs with large drive currents.

# Growth and structure of cobalt ferrite thin films with large inversion parameter

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Cobalt ferrite ultrathin films with inverse spinel structure are among the best candidates for spin-filtering at room temperature. We have fabricated a few nm thick high-quality epitaxial CoFe2O4 films on Ag(001) following a three-step method: an ultrathin metallic CoFe2 alloy was first grown in coherent epitaxy on the substrate, and then treated twice with O2, first at RT and then during annealing. The epitaxial orientation, the surface, interface and film structure were resolved combining LEED, STM, Auger and in situ GIXRD. A slight tetragonal distortion was observed, that should drive the easy magnetization axis in plane due to the large magneto-elastic coupling of such a material. The so-called inversion parameter, i.e. the Co fraction occupying octahedral sites in the ferrite spinel structure, was obtained through in situ x-ray resonant diffraction measurements collected at both the Co and Fe K edges. It is a key element for its spin-dependent electronic gap. The data analysis was performed using FDMNES, an ab initio code already extensively used to simulate x-ray absorption spectroscopy, and shows that Co ions are predominantly located at octahedral sites with an inversion parameter of 0.88±0.05.

# Strain mapping with coherent scanning X-ray diffraction at NanoMAX beamline

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At the 4th generation synchrotron light source MAX IV in Lund, Sweden, the high brilliance is ideal for pushing the limits of resolution for coherent x-ray diffraction. X-rays are highly energetic and highly penetrable which enables us to probe the inner structure of materials. With their short wavelengths, it is possible to get a resolution on the nanoscale. With x-ray diffraction (XRD) we can investigate the structure of crystalline materials and detect strain and stacking faults. These properties are important for nanowires (NWs) that are used to build solar cells. Strain in NWs can affect the transport properties, and thereby the performance of the solar cell devices. We performed scanning XRD on a single nan-owire at the hard x-ray nanoprobe beamline NanoMAX at MAX IV, to create maps of the strain varia-tions in the NWs.

# Local Energy Landscape in Small Molecule Organic Donor–Acceptor Heterojunctions

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Organic solar cells show great promise for low-cost, flexible devices with low embodied energy. However, their power conversion efficiencies are currently too low for large-scale commercialization. A key reason for this is the high exciton binding energy in organic semiconductors. The driving force for exciton dissociation is the local energy landscape around the donor-acceptor interface. To optimize device efficiency, we therefore need to better understand the pathways of exciton dissociation at interfaces in OPV materials and how we can design the energy landscape to optimize efficiency. We use scanning tunnelling microscopy and spectroscopy (STM/S) to investigate the local energy landscape with sub-molecular spatial resolution. As a model system, we study C60 thin films with single impurity molecules of pure and fluorinated zinc phthalocyanine (ZnPc, F4ZnPc, and F8ZnPc) added. The impurity molecules cause the frontier energy levels in the surrounding C60 film to shift, as measured by STS. The magnitude and degree of localization of this shift depends strongly on the degree of fluorination. While pure ZnPc only induces a ~10 meV shift of the energy levels of the nearest few C60 molecules, F8ZnPc causes the energy levels to shift by ~150 meV over several nanometres. This large and long-range shift induced by some fluorinated phthalocyanines promises opportunities for controlled design of the organic heterojunction energy landscape to optimize charge transfer efficiency.

# Room temperature magnetic skyrmions in ultrathin magnetic nanostructures and their manipulation by electrical currents and light

Olivier BOULLE

Magnetic skyrmions are nanoscale whirling spin configurations. Their small size, topological protection and their manipulation by electrical current have opened a new paradigm to manipulate magnetization at the nanoscale. This has led to novel proposal of memory and logic devices in which the magnetic skyrmions are the information carriers [1]. The recent observation of room-temperature magnetic skyrmions [2,3,4] and their current-induced manipulation [4,5] in ultrathin sputtered magnetic nanotracks have lifted an important bottleneck toward the practical realization of such devices.

In this talk, I will show that magnetic skyrmions can be stabilized at room temperature in magnetic nanostructures patterned in an ultrathin Pt/Co/MgO multilayer stack. Using high spatial resolution X-ray magnetic microscopy technique, we were able to observe the internal topological spin texture of the skyrmion as well as its homochiral Néel internal structure [3]. The skyrmions can be manipulated with small electrical currents with velocities up to 100 m/s which is promising for lower power skyrmion-based memory and logic devices. Using specifically engineered magnetic stacks, I will also show that magnetic skyrmions can be stabilized at room temperature and zero magnetic field with diameter smaller than 30 nm. Finally, I will show that skyrmions can be controllably created/annihilated using electrical currents as well ultrafast laser pulses [6], which can be used for the writing operations in memory and logics devices.

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# Atomic engineering of monolayer graphene: selective symmetry breaking and Kekulé bond order via lithium deposition

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The Kekulé distortion (KD) periodically alters the carbon-carbon hopping strengths in graphene, resulting in a sqrt(3)\*sqrt(3) R30 deg superstructure and symmetry breaking between three previously equivalent hexagonal plaquettes. Such a KD phase is induced in monolayer graphene by low-flux deposition of a small number of lithium adatoms and studied via angle-resolved photoemission spectroscopy (ARPES). In a regime where no charge-transfer doping by the lithium is apparent, the superstructure periodicity is observed in a sharp backfolding of the Dirac cones to the Gamma point, as well as the appearance of corresponding peaks in low-energy electron diffraction (LEED). A gap opening 2\*Delta = 0.19 meV is observed at the Dirac point. Above approximately 30 K, the new features vanish, the gap closes, and neither is recovered upon subsequent cooling. A Monte Carlo toy model demonstrates that during low-flux deposition, adatoms prefer to occupy the same set of inequivalent plaquettes even when separated by many sites, producing a self-reinforcing, long-range order that is not observed at high flux.

#### Tunable orbital transitions and tunnelling readout in a dilute Si:P delta-layer near an interface

Neil Curson, Guy Matmon

Recent progress towards fabricating and measuring novel device structures based on donors in silicon will be described. In particular the optical response of a 2D isolated donor system will be discussed. For this device we fabricated a dilute disordered phosphorus (P) delta-layer ~15 nm below the surface of bulk silicon. 2D metallic P contact pads were fabricated in the layer using hydrogen resist lithography, where the resist patterning is performed using scanning tunneling microscopy (STM). These buried contact pads were connected to large aluminium (AI) contact pads on top of the sample using AI vias.

Measurements were performed to determine the optical response of the donors to THz radiation at different temperatures and bias voltages. We find two main differences between the delta-layer and equivalently-doped bulk silicon. Firstly, the Rydberg states of the phosphorus donors are shifted to higher energies, which our modelling shows originates from the proximity of the donors to the surface. Secondly, we measure a strong signal down to 200 mK, that cannot not be explained by photothermal ionization (PTI), and we describe a new low-temperature conduction mechanism. These findings open the way to selective optical manipulation of donors/qubits. By patterning the silicon overlayer we can control the transition energies of individual donors. Additionally, a direct electronic readout is available even at a temperature that is considered too low for PTI. Furthermore, we show we can use the line shape of the transitions to nondestructively determine the depth and thickness of our delta-layers.

# Single Metal Zirconium Non-Evaporable Getter Coating

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The non-evaporable getter coating (NEG) is widely used in particle accelerators and colliders. Not only it provides distributed pumping speed, but also reduces thermal, electron-, photon- and ion-stimulated desorption, which is important for maintaining high vacuum and mitigating beam-induced effects in accelerator beam chambers. However, compound material deposition targets, like most widely used TiZrV or TiZrHfV alloys or twisted wires, are hard and expensive to manufacture. Therefore, single metal zirconium was tested as a substitute coating material which could potentially make the production of uniformly coated vacuum chamber parts of various shapes more efficient and cheaper due to the greater availability of Zr. In this work, analysis of two NEG-coated tubular stainless-steel samples with dense and columnar Zr film structure will be demonstrated, providing results of sticking probability measurements, electron-stimulated desorption (ESD) yields and surface characterisation using various techniques. The findings show that columnar Zr coating activated at 160°C has a sticking probability and pumping capacity comparable to that of TiZrV activated at the same temperature. In addition, the desorption yields from dense Zr are similar to the ones measured from ternary film samples. The results show that single metal Zr coating demonstrates properties good enough to be considered a possible alternative to TiZrV films in vacuum chambers.

#### Spatial extent of Yu-Shiba-Rusinov states of individual magnetic atoms on 3D and quasi-2D superconductors

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Magnetic impurities in conventional superconductors induce a pair-breaking potential, which leads to bound states inside the superconducting energy gap. These states are called Yu-Shiba-Rusinov states, or short: Shiba states, and can be probed by scanning tunneling spectroscopy at the atomic scale.

Here, we explore the Shiba states of individual magnetic atoms on superconducting substrates. The patterns of Shiba states of individual Mn atoms on a Pb(100) surface exhibit the shape of the corresponding spin-carrying d-orbital [1]. When the adatoms are brought into sufficiently close distance, they hybridize by forming symmetric and anti-symmetric linear combinations of the Shiba wave functions [2].

NbSe2 is a van der Waals-layered material with quasi-2D character. In addition to its superconducting properties it hosts a chargedensity wave (CDW) at low temperatures. Magnetic atoms and molecules have been shown to give rise to long-range oscillatory Shiba states [3,4]. Here, we show that the CDW affects the energy and symmetry of Shiba states around individual Fe atoms.

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# Areal strain profiles of suspended germanium microstructures via Raman mapping

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Strain engineered germanium (Ge) microstructures have attracted a great deal of attention in recent years because of the potential for dramatically altering the electronic band-structure. It is predicted that, even for moderate (tensile) strain, on the order of a few percent, the material bandgap can be converted from indirect to direct, opening up the possibility for a class of CMOS compatible opto-electronic devices with enhanced performance; channel MOSFETs, photo-detectors and even laser sources. So important is this topic that in just four short years since the seminal Ge micro-bridge work, we have already seen demonstration of low-threshold optically pumped lasing from this type of structure. Various structures were reported showing very high levels (up to 5.7%) of uniaxial tensile strain, as well as bi-axially strained structures, fabricated either from germanium-on-silicon-on-insulator (Ge-SOI) or germanium-on-insulator (GeOI) starting wafers, using standard (e-beam-, photo-) lithography techniques. In this contribution, we present high resolution Raman mapping of various Ge micro-bridge structures, prepared from both Ge-SOI and GeOI using photo-lithography. We discuss how the microstructure geometry influences the level of strain and, critically, the strain distribution and we show the effects of natural strain relaxation through the formation of curved micro-bridge structures. Potential routes to realising practical devices from these microstructures will also be discussed.

# Surface diffusion and growth. C60 on Cu(111)

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Surface diffusion is probably the most significant phenomenon in the atomic scale during the epitaxial growth. The growth involves the surface diffusion, island nucleation and, nucleation at (or jumping over) step edges. In this context, it is tempting to affirm that a better, more ordered growth, would happen for larger diffusion lengths (smaller barriers). Although this is true in the step flow regime, in which the atoms only nucleate at the step edges, it is not so for more typical growth conditions that lead to island formation. The case of homo-epitaxial growth of Cu on Cu(100) and Cu(111) is a good example of a layer by layer growth (LbL) for the surface with greater diffusion barrier: Cu(100). This is due the relation between the surface diffusion and the step jumping process (Erlich-Schwoebel barrier) and the different diffusion mechanisms in both cases i.e. atomic interchange in the (100) face and jumping in the (111) one.

In this work we present results, based on Auger electron spectroscopy (AES) and molecular dynamics simulations (MD) on the diffusion of C60 on Cu(111). This is a quite interesting system; in the first place, the C60 molecule is tridimensional allowing the rotation as an alternative displacement possibility respect to the atom and island diffusion. The other interesting point is the large difference in the diffusion barriers, of an order of magnitude, in between the C60 on Cu(111) and on a C60 adlayer. With such a configuration there are two clearly different diffusion systems, one at low temperatures that is random in nature (with translations proportional to the square root of time) and another at higher temperatures signed by a deterministic evolution (in which displacements are proportional with time), for short diffusion times, retrieving the random behavior for larger ones. In contrast, for C60 on C60 the diffusion is always random in nature.

# two-dimensional spot-shape analysis in X-ray diffraction for strain-distribution evaluation

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Two-dimensional (2D) reciprocal space mapping (RSM) has been utilized for displaying anisotropic strain of single-crystalline films in in-plain and/or out-of-plain X-ray diffraction. Most papers discuss the averaged strains from peak-center positions of 2D spots, however, could not discuss strain distribution which can be achieved by a peak-shape analysis. Such a peak-shape analysis is not yet demonstrated in 2D RSM because of no guide line.

In this presentation, we demonstrate new fitting analyses for 2D peak shapes in in-plane RSM for crystalline ultra-thin (~1.5 nm) film of beta-FeSi2(100) [1] epitaxially grown on Si(001) substrate. The first analyses display residual maps as a function of strain (epsilon) or domain size (D), reflecting the existence possibility of a homogeneous domain. The 2D Laue fit with the convolution of instrument broadenings showed small residuals around strains epsilon\_b = 0.0% and epsilon\_c = -0.3% along the b and c axes of beta-FeSi2, respectively, at D ~ 23 nm with R\_min = 0.10 in the residual map by the strains.

The 2D fit can also display an inhomogeneous domain distribution, by the superposition from the components with different strains. The next analysis displays the population map by the strains, indicating that the main strain components (>65%) are around epsilon\_b = 0.0% and epsilon\_c = -0.3% achieving R\_min = 0.09. The analyzed results indicate that the beta-FeSi2 nano film was mostly strain-free, implying weak interaction between the film and substrate.

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# Fabry-Perot cavity-based refractometry utilizing gas modulation for assessment of pressure with sub-ppm precision.

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In this presentation we will present the basics of Fabry-Perot cavity (FPC) based refractometry in general, and the gas modulation refractometry (GAMOR) methodology in particular. We will present our latest results in the field, including a novel and significantly improved realization of the GAMOR method that improves both the short- and the long-term characteristics. Using a dead weight piston balance set to 4303 Pa as a reference, and for measurement times above 20 minutes (about measurement 10 cycles), the improved GAMOR system is limited by flicker noise, which when expressed in terms of an Allan deviation is 1 mPa (corresponding to 0.25 ppm). This thus corresponds to a precision, defined as twice the Allan deviation, of 0.5 ppm.

While we so far mostly have been focused on the short- and long-term stabilities of the system, we will in this presentation also present recent assessments of the linearity and accuracy of the system by comparing it to a dead-weight piston balance. Finally, we will discuss how the properties of GAMOR justify the use of the methodology for transfer of calibration between widely different pressure ranges, discuss the advantages and disadvantages of the technique, and touch on the possibilities of FPC-based refracometry to in future, become a primary standard for pressure.

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#### Vacuum resonance states as atomic-scale probes of non-collinear surface magnetism

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Developing future spintronic devices requires the full understanding of the interaction of electrons with localized spins. Up to now, atomic-scale variations of the spin-dependent electron scattering process at surfaces remained inaccessible, due to the laterally averaging nature of the established electron reflection techniques. Utilizing spin-polarized scanning tunneling microscopy (SP-STM), we realize a spin-resolved electron vacuum interferometer on the atomic scale by placing a biased magnetic probe tip in front of a magnetic surface. By tuning the bias, spin-polarized electrons from the tip are injected into individual resonance states evolving in the vacuum between the tip and the surface, and the resulting spin-resolved tunnel current is recorded as a function of tip position [1]. Our experiments on the double layer Fe/W(110) and the double layer Fe/Ir(111) include a variety of resonances, ranging from Stark-shifted image-potential states to field states [2]. With increasing electron energy, topographic features like atomic step edges tend to smear out in the microscopy image. However, the magnetic image contrast and local spin-resolved spectroscopy reveal that all resonance states with up to 20 eV above the surface Femi level exhibit a local spin quantization axis that rotates on the atomic scale with the surface spin texture. Our findings indicate that spin-dependent electron scattering at surfaces and interfaces is affected by all the magnetic ground state interactions like Heisenberg exchange, Dzyaloshinskii-Moriya and spin-orbit interactions, even for energies far above the vacuum level.

[1] A. Schlenhoff et al., Phys. Rev. Lett. 109, 097602 (2012).

[2] A. Schlenhoff et al. (submitted).

# Cross-sectional X-ray Nanodiffraction Characterization of Radiation Damage, Stresses and Microstructure in W Thin Film

Kostiantyn Hlushko<sup>1</sup>, Anna Mackova<sup>2</sup>, Juraj Todt<sup>3</sup>, Jakub Zalesak<sup>3</sup>, Rostislav Daniel<sup>1</sup>, Jozef Keckes<sup>1</sup>

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A better understanding of depth-dependent radiation damage in protective thin films used in fusion and fission reactors as plasmafacing components is an essential pending step for further development of novel film types and microstructures that are capable of withstanding severe environments over long time periods. Nanocrystalline tungsten is a perspective material for plasma-facing components of a fusion reactor due to its high radiation resistivity, high thermal conductivity and high melting point. In this contribution, a 8µm thick nanocrystalline tungsten film on WC substrate was irradiated using Si ions with an energy of 5MeV and a fluence of 2x1016 ions/cm2. In order to investigate depth-dependent changes in residual stresses and microstructure induced by the irradiation, cross-sectional X-ray Nanodiffraction (CSnanoXRD) with a beam size of 30nm was applied at European Synchrotron Radiation Facility in Grenoble, France, to scan 50µm thick samples at the film cross-section. The experimental results revealed significant changes in the depth-dependent gradients of residual stresses as well as changes in unstressed lattice parameters and the coating microstructure, which will be presented together with the data from transmission electron microscopy.

The research has been carried out at the CANAM infrastructure LM 2015056 and the work was supported the project CANAM OP, CZ.02.1.01/0.0/06\_013/0001812 and the Czech Science Foundation (GACR No. 18-03346S).

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# Label and Metage Symmetries and Stability of Fusion Plasmas

Asher Yahalom

Label symmetries are related through the Noether theorem to important conservation laws. Among those are local conservations laws of potential vorticities and global conservation laws of circulation in barotropic flows. Subgroups of the labelling group are connected to topological conservation laws. For example it was shown that the Metage symmetry group is connected to the conservation of Helicity in barotropic flows and the conservation of cross helicity in barotropic magnetohydrodynamics. In both cases the choice of the labels is restricted by attaching them to comoving physical lines. Those are vortex lines for the fluid dynamical case and magnetic lines for the magnetohydrodynamic case. It should be remarked that recently a way was found to expand the realm of Metage symmetries also to non-barotropic magnetohydrodynamics and thus obtain a generalization of the cross helicity conservation law for this case. This new topological constant of motion was also found using non-single valued variational variables. In this talk we will review some of the results associated with label symmetry sub groups and the associated conservation laws and relate them to the stability of fusion plasmas.

## phase guided decomposition in metastable Zr1-xAlxN thinfilms

Samira Dorri, Jens Birch, Naureen Ghafoor

At elevated temperatures and pressures the mechanical stability of hard coatings, constituting metastable transition metal ternary aluminum nitrides, correlates to decomposition rout and decomposed structure. Zr1-xAlxN is a potential alloy for coating applications and can be deposited both in cubic and wurtzite phase depending on aluminum content. However, at elevated temperatures decomposition into ZrN and AlN rich domains is expected due to high immiscibility of the constituent in the entire composition range. We investigate two compositions Zr0.75Al0.25N and Zr0.5Al0.5N deposited as 0.5 micron thick films on MgO (001) substrates using DC magnetron sputter deposition. The depositions were made at 900 °C to allow surface diffusion during growth, as well as at 500 °C to facilitate formation of single-phase homogeneous alloys. The 500 °C deposited films were further annealed to 1000 °C and the decomposed nanocomposite structures were compared with 900 °C as-deposited films to understand the decomposition mechanism.

The phase evolution during growth and annealing was monitored using in situ wide-angle high-energy X-ray scattering. The decomposed structure in the films was characterized using scanning TEM whereas XPS was used to find the bonding structure. We will show comparison between the two decomposition routs and that despite a predicted large driving force for phase segregation a slow diffusion occurs in high Al containing wurtzite phase alloys during both decomposition routs.

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# Improved pumping speeds of oxygen-free palladium/titanium nonevaporable getter coatings and suppression of outgassing by baking under oxygen

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Oxygen-free palladium/titanium (Pd/Ti) is a new nonevaporable getter material with an activation temperature as low as 133 °C [1]. Because pumping speeds of oxygen-free Pd/Ti for H2 and CO have been reported to be improved by baking under an O2 atmosphere, we investigated oxygen-free Pd/Ti samples heated in an ultrahigh vacuum (UHV) or under an O2 pressure of 1.3 × 10 –4 Pa by X-ray photoelectron spectroscopy (XPS) [2]. We found that carbon contamination decreased to an extent on heating in UHV, but decreased considerably on heating in O2. Pressure-curve measurements in an oxygen-free Pd/Ti-coated chamber show that pumping speeds for H2 and CO were considerably improved after baking the chamber under an O2 pressure of 1.3 × 10–4 Pa (O2 baking) in comparison with baking in UHV. Furthermore, partial-pressure measurements suggested that O2 baking removes adsorbed carbon and hydrogen, and consequently suppresses the formation of H2, CO, H2O, and CH4. Catalytic chemical reactions on the Pd surface appear to be responsible for the removal of adsorbed carbon and hydrogen. The pumping speeds of the oxygen-free Pd/Ti coated chamber for H2 and CO were measured by using the orifice method, and were found to be improved after O2 baking. O2 baking is therefore useful for improving pumping speeds for H2 and CO, and for reducing the partial pressures of H2, CO, H2O, and CH4.

## References

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# Frontiers of force microscopy in liquid: From single adsorbed ions to single cell nanomechanics

RICARDO GARCÍA

This contribution introduces some of the main challenges faced by force microscopy to image with subnanometer-scale spatial resolution solid-liquid interfaces. The presentation is divided in three sections. The first section is devoted to introduce the capabilities of 3D-AFM to image with atomic resolution the three-dimensional interfacial structure of surfaces immersed in aqueous solutions (1-2). Those images enable the identification of ions on solid-liquid interfaces. The second section, will illustrate how bimodal force microscopy provides high speed nanomechanical maps (1 frame/s) of polymer surfaces (3). The third section discusses some fundamental issues involving the imaging and nanomechanical characterization of live cells with the AFM (4-5).

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## Molecular Beacons: an investigation of uptake and distribution

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Molecular beacons (MBs) are fluorescent probes based on oligonucleotides which bind to specific RNA sequences within cells. The ability of these beacons to target specific RNA sequences among the vast informational content in the cytosol enables a live and detailed snapshot of a cell's state and thus an indication of its fate.

These probes are constructed of three main parts which together form a hairpin shape: i) a long single nucleotide strand complementary to a specific target sequence, ii) a short stem of complementary nucleotides, and iii) a fluorescent reporterquencher pair, bound to the ends of the stem sequence. Upon binding, the hairpin loop opens up, and the reporter fluoresces, indicating the target sequence.

Reports of using MBs for biomolecular targeting have been and still are, however, highly controversial. The mechanisms by which MBs enter the cell and how they are distributed thereafter are unclear. Further, the pathway to their target sequence is hindered, and may even be interrupted, by several unknowns, e.g. spontaneous rupture, endosomal trapping or permanent binding to mitochondrial structures. Thus, conclusions about a cell's state and fate cannot be drawn before the specificity of the MB signal is confirmed.

Here we investigate the MB signal in living A549 cells. The MB signal is co-localized mainly with lysosomes and mitochondria. We discriminate these signals through a series of controls, and use quantitative image analysis based on confocal fluorescence microscopy in order to map out the true signal of the molecular beacon which has reached its target RNA.

# synthesis of ingan sub-micron-platelets and applications towards green and red light emitting diodes

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Blue nitride LEDs can reach an external quantum efficiency (EQE) of >80% with InGaN/GaN actively layers (ALs) grown on a GaN buffer layer. However, when indium content in InGaN/GaN ALs is increased for green and red light emissions, the EQE drops drastically (2-3% for red LEDs) due to the increased strain and quantum confined Stark effect in ALs. A solution to this is to replace the GaN buffer layer with an InGaN layer that has indium contents closer to the InGaN/GaN ALs.

We present a method to synthesize InGaN sub-micron-platelets by metal-organic vapor phase epitaxy (MOVPE). The InGaN platelets are about 200 nm thick and have a smooth top c-plane with an extension of a few hundred nanometers, able to be used as a buffer layer for green and red nitride LEDs. The platelets were prepared by in-situ annealing of hexagonal InGaN pyramids, grown by selective area MOVPE. The annealing etched down the pyramids from the top apex, forming a c-plane surface. As-formed rough c-plane can be flattened by InGaN regrowth, showing single-bilayer steps. The InGaN platelets show narrow room temperature photoluminescence peaks with linewidths of 107 meV for In0.09Ga0.91N and 151 meV for In0.18Ga0.82N. Single InGaN QW, emitting green and red light, can be grown on such InGaN platelets with sharp interfaces. Prototype LEDs were demonstrated with the green on In0.09Ga0.91N platelets and the red on In0.18Ga0.82N platelets.

# XPS/HAXPES analysis of biofunctional strata prepared by titanate assisted organosilanization

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Titanate assisted organosilanization (TAO) is a technique for surface functionalization that is gaining relevance due to both, the different types of substrates it can functionalize and the alternative functional groups that can be integrated on the surface. In this work, we have carried out an X-Ray photoelectron spectroscopy (XPS) and hard X-ray photoelectron spectroscopy (HAXPES) characterization of a set of surfaces produced by TAO. XPS has been used for the inspection of films of octyl-silane (OCTS) and mercaptopropyl-silane (MPS) with respect to a titanate control film (TIPT). In spite of the smaller concentration of the silanes with respect to the condensing titanate in the sol ([Ti]/[Si]= 40), it has been observed that, upon condensation, the organosilane migrates to the surface reverting considerably the molar concentration on the surface. An additional organosilane (perfluorodecyl silane, PFDS) was probed by HAXPES. The results for this silane show that the concentration of organic species increases with respect to the Ti signal as the excitation energy of the X-ray beam is reduced (reduced probed depth). This trend is accompanied by an increase of F concentration with respect to that of Si (for reduced X-ray beam energy). Not only the relative stoichiometry of the elements suggests an organization of the organosilane towards the surface of the film, but also the relative components of core level peaks of specific elements. Selective cell adhesion, DNA immobilization and virus like particle organization have been achieved by this straightforward method.

# Ultra-thin films of In on Pd(111) characterized by X-ray photoelectron diffraction

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Metallic surfaces involving transition metals are widely used in the preparation of catalysts. The conversion rates and the selectivity can be improved, in many instances, by a surface alloy formed by a transition metal with a less reactive sp metal. Bimetallic systems based on Pd-In have been shown to be efficient catalysts for nitrate reduction in water. The catalytic reaction depends on both the electronic structure and the geometric arrangement of the surface alloy atoms. Even though In is barely miscible with Pd in the bulk, it forms ordered surface alloy phases. Recently a similar system was studied by our group, ultra-thin films of Sn deposited on Pd(111), and we observed the formation of a corrugated bi-dimensional Pd2Sn surface alloy. In the present study, we have investigated the growth and the surface alloy formation of a ultra-thin film of In deposited on a Pd(111) single-crystal substrate surface. The electronic structure and the surface structure have been determined by a combination of low energy electron diffraction (LEED) and X-ray photoelectron diffraction (XPD).

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# Design and Fabrication of GeSn/SiGeSn Multiple Quantum Well Laser

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GeSn has been proven to exhibit a direct bandgap for Sn concentration larger than 8.5%. The successful deposition of GeSn alloys with Sn concentration far beyond the solid solubility level of about 1% Sn in Ge is achieved by reactive gas source epitaxy at low temperatures. Optical pumped lasing was observed from this material. Recently high temperature operation was achieved by increasing the Sn concentration beyond 16%, which is explained by the increase of the energy splitting between the Gamma and the L-valley, the so called directness of the bandgap. Employing GeSn/SiGeSn multiple quantum well structures on relaxed GeSn buffer layers the threshold currents could be significantly reduced to 40kA/cm2, which is attributed to a lower defect density inside the optically active material. Optically pumped Fabry-Perot as well as microdisc laser could be demonstrated using this technology. However, at high Sn concentrations, required for room temperature operation, the material is vulnerable making device fabrication technology for electrical pumped laser challenging. In this paper we will discuss the impact of tensile strain on the band structure GeSn alloys. Tensile strain will reduce the bandgap and at the same time increase the directness of the bandgap. Furthermore tensile strained GeSn layers are expected to be beneficial for the optical gain. It is argued that GeSn alloys with a Sn concentration of 10% combined with an applied tensile strain in the range of 1% is a suitable pathway towards electrical pumped laser operating at room temperature.

## Vacuum Technology in Nuclear Fusion – Review and Current Trends

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Vacuum technology is of paramount importance for the design and operation of nuclear fusion devices. Since the start of the first tokamak and stellarator machines in the 60s, vacuum requirements in the harsh fusion environment turned out be design driving. One has to know that, contrary to the accelerator community, where there is a quest for lowest pressures, the pressure requirements in fusion (during the plasma pulse) are relatively moderate (1 Pa range). The pumping speed challenge in fusion, in particular for the larger devices, is not driven by low pressures but comes from the high throughput needed to compensate for the low burn-up of the injected deuterium-tritium fuel.

The first lab-scale machines triggered the development of high throughput turbomolecular pumps. With increasing size, pumping speed requirements became larger and larger. Nowadays, most medium-size fusion devices are equipped with cryogenic pumps. A highlight of this technology is ITER, where the use of tritium poses additional requirements on the vacuum system design.

The next step after ITER, then producing its own tritium and providing electricity to the grid, will be a demonstration fusion power plant (DEMO), the pre-conceptual design of which is under elaboration in different places on the world. On DEMO scale, accumulation pumps would build up excessive tritium inventories which imply regulatory issues. This is why a R&D programme has been launched in Europe to develop alternative pump technology.

The paper will introduce in how the requirements and challenges have evolved over the last five decades of nuclear fusion vacuum technology. Examples will be given for turbomolecular and cryogenic pumps. The DEMO development programme which looks into tritium-compatible mercury driven diffusion and liquid ring pumps as well as high capacity getter pumps will be reviewed and recent highlights be presented.

# Nanobeam X-ray fluorescence investigation on in situ Zn-doped nanowires reveals gradients and background doping

Andrea Troian<sup>1</sup>, Gaute Otnes<sup>2</sup>, Xulu Zeng<sup>2</sup>, Lert Chayanun<sup>1</sup>, Vilgailė Dagytė<sup>2</sup>, Susanna Hammarberg<sup>1</sup>, Rainer Timm<sup>1</sup>, Daniel Salomon<sup>3</sup>, Anders Mikkelsen<sup>1</sup>, Magnus Borgström<sup>2</sup>, Jesper Wallentin<sup>1</sup>

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Controlled doping is essential for functionalization of III-V nanowire (NW) devices. However, doping evaluation in nanostructures is challenging, requiring high resolution and detection limits and possibly minimal sample preparation.

Here we demonstrate a quantitative evaluation of Zn doping profiles of in situ doped III-V NWs, based on X-ray fluorescence with a nanofocused synchrotron beam, with a 50 nm lateral resolution and around 7 ppm detection limit.

Three distinct batches of III-V NWs were grown via metal organic vapor phase epitaxy, with in situ Zn doping via diethylzinc (DEZn). After transferring the NWs from the growth substrate to a Si3N4 wafer, the samples were scanned under the beam.

We found that Zn concentration in a GaInP NW grown under a constant flux of DEZn is in direct correlation with the Ga concentration.

We then studied InP NWs used as template for solar cells, with a p-i-n axial structure, observing an unexpected non-intentional Zn doping in the nominally undoped middle segment.

Finally, we studied the switching dynamics of Zn during growth in a multi-segment InP NW, with an axial sequence of nonintentionally doped alternated by increasingly p-doped sections.

After switching on the DEZn source, Zn concentration in the p-doped segments increases slowly, whereas Zn concentration decreased relatively abruptly after switching off the DEZn source.

The results showed complex dopant incorporation mechanism during in situ NWs doping. Moreover, the methodology presented here can be adapted for quantitative mapping of a wide variety of dopants in many types of nanostructures.

#### Thermal evaporation of black phosphorus onto (111) terminated bismuth

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Two-dimensional (2D) materials have a very wide range of interesting and unique properties, which can not be realised in bulk form. Therefore, 2D materials have the potential to become key players in the fields of energy, electronics and catalysis, to name but a few. Recently, there has been an increased effort to synthesise and study new 2D materials. One such material is phosphorus, which can form several allotropes with different properties. In terms of surface science, a new allotrope has been observed in ultra-thin form when black phosphorus was evaporated on Au(111) [1]. In this work, phosphorus has been grown on cleaved Bi(111) by thermal evaporation of black phosphorus. The analysis is performed by the combination of in-situ low-energy electron diffraction (LEED), low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) techniques. Initial analysis of the atomic structure indicates the synthesis of a new phase of phosphorus. The underlying substrate dictates the crystal structure of this phosphorus allotrope. Although intercalation of phosphorus below the bismuth termination is not ruled out.

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#### Perfect Patterning of Atomic Silicon Computational Elements

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Atomic circuitry composed of silicon surface dangling bonds has the potential to address the shortcomings of CMOS – power density and speed – and as well to enable powerful new devices not achievable with conventional transistor based circuitry.

It will be shown that paired atoms form a double well potential occupied by one electron. This serves as an ideal bit. Such a bit can be biased to yield a preferred occupation of one side or the other of the double well, thereby spatially mapping binary 0 and 1 states. Larger ensembles create "binary wires" and logic gates. Together, these enable ultra-low power, ultra-fast "Binary Atomic Silicon Logic", Nature Electronics 1, 636 (2018).

Ensembles of coupled and thermally driven multi-electron-state atom-defined entities also enable a new kind of device: an atomic embodiment of an Ising model Hamiltonian. This can be viewed as a simulator from which the particular state of the system read out as a binary string. By repeatedly reading the state (the electron position in each atom pair) we can trivially collect a "Gibbs sample" – that is – the fluctuations in energy of this "machine" as it experiences thermal buffeting by the environment. Phys.Rev. Lett, 121, 166801 (2018). Effective hardware-derived Gibbs sampling has the potential to obviate expensive Markov Chain Monte Carlo approximations to Gibbs sampling and thereby enable the next wave of machine learning.

Machine learning-based automated processes for repair of the scanning probe and for truly perfect atomic circuit patterning will be described.

# Virtual substrate method for nanomaterials characterization

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Surface analysis techniques such as x-ray photoelectron spectroscopy (XPS), and Auger electron spectroscopy (AES) are nowadays intensively employed to study substrate-supported nanomaterial. However, target nanomaterial information is always diluted by signals originating from underlying substrate by these techniques even in a low-energy electron operation mode. Here, we develop a new method, named virtual substrate method [Nature Commun. 8 (2017) 15629], to extract pure electron-electron (e-e) interaction information of target nanomaterial with an extremely high efficiency because of employment white-beam technique in this method (Fig. 1). Based on this new method, we can identify and drive part of SEs excited in substrate as "white-beam electrons" to probe the e-e interaction information of supported nanostructured material. Precisely because of using common SEs as information carrier instead of core-level electrons, this new method can work in very low energy range, even down to several electron volt. We believe that this new method will be a new benchmark method to study substrate-supported nanomaterials. Furthermore, characterizing materials with ordinary SE signals instead of core-level signals increases the signal-to-noise ratio by several orders of magnitude, which has great value for manufacture and quality control.

# scanning kelvin-probe study of photo-induced charge transfer in organic nano-crystalline donor-acceptor heterojunctions

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Organic solar materials are of great interest due to their cheap and easy production, possibility for thin film formation, and tunable visible spectrum. The perylene-diimine (PDI) – copper pthalocyanine (CuPc) pair shows promise due to stability, robust mechanical properties, and favorable spectral characteristics. The tendency of PDIs to aggregate has hampered the search for optimal geometries for charge generation and collection. In this work, we studied and compared the charge generation, transport, and recombination in these donor-acceptor pairs using Scanning Kelvin Probe Microscopy (SKPM). These microscopic results are supported by theoretical calculations, and spectroscopic and time-resolved fluorescence studies. Three different PDI derivative were tested and measurements revealed the charge distributions both in the dark, and under light. Two illumination types were used: the CuPc only was excited using a red laser, or LED illumination was employed to excite both species. Varying the preparation methods allowed changing the geometry of the interface to include PDI nanocrystals lying on a CuPc film (type 1), PDI nanocrystals decorated by CuPc leaflets (type 2), as well as a junction between two films as prepared by plasma vapor deposition (type 3). The type 1 interface gave the highest achieved by choice of the particular PDI derivative used. The dependence of the energetics on morphology and molecular structure will be discussed, as well as recommendations for optimizing photovoltaic performance.

# Plasmonic Au/Au-Pd nanoparticles on TiO2(110) : coupled optical and structural in situ characterization during growth

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Recent experiments showed an important increase of the catalytic activity for chemically synthesized gold or gold alloyed nanoparticles under visible light (VIS) exposition. Such phenomenon, attributed to surface plasmon resonance modes localized on nanoparticles (LSPR), is extremely relevant in the context of energy-efficient processes using solar light, in order to transform VIS into chemical energy via photocatalytic reactions.

Combination of gold, known for its LSPR, with palladium, characterized by important catalytic properties, is very promising, but very little is known about plasmonic properties of Au-Pd nanoparticles (NP). A deep comprehension at the nano/atomic level is a key step in order to allow large scale development of plasmon assisted photocatalysis.

In the aim of exploring the link between plasmonic properties and structure of the NPs, our approach consists in studying model systems, namely Au and AuxPd1-x nanoclusters deposited by molecular beam epitaxy (MBE) onto TiO2(110). For the first time, we succeeded in performing in situ coupled measurements of the morpho-structural and optical properties during the growth of few nanometers sized bimetallic nanoparticles. Experiments were done at SOLEIL synchrotron (France) by means of Grazing Incidence Small Angle X-ray Scattering, providing size, shape and inter-particle distance, Grazing Incidence X-ray Diffraction for crystallographic properties and UV-Vis Surface Differential Reflectivity Spectroscopy for optical plasmonic response.

We will discuss the original results obtained during the Au NP growth concerning the influence of the substrate and of NP size on the plasmonic response. We will then consider the influence of Pd adding, both in sequential and co-deposition.

# Potential dependent in situ Surface Resonant X-Ray Diffraction of Pt(111) electrolyte interface

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Platinum is widely used in electrocatalysis, particularly as catalyst of low-temperature fuel cells and water electrolyzer. Competitive adsorption of anions hindering the kinetics of the processes involved in these applications still needs to be fully understood. In this context, Pt(111) is a particularly interesting model surface. Although this system has been extensively studied, the description of adsorbed sulfates in acidic media as a function of the applied potential and of the related charge exchange is still controversial.

Aiming to specifically investigate the valence state of the surface Pt atoms and the structure of the ordered adsorbed species, we have performed in situ Surface Resonant X-Ray Diffraction (SRXRD) and Surface X-Ray Diffraction (SXRD) experiments on Pt (111) in 0.1MH2SO4. The unique sensitivity of SRXRD, merging diffraction and x-ray absorption spectroscopy into a single experiment, provides site selected information about electronic density. We made experiments in i) in the (0.4-0.6VRHE) interval, also called "unusual state", associated to (hydrogeno)-sulfate) desorption/adsorption, whose description remains controversial and ii) in the oxidation potential region above +0.8VRHE.

We present the polarization dependent SRXRD spectra recorded across the Pt LIII edge using our home-made "thin-layer" electrochemical cell well suited for in situ diffraction experiments, allowing and polarization scans for the decoupling of contributions in the two directions.

For the interpretation of SRXRD experimental data, we use FDMNES software recently extended to the simulation of surface diffraction experiments. FDMNES permits for the first time the simulation of both resonant spectra (SRXRD) and diffraction truncation rods (SXRD).

# Deprotonation process of biphenyl dicarboxylic on Ag(100)

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Molecular self-assembly of organic molecules on metal surfaces typically leads to a formation of regular molecular networks. Stability and structure of these molecular phases is usually governed by equilibrium between molecule-substrate and intermolecular interactions. These interactions can be, however, rapidly modified by molecular deprotonation induced by thermal annealing of the substrate, which results in a molecular phase transformation and formation of new stable or metastable molecular structures.

In this presentation we describe thermally induced deprotonation process of 4,4' biphenyl dicarboxylic acid (BDA) molecules on Ag (100) surface accompanied by presence of three subsequent phase transitions and four different and stable molecular phases (alpha, beta, gamma and delta) which correspond to a different ratio of protonated / partially protonated / deprotonated BDA molecules. Whereas Low Energy Electron Microscopy (LEEM) allowed us to characterize molecular islands on the large scale, molecular dynamics during phase transitions, diffraction patterns from individual islands and dark field imaging, Scanning Tunneling Microscopy (STM) was subsequently used for the molecular structure characterization on the atomic scale level. Moreover, the combination of LEEM and STM techniques allowed us to observe molecular phases which are stable only in a very narrow temperature interval.

# Doping of GaAsP nanowires grown by aerotaxy

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Nanowire (NW) Photovoltaics are a promising route for low-cost multi-bandgap tandem cells, which is taxing in terms of processing and lattice matching in traditional planar geometries.[1] III-V nanowires are more suitable for monolithic integration as they can assimilate the lattice mismatch to a larger extent.[2] GaAsP is a material that offers a wide tunability of the band gap from near infrared (Eg = 1.42 eV) to visible regions (Eg = 2.3 eV) and is one of the best-suited materials for growth on silicon.[3]

Controlled synthesis of GaAs(1-x)P(x) NWs with a bandgap ranging from 1.42 to 1.90 eV (at 300K) through the scalable Aerotaxy [4] technique has already been reported.[5]

The present work concerns doping of GaAsP NWs by controlling precursor (DEZn) flows during growth by Aerotaxy. Here we present structural, optical and electrical studies of doped GaAs(1-x)P(x) NWs by high-resolution TEM, Photoluminescence, 4-point probe and Hall measurements.

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# TiB2 coatings deposited via high power impulse magnetron sputtering

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Titanium diboride (TiB2) is a versatile high potential material for thin film applications due to its high strength, melting point and conductivity. It crystallizes in the hexagonal AlB2 type structure, where close-packed Ti layers are interleaved by B atoms, which are arranged in a honeycomb pattern. The crystal orientation of TiB2 coatings is essential for the film properties, including hardness. Indeed, the highest hardness values (H > 40 GPa) are reported for (001)-textured films and therefore such orientation is highly desired. There are several studies of magnetron sputtered TiB2 coatings in the literature. Depositions are generally performed using TiB2 compound targets and often result in overstoichiometric coatings, i.e. B/Ti > 2. Coating microstructure and hence properties are heavily influenced by the sputtering parameters. This study is devoted to deposit stoichiometric boride layers and to investigate the influence of HiPIMS frequency, substrate temperature and bias on the resulting microstructure and mechanical properties.

# Accurate many-electron description of ZrO2 polymorphs

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Zirconia (ZrO2) has been investigated in numerous experimental studies due to its technological importance for applications including sensor materials or fuel cell components. Yet an accurate theoretical description of the three most stable polymorphs (cubic, tetragonal and monoclinic) remains challenging: While most density functional theory (DFT) based approaches, including standard GGA functionals (PBE) or hybrid functionals (HSE), tend to capture the correct energetic order, the actual energetic differences are very sensitive with respect to the chosen functional. In addition, several functionals severely overestimate the stability of various metastable phases. In this presentation, I will show that many-electron (RPA) calculations [1,2] using the Vienna Ab-Initio Simulation Package (VASP) offer a highly accurate description of the ground state properties, allowing to resolve this disambiguity. In addition we find that the predicted values for the bulk modulus are in excellent agreement with the experimental data.

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## Buckling of graphene by the intercalation of Co

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The intercalation of cobalt between graphene and Ir(111) results in a highly corrugated network of strongly and weakly bound carbon[1]. Utilising the normal incidence X-ray standing wave method and the two distinct chemical-state resolved C 1s photoemission components[2], we have demonstrated that the strongly bound carbon atoms adsorb with a mean adsorption height, above the Co layer, of  $2.06 \pm 0.03$  Å, almost three quarters of an angstrom lower than the mean adsorption height of the weakly bound carbon atoms ( $2.76 \pm 0.05$  Å). Density functional theory calculations using DFT-D2 and vdW-DF dispersion force corrections predict a subtly, but significantly different, corrugation structure of the intercalated graphene, with the DFT-D2 calculations result in a structural model that more closely matches the experimental results, with the vdW-DF calculations predicting a mean adsorption height that is 0.10 and 0.37 Å closer to the Co intercalant than is measured experimentally. Despite this difference, both functionals predict a covalent like interaction between the Co and the C, resulting in a weak neighbour-to-neighbour buckling, in addition to the long range corrugation, of the graphene layer.

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## Imaging hot electron dynamics in single semiconductor nanowires

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The ability to harvest the excess energy of photoexcited 'hot' carriers before it is dissipated would be highly beneficial for applications such as catalysis and light harvesting. III-V semiconductor nanowires are promising building blocks for hot carrier photovoltaic devices. However, to design optimal structures, the relaxation and diffusion dynamics of hot carriers need to be understood down to femtosecond (fs) time and nanometer (nm) length scales. Here, we investigate the ultrafast hot carrier dynamics in single indium arsenide nanowires with 20fs/50nm spatiotemporal resolution by combining photoemission electron microscopy with optical pump probe techniques. We find that by tuning the intensities of the pump and probe laser beams we can track the evolution of the initial non-equilibrium hot carrier distribution in a single nanowire during the first few picoseconds after photo-excitation. We interpret the observed signals as signatures of different electron relaxation processes (electron-electron followed by electron-phonon scattering). Further, we observe differences in the dynamics between ordered segments in the nanowires with different (wurtzite and zincblende) crystal structures. This work establishes time resolved photoemission electron microscopy as a tool to follow hot electron relaxation in semiconductor nanostructures with high spatiotemporal resolution. The technique should be applicable to a wide range of semiconductor or metal nanostructures in which hot electron dynamics are important.

## sustainable glasses for luminescent solar concentrator applications

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Luminescent solar concentrators (LSC) appear as a new technology that promises to achieve the goal of transforming conventional energy-passive glazing systems into semi-transparent photovoltaic (PV) windows 1. LSC consist in a material doped with a fluorophore that down-converts solar light through luminescence which is waveguide-propagated to the window edges where it may be converted into electricity by PV devices 2.

Towards this goal, environmental-friendly transparent glasses with high photoluminescence yield and high Stokes shifts have received special attention due to their stability and luminescent optical properties 3. In this work aluminoborosilicate glass is used as matrix for luminescent centers such as copper, tin and manganese. The glasses were tested with organic PV solar cells under a simulated sunlight irradiation where the geometrical factor of the samples was considered. In all cases it was verified an increase of the open-circuit voltage (Voc) and short-circuit current density (Jsc) coupled with an increase of efficiency compared with the blank (without glass). These glasses were also tested with mirrors in the edges to increase the interior reflection.

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# Synchrotron X-ray studies of the onset of galvanic corrosion in steel by controlling the electrochemical potential

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Because of its economic impact, corrosion of metallic alloys like steel has been studied in various aqueous environments (seawater, rain, surface- or ground water, etc.) for decades [1-2]. An estimated 3% of the world's GDP is lost due to corrosion [3]. For stainless steel (SS), corrosion can be strongly enhanced locally, at atomic level, leading to pitting, responsible for structural weakening and subsequent failure [4]. Our main aim is to understand the very early stages of pitting of steel alloys at the nanometer level. Ultra-thin films of two different types (304L and 316) of SS have been deposited (at UGC-DAE CSR, Indore, India) on silicon and multilayer substrates using DC magnetron sputtering [5] to investigate early stages of corrosion, using bulk steel foils as references. Synchrotron based X-ray techniques (X-ray fluorescence and absorption spectroscopy, X-ray standing wave, etc.), applied ex situ and in situ, are complemented by electrochemical characterisation on the corrosion of SS in 0.1 M KCI and H2SO4 [6]. First results regarding the onset of galvanic corrosion will be discussed.

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# Kinetics of deprotonation induced phase transition of self-assembled 4,4'-biphenyl dicarboxylic acid on Ag(001) surfaces

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Carboxylation (or deprotonation) of carboxylic groups on surfaces is one of basic reaction steps leading to phase transitions and formation of new molecular surface phases. In this contribution we describe the kinetics deprotonation induced irreversible phase transitions of 4,4'-biphenyl dicarboxylic acid on Ag(001) surface. The real-time view by low energy electron microscopy (LEEM) complemented with low energy electron diffraction (LEED), STM, non-contact AFM and XPS, supported by DFT and kinetics Monte Carlo simulations provides new insights on the deprotonation reaction. In this way we were able to reveal and describe intermediate phases and describe how these phases are transformed in the subsequent ones. We point out to significant role of surface step-edges on this process and nucleation limiting kinetics.

# Ferroelectricity in dopant-free hafnium oxide using plasma enhanced atomic layer deposition

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The well-established method for improving transistor device performance by scaling device dimensions is challenging for future generations. Power dissipation in electronics is a big concern and new approaches are required in order to obtain low power consumption. A promising approach is the integration of ferroelectric materials in the gate electrode, enabling a negative capacitance effect, which allows a subthreshold slope below the Boltzmann limit of 60 mV/decade and thus making possible a substantial reduction in drive voltage and power consumption.

In this work, we present for the first time ferroelectric characteristics in crystallized hafnium oxide thin films grown using plasma enhanced atomic layer deposition. The films are characterized by x-ray diffraction, atom force microscopy and by pulsed electrical measurements after integration into a titanium nitride metal-insulator-metal (MIM) device. The presence of ferroelectricity has been confirmed with values of the remanent polarization of 5  $\mu$ C/cm2 for 10 nm thick films with a dielectric constant of 30. We further evaluate the effect of film thickness, varied oxygen vacancy concentration controlled by the O2 plasma conditions, and post-deposition annealing temperature on the ferroelectric properties.

Dopant-free ferroelectric hafnium oxide is ideally suited for industrial scale production due to its excellent compatibility to already existing manufacturing methods in silicon technology. Not only for low-power negative capacitance field effect transistors but also for non-volatile memory such as ferroelectric field effect transistors, ferroelectric random-access memory, and neuromorphic applications.

## STM and Photoemission Studies of Ag films on In/Si(111)-root3xroot3

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Over the past decades, a large number of studies have been devoted to metal thin films on metal substrates, though the observations of quantum-well states (QWS) have been restricted to a few systems. In recent years several studies have reported thin metal films grown on clean Ge or Si surfaces at reduced sample temperature [1]. These films show an energy quantization effect in their valence band states. Inspired by these findings, we have investigated the electronic structure of Ag films on the In/Si (111)-root3xroot3 surface by scanning tunneling microscopy and ultraviolet photoelectron spectroscopy.

Ag were deposited on In/Si(111)-root3xroot3 at RT. At the initial stage, the silver atoms bind to the topmost In and Si atoms and form short line structures. The first layer of Ag grows in atomic rows with three-fold symmetry. These rows are oriented 30° with respect to the root3xroot3 surface unit cell directions and thus follow the 1x1 direction of the underlying Si(111) substrate. The electronic structure of the valence band was also studied with a photon energy of 21.2 eV for different thin Ag films at RT. We find that the very first QWS shows up at a Ag coverage of 2 monolayer. The fine coupling features between the QWS and the Si bulk bands will also be discussed.

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## Structural studies of short period superlattices grown by molecular beam epitaxy

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Wide band gap MgxZn1-xO semiconductor alloys offer the possibility of tuning the band gap by changing the Zn/Mg ratio. This alloy is expected to display an enhanced UV or blue light emission which is very important for light emitting devices. However MgxZn1-xO alloys have tendency to form metastable phases due to different ZnO and MgO crystallographic structures. One possibility to overcome this drawback is the growth of pure multilayers in a superlattice (SL) structure Furthermore in ZnO/MgO SL structures it would be possible to manipulate the layer thicknesses to avoid metastability and get the whole SL in the wurtzite structure. One of the advantages of SLs is that their band gap can be tuned by the thicknesses of the constituent binary layers allowing modulation of the band gap energy.

In the present work SL structures with 30 - 80 pairs of ZnO/MgO thin layers were grown by molecular beam epitaxy (MBE). The crystalline quality was studied by high resolution X-ray diffraction and ion beam channelling. The minimum yield below 3% clearly shows an excellent crystalline quality for multilayers with periods below 2 nm. Reciprocal space maps and detailed angular scans across off-normal axis were measured to determine strain distribution in the structures. The multilayer structure of the superlattices was confirmed by high resolution transmission electron microscopy excluding the possibility to mix or alloy the two oxides during the growth. The structural results will be discussed and correlated with preliminary results of the optical properties of the SL.

# Block Copolymer Mask for 50 nm Pitch Pattern Transfer into Silicon Nitride

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Block copolymer (BCP) lithography can provide highly dense patterns at low cost. As dense patterning can be critical to achieve functionalities often required in high technology devices, such as high sensitivity biosensors or bit-patterned media, research on BCPs as masks in plasma processes is expected to be of use in both academia and industry. This work has studied the use of spin-coated Polystyrene-block-Poly-4-Vinylpyridine (PS-b-P4VP, Mn=50.0-b-17.0 · 103 g/mol, Mw/Mn=1.15, Polymer Source Inc.) as an etch mask to transfer the resulting 50 nm pitch hexagonal pattern of cylinders into a Silicon Nitride layer. By utilizing surface reconstruction in a preferential solvent for the P4VP cylinders, pores were opened in the BCP layer. The lateral size of these pores could be controlled by the temperature of the solvent, in the span 19 to 70°C. The BCP pattern was exerted to a gentle oxygen plasma in a reactive ion etching system with inductively coupled plasma (ICP-RIE), to remove residual polymer at the bottom of the structures. The BCP pattern was thereafter used as an etch mask in ICP-RIE to transfer the pattern into Silicon Nitride using Nitrogen and Trifluoromethane (80:20 sccm) plasma, at 10 mbar with 14 W radio frequency and 270 W ICP, with an etch selectivity of 5.7 of Silicon Nitride to PS-b-P4VP blanket films. As PS-b-P4VP is a so-called high-Chi material, there are also possibilities to scale down the pattern, simply by utilizing BCP with smaller molecular weights, enabling an even denser pattern for high performance device functionalities.

## Theoretical Design of Organic Semiconductors based on First-Principles Charge Transport Calculations

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Organic semiconductors have attracted much attention for the applications to flexible, lightweight, and low-cost electronic devices. For development of high performance organic semiconductors, detailed analyses of transport properties at the atomistic levels are important. Transport properties are sensitive to molecular orbitals, structures, orientations, and thermal fluctuations in the crystal. [1-3] We have developed a first-principles method for calculating charge transport in organic semiconductors based on density functional theory. [4] The time evolution of wave packets of carriers is calculated, and mobility, mean free path and the relaxation time of carriers are analyzed by considering the effects of electron–phonon scattering and the thermal fluctuation of molecular vibration. An order-N calculation has been successful and the transport calculations for 100 million atoms can be performed. We demonstrate that our calculations show good agreement with experimental results for various molecular systems, and show our theoretical design scheme using the method.

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# COHERENT DIFFRACTION FOR A LOOK INSIDE NANOSTRUCTURES: CATALYSIS AND INTERFACE

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Characterising the structural properties (strain gradients, chemical composition, crystal orientation and defects) inside nanostructures is a grand challenge in materials science. Bragg coherent diffraction imaging (Bragg CDI) can be utilised to address this challenge for crystalline nanostructures. A resolution of the structural properties of less than 10 nm is achieved up-todate [1]. The capabilities of the Bragg CDI technique will be demonstrated on single nanoparticles for enhanced catalysis.

As an example, the Bragg CDI technique allows understanding the interplay between shape, size, strain, faceting [2], composition and defects at the nanoscale. We will demonstrate that Bragg CDI on a single particle model catalyst makes it possible to map its local strain/defect field and directly images strain build-up close to the facets. The localised strain modifies sorption energies of the reactants. In situ [3,4] and operando Bragg CDI was also performed: it was possible to track a single particle in liquid and gas phase environments, to monitor its facet changes and to measure its strain response to gas or electrochemical reaction.

This technique opens pathways to determine and control the internal structure of nanoparticles to tune and optimise them during catalytic and other chemical reactions.

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# Low Temperature Scanning Tunneling Microscopy and Spectroscopy of Semiconductor Nanowire Device Surfaces

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III-V semiconductor nanowires (NWs) show considerable promise as components in efficient and fast electronics as well as for quantum computing. In particular, the surfaces of the NWs play a significant role in their function due to the large surface to bulk ratio. Further, as the incorporation and activation of the nanowires in a device can affect their structure, it is relevant to study the surface structure and its influence on electronic properties in devices and during operation.

We use atomically resolved Scanning Tunneling Microscopy/Spectroscopy (STM/S) to study InAs and GaAs NWs in planar device configurations. We use atomic hydrogen cleaning at 400C to obtain well-defined surfaces that can be scanned with STM while the complete device is still fully functioning[1]. We study both NWs grown directly in a planar configuration as well as wires harvested from a growth substrate and placed on top of predefined metal contacts with ~100nm precision using a micro/nano probe. In our new <10K closed-cycle STM we can identify the individual device NWs simultaneously as we can apply voltages across the devices using four additional contacts in the STM. We initially investigate NW geometric structure and morphology with high precision. Then we continue to perform low temperature STS to investigate electronic structure and potential quantum confinement effects as well as the influence of defects. These measurements can be performed while external biases are applied to the device and the I(V) characteristic across the NW is obtained.

[1] Webb, J., et al, Nature Scientific Reports, 7(2017)12790.

# High quality GaN templates by coalescence overgrowth of GaN nanowires by MOCVD

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GaN has recently gained renewed scientific attention as one of the most promising wide-bandgap semiconductor materials for high-frequency power devices [1]. Due to the difficulty to produce GaN crystals from the melt and the high cost of GaN bulk substrates, the heteroepitaxy approach has been widely used for fabrication of GaN-based electronic and optolectronic devices [2, 3]. The crystal quality of heteroepitaxial GaN layers is strongly influenced by the lattice and thermal mismatches with the substrate, resulting in strain and structural defects which limit the device performance. To solve these issues, homoepitaxy seems to be the best approach enabling the reduction of the dislocation density in the GaN layers and providing enough crystalline quality to improve the production of vertical electronic power devices. An alternative to the use of GaN bulk substrates is to obtain high-quality coalescence overgrowth templates from a patterned-grown GaN nanowires (NWs). Previous studies have demonstrated that the quality of the coalesced layer is directly related to the regularity and the quality of the NW array [4].

In this work, we study the dependence of the NW reformation and coalescence experimental growth conditions on the quality and morphology of a subsequent 2-µm thick GaN layer grown by Metal Organic Chemical Deposition (MOCVD). For that, different annealing conditions together with different nucleation temperatures and V/III ratios have been investigated in terms of effects on the properties of the subsequent GaN film. The structural quality of the homoepitaxial GaN films has been evaluated by high-resolution X-ray diffraction, revealing a dislocation density in the order of 2x107 cm-2. Morphological studies performed with Atomic Force Microscopy (AFM) over an area of 10x10 µm2 have shown smooth surfaces with the rms values between 0.12-0.15 nm. Atomically step-liked surface area where no spiral steps have been observed suggests that the growth took place following the step-flow mode. The sample with the smoothest surface had the lowest screw dislocation density, the lowest value of strain along the c-axis and the highest transmittance. The thermal conductivity measurements performed by time-domain thermoreflectance (TDTR) revealed that the smoothest sample exhibits an out-of-plane thermal conductivity of k= 206 W/mK, approaching the bulk value. This improvement in the quality of the GaN layers arises from the optimization of the reformation process where different annealing and nucleation conditions have been employed. In that regard, we conclude that annealing at an optimized temperature in presence of ammonia followed by a nucleation under high V/III ratio lead to the best properties among all compared samples.

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#### Protective graphene single-layer grown on epitaxial FeRh thin films

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Epitaxial FeRh thin films are magnetic materials which feature a first-order antiferromagnetic (AF) to ferromagnetic (FM) phase transition present around 360 K. FeRh is a highly tunable material [1] where the phase transition can be controlled by different stimuli: temperature, magnetic field, strain, electrical current and optical pulses. To ensure stability of such a material under air conditions, capping layers like metallic (Pt, Au) or insulating (Al2O3) ones have ben generally used. We report on an alternative way of such a protection using a graphene layer formed in situ by the simple thermal annealing of a magnetically active epitaxial FeRh thin film prepared by magnetron sputtering. The quality of the graphene layer was characterised using X-ray Photoemission and X-ray Absorption Spectroscopy (Synchrotron Soleil), and Low Energy Ion Scattering, Scanning Tunneling Microscopy, and Low-Energy Electron Microscopy (complex UHV system at CEITEC). It has proved that graphene is polycrystalline and covers at least 97% of the FeRh (001) surface. Two preferential orientations of graphene domains mutually rotated by 30° has been identified. We will propose the mechanism of formation of graphene on the FeRh (001) surface and show that the graphene layer is capable of protecting the film from oxidation when exposed to air for several weeks, which enables production of functional devices based on stacking of 2D materials on tunable magnetic surfaces.

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[1] S. Maat, J.-U. Thiele, and E. E. Fullerton, Temperature and field hysteresis of the antiferromagnetic-to-ferromagnetic phase transition in epitaxial FeRh films, Phys. Rev. B 72,214432 (2005).

# Crystal Phase Selective Bi Incorporation in GaAs Nanowires

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Bi incorporation and alloying in III-V semiconductors such as InAsBi and GaAsBi have become a popular topic during recent years, due to a number of promising properties including band gap engineering, a large spin-orbit splitting, and predicted band inversion and topological behavior in the case of high Bi concentrations [1]. However, the realization of allows with high Bi content by epitaxial growth has remained challenging.

We follow a different approach and deposit Bi onto GaAs nanowires (NWs) containing both zinc blende (Zb) and wurtzite (Wz) facets, allowing us to study the incorporation of Bi atoms in different surface facets by scanning tunneling microscopy and spectroscopy (STM/S). Our previous STM/S studies on GaAs:Sb NW surfaces showed a preferential incorporation of Sb into GaAs {110} surfaces of Zb segments compared to GaAs{11-20} surfaces of Wz segments [2].

Here, we present STM/S studies obtained at 5K on the effect of Bi deposition on the morphology and electronic properties of GaAs NWs. We observe that Bi tends to replace the As atoms in the GaAs NW surfaces, resulting in band gap reduction. We also find a crystal structure dependent surface alloying process, where ordered Bi layers and atomic chains are formed on Wz {11-20} facets, while randomly distributed single Bi sites are found on Zb {110} facets. Signs of a length-dependent confinement effect in the Bi-chains of the Wz {11-20} facets are observed via STS.

[1] Chuang et al., Nano Lett. 14, 2505 (2014)

[2] Hjort et al., Nano Lett. 17, 3634 (2017)

# Towards single molecule detection of unbound agents in molecular motor systems

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Molecular motor proteins which propel cytoskeletal filaments have found recent use in synthetic macroscopic environments performing tasks such as cargo transport, surface imaging, molecular biosensing or biocomputation (Nicolau et al, PNAS 113(10) 2016). Observation has so far exclusively relied on optical microscopy, requiring bulky additional instrumentation and limiting the overall area of observation, which impedes large-scale and high throughput applications. We aim for microscope-free monitoring of the actomyosin and kinesin-microtubule molecular motor systems in real-time, by implementing nanoscale checkpoints which detect closely passing filaments by capacitive gating of electrical transistors. This requires that the detectors are positioned directly inside the nanochannels that direct the propelled filaments. We have observed motility across many nanostructures situated this way such as: isolated carbon nanotubes, carbon nanotube networks, and nanoscale parylene surfaces. In operation, the travelling height of these propelled filaments is many times the Debye length of the surrounding electrolyte. We present architectural elements integrated into a guiding nanochannel which ensure close passing of the filament to the detector with minimal impedance to agent motility. Since the detection takes place without binding or unbinding events, the function of the molecular motor system is not altered. Such a detector can be monitored simultaneously with conventional optical microscopy of the checkpoint region and both signals correlated. Full realization this device could count passing filaments and measure their gliding velocity in real time, relevant for point-of-care medical diagnostics and large-scale biocomputation.

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# Charge Transport though Individual Graphene Nanoribbons

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Graphene is a zero-gap semiconductor and its band structure of low-energy  $\pi$ -state is characterized by electron–hole symmetry. High carrier mobility, high thermal conductivity, and ambipolar transfer characteristics make graphene attractive for many electronic applications. However, despite its outstanding properties, one of the hurdles for graphene to be useful as an electronic material is the lack of an electronic gap. One of the ways to open a gap in its electronic spectra is to reduce the width of the graphene. Recent advances in surface chemical reactions allows us to precisely prepare graphene with nanosized widths called graphene nanoribbons (GNRs). Despite the development of the synthetic method for GNRs, its transport property remains largely unexplored due to the lack of appropriate technology platform to make electronic contact with individual GNRs and measure its electric current. Here we present single-molecule transport study on GNRs using scanning tunneling microcopy-based break junction (STM-BJ) technique. The GNRs were prepared by surface assisted polymerization of halogenated acene derivatives on Au(111). STM-BJ measurements on individual GNRs revealed that single-molecule junctions correspond to dimmer and tetramer of the precursors. We demonstrate that the individual GNRs are highly conductive with the electronic conductance of 0.1 and 0.4 G0 (G0 = 2e2/h).

## Preliminary study to develop a compact sputtering source for Ti-Zr-V non-evaporable getter coating

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Non-Evaporable Getter (NEG) coating was originally developed at CERN to elevate vacuum properties of particle accelerator beam chambers. In order to meet increasing demands for the NEG coating to be applied in various vacuum systems where further reduction in vacuum pressure is required to improve their performance, we have started a study for the development of a compact magnetron-sputtering source that can deposit the NEG thin film on common vacuum chambers. This will be enabled by mounting the sputtering sources in the vacuum system as many as possible to coat the inner surfaces with NEG. As compared to the conventional NEG-coating method, the compact sputtering sources should have: 1) an individual magnetic circuit formed by permanent magnets (e.g. Sm-Co) instead of a long solenoid magnet, and 2) a Ti-Zr-V alloy target compatible with any structure (e.g. length and diameter) of the chambers to be coated. So far, we have succeeded in producing Ti-Zr-V ternary alloy that can be machined to any shape, and have tried a deposition with a prototype of the compact sputtering source by mounting it to a test chamber with a DN63 flange. We will present these preliminary results including the vacuum properties of the coated chambers after the NEG-coating activation, as well as the characterizations of the deposited NEG films by SEM for morphology analysis, by EDS for Ti-Zr-V composition, and by XRD for crystal structure of the film. The presentation also includes the design of the compact sputtering source and its possible further improvements.

# Growth of arc deposited TiAIN coatings studied in situ by high-energy x-ray scattering

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We use a state-of-the-art arc deposition system, designed for in-situ studies of the coating growth at industrial conditions [1], to study the effect of growth parameters on the nucleation and growth of TiAlN coatings. TiAlN coatings were grown on Si wafers to a total film thickness of ~800 nm at 4.3 Pa N2 pressure, using a Ti33Al67 alloy target and an evaporation current of 90 A. The growth was studied in situ by high-energy x-ray scattering at beamline P07, Petra III. 6 s long exposures were recorded every 16th second by a 2D detector. The first diffraction signal is obtained after 16 s of growth, corresponding to a film thickness of approximately 20 nm. Coatings grown with substrate bias VS = -30 V are dominated by a hexagonal TiAlN phase. Hexagonal and cubic phases nucleate simultaneously while the hexagonal phase is dominant already at 20 nm film thickness. Growth of the cubic phase is dominant at the initial stage of growth while a small amount of hexagonal phase also exists in the coating. For all coatings, the ratio between cubic and hexagonal phase remains approximately constant with deposition time, thus segregation occurs already at the initial growth stage.

[1] J.L. Schroeder et al., Rev. Sci. Instr. 86(9) (2015) 095113.

# Fabrication of RGB LEDs based on nanowire technology

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Achieving high efficiency in nitride LEDs outside of the standard blue and near UV spectral regions is very challenging due to the high density of crystal defects and the difficulty of growing high-quality InGaN layers having sufficiently high In-compositions that enable green and red emission. In this work, we demonstrate a method to fabricate LEDs based on a new kind of MOCVD-grown nanostructure reformed in-situ to develop smooth c-plane top facets. This approach combines the advantages of dislocation-free, high quality nanostructures with the growth of active layers on the c-plane and enables growth of In-rich quantum wells on relaxed, high-quality InGaN barrier layers for green and red light emission. This presentation focuses on the challenges and possibilities associated with fabrication and characterization of nanostructure-based LEDs. We will present the fabrication procedures, IV-characterization and light-emission in blue, green and red for arrays of nanostructures as well as for single sub-micron-sized light emitters. We believe that this concept has the potential to become an important technology for future high-performance nitride optoelectronics.

#### Evolutional selection of crystal orientations in obliquely deposited thin films

Susann Liedtke-Grüner<sup>1</sup>, Christoph Grüner<sup>1</sup>, Andriy Lotnyk<sup>1</sup>, Jürgen Gerlach<sup>1</sup>, Bernd Rauschenbach<sup>1</sup> <sup>1</sup> Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany Vertically deposited metal thin films often show a polycrystalline, columnar morphology. If the incident particles hit the substrate in an oblique manner, the columns will grow tilted into the direction of the particle source. At highly oblique incidence angles, the columns start to separate, forming isolated single-crystalline nano-needles, even at room temperature. An interplay of selfshadowing and growth competition leads to the formation of an overall biaxial texture. Aim of this presentation is to explore the mechanisms behind the formation of the single crystalline structures as well as the evolution to the final film texture. This is achieved by a detailed investigation of individual nanostructures as well as the complete thin film by TEM, electron, and X-ray diffraction techniques. The studies are carried out exemplarily for Ti and Mo thin films obliquely deposited by electron beam evaporation at room temperature. A model is presented, allowing to explain the morphology of the obliquely deposited thin metal films. Such highly porous thin films can serve as substrates for plasmonic sensing devices or can be utilized in catalysis, for instance. As purely vertical deposition is a rather idealized case, the presented effects may appear in the majority of deposition systems.

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## reflectance analysis of polyaniline-chitosan hydrogels

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The optical property of biomaterials is an important parameter to fabricate devices for biomedical applications such as biosensors, bio-imaging, and biophotonics. Reflectance is a straight-forward, non-destructive characterization technique that can be used to identify the material's optical conductivity. This study will utilize the reflectance analysis to investigate the optical properties, such as refractive index and optical conductivity, of the polyaniline-chitosan (PAni-Cs) hydrogels (with varying ratios). The materials that will be used in this study are PAni, due to its high conductivity, and Cs because it is non-toxic and biodegradable. By modifying chitosan with polyaniline, we are expecting to change the optical conductivity of chitosan. To tailor the experiment, the Helium (He)-Neon (Ne) Laser will be used in the study. Logarithmic reflectivity vs. incident angle plots of the samples will be analyzed and their degree of polarization will be measured. The refractive indexes and the Pseudo-Brewster angles in the p-polarized logarithmic plots of the samples will be determined. The refractive indexes and the optical conductivity experiment. The PAni-Cs ratio will then be compared. UV-Vis spectroscopy will be used to support the results of the reflectivity experiment. The PAni-Cs samples are expected to have the highest polymerization yield and highest conductivity. Also, they are expected to have the highest oxidation state. The PAni-Cs hydrogels are expected to have granular, unique and homogenous structure which could be a reason for their high conductivity. The results of this study will be useful for the characterization of polyaniline-chitosan using reflectance analysis.

# Tuning the structure of ultrathin iron oxide islands on Ru(0001) by UHV annealing

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Ultrathin iron oxide (FeO) islands and films grown on Pt(111) exhibit unique electronic [1], magnetic [1,2] and catalytic [3] properties not observed for bulk iron oxides. We studied ultrathin FeO islands epitaxially grown on another close-packed metal substrate – Ru(0001) – by room temperature iron deposition, post-oxidation in molecular oxygen and annealing in ultra-high vacuum (UHV). The performed scanning tunneling microscopy (STM), low energy electron microscopy (LEEM), local low energy electron diffraction (micro-LEED) and X-ray photoelectron spectroscopy (XPS) experiments revealed that vacuum annealing leads to the coalescence of initially-formed well-dispersed iron oxide islands and formation of larger structures. The obtained scanning tunneling spectroscopy (STS) dl/dV maps indicated the presence of potentially catalytically-active undercoordinated iron sites (CUFs) [4] at the perimeter of the annealed islands and within the islands, which makes FeO(111)/Ru(0001) an interesting material for model catalytic studies.

## Acknowledgements

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# Structural Colors from Self-assembled InP Nanopillar Metasurfaces

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Metal and dielectric metasurfaces display interesting optical features depending on nanostructure shape, size, choice of material and surrounding media. One such property is structural color that originates from light interacting with nanopatterns through phenomena such as interference, scattering, diffraction or absorption. Recently, structural colors have been produced from nanopatterned silicon and III-V semiconductors. Most of these fabrication approaches are either multistep procedures or limited to smaller areas (<mm2). Here, we address generation of spectral colors from self-organized InP nanopillars fabricated using a novel single step wafer scale ion beam etching (IBE) method. Preferential etching of phosphorous (P) leads to formation of indium (In)-rich nano-clusters which serve as etch-masks. The formed InP nanopillars are crystalline with a ball-shaped In-rich cap and a thin amorphous InP shell. The nanopillar height as well as their orientation with respect to the substrate can be controlled by tuning the etch parameters. The spatial arrangement of the InP pillars is highly disordered with subwavelength interpillar spacings. We observe vibrant spectral colors in reflection from the nanopillars. By controlling the nanopillar height and shape the spectral characteristics of the generated colors can be varied. Using finite difference time domain (FDTD) simulations the spectral features in the specular and diffused reflectance are explained by wavelength dependent absorption and scattering from individual pillars. The results show that spectral features are primarily determined by the height and the shape of the individual pillars and their material properties rather than their spatial arrangement.

# Towards scale-up of parallel, network-based biocomputation: Fabrication of dynamically programmable gates via thermoresponsive polymer

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Network-based biocomputation (NBC) is a parallel computing paradigm in which com¬binatorial problems are (i) encoded into nanofabricated graphical networks and (ii) solved by exploring the networks in a parallel fashion using a large number of independent, biological agents, such as molecular motors. Exploration of these paths by the agents then finds all possible solutions to the combinatorial problem.

A key aim in the upscaling of biocomputation devices is to be able to use the same device 1 to solve multiple, different instances of a problem. By locally depositing a switchable polymer in the junctions, it is possible to switch the functionality from a split to a pass junction and back. This would essentially establish programmable devices. To achieve reversible switching, we use the thermally responsive polymer poly(N-isopropylacrylamide) (PNIPAM) anchored to Poly(glycidyl methacrylate) (PGMA)2 to locally block and unblock pathways within the junctions. PGMA is a negative tone resist that can be locally patterned using electron beam lithography. The key to the selective binding would be achieving PGMA deposition inside the deep SiO2 channels(~450nm) to enable testing of the junction programmability. High aspect ratio Atomic Force Microscopy is employed to characterize the topography in the bottom of the channel. A proof-of-concept network has been designed by switching all the split junctions in selective rows to pass. This work will not only be a necessary element for large-scale biocomputation networks but also explores the possibility of precise patterning in nanostructures.

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# Magic number (C60)7-Au19 clusters on highly-oriented pyrolitic graphite

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We report the synthesis of (C60)7-Au19 clusters on graphite substrates in ultra-high vacuum. This follows our recent work on magic number (C60)7-Au19 clusters formed on the Au(111) substrate [1,2]. The interaction between C60 molecules and Au atoms leads to the preferential formation of two-dimensional Au19 clusters with a perfect hexagonal shape. There are six C60 molecules, one attached to each edge of the Au19 hexagon, and one additional C60 molecule sitting directly above the Au19 cluster. The (C60)7-Au19 cluster has excellent stability at RT and is stable against exposure to atmosphere.

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# Blood cell visualization using PEEM and imaging XPS

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Photoemission electron microscopy (PEEM) and X-ray photoelectron spectroscopy (XPS) have the potential for biomedical visualization. The aim is to increase the understanding of biological processes on the cellular level, with topographical and threshold imaging using energy-filtered capabilities and laterally resolved element and chemical state mapping.

This is hereby demonstrated by combined PEEM and Imaging XPS investigation of neutrophils and their activation processes. Neutrophils are white blood cells and a predominant part of the innate immune system and vital components in the human defense system, with the fundamental role to fight invading pathogens. Neutrophils are also able to release and form extracellular web-like structures composed of decondensed chromatin and called neutrophil extracellular traps (NETs) to capture and occasionally kill intruding microbes.

Here we report neutrophils triggered by external treats, in this case nanoparticles (NPs). The neutrophils and NETs formation are imaged in presence of NPs and we report elemental composition of single-cells and structure of NETs. Active cellular uptake of nanoparticles is imaged before and after NETs release. This shows the potential for element specific bio-related cell studies on surfaces and nanoparticle tracking on the cellular level.
### Semiconductor nanostructure-based metasurfaces for light manipulation functions

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Dielectric metasurfaces, by appropriate choice of their geometrical and material properties, can offer new or added light manipulation functionalities in surface optical coatings and optical interfaces in optoelectronic devices. Here, we present our investigations of the optical properties of sub-wavelength semiconductor nanodisk arrays, including electromagnetic design and simulations, spectrophotometric analysis and device applications. In particular, Mie resonances in a-Si and TiO2 nanodisks are investigated in detail and their spectral characteristics utilized to achieve NIR spectral filters and anti-reflection in solar cells, respectively. Stand-alone spectral filters in reflection and transmission modes were made by embedding substrate-free a-Si nanodisk array in a flexible transparent matrix. With appropriate geometric parameters of the a-Si nanodisk arrays, filters with high (> 75%) transmittance and reflectance are obtained in the NIR region. We demonstrate a pattern embossing method by which sub-wavelength TiO2 colloidal nanoparticles can be packed into pre-designed nano- and microstructures on device surfaces. The embossing method is a low pressure (~0.1 bar) and low temperature (<100 °C) process and thus surface structures can be added-on without adversely affecting the fabricated devices. Using reflectivity data and a Bruggeman model, an effective index of ~1.9 was determined for the TiO2 nanoparticle-air film. For this refractive index value, the lowest solar (AM 1.5) weighted reflectivity of ~ 7% was obtained by optimizing nanodisk array parameters. Single junction planar solar cells (Si, GaAs and InP) embossed with the optimized TiO2 nanodisk-based metasurfaces show appreciable improvement (~ 30%) in the short circuit current densities.

#### **Bio-applications of semiconductor nanowires**

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Semiconductor nanowires are very promising tools for biological applications. Their small dimensions, which are on the same length scale as many cell components, make them an ideal tool to probe and stimulate cells with minimal perturbation. In this talk I will review our work towards using nanowires for neural implant [1,2] and biosensor applications [3–5], as well as our studies towards understanding and controlling the cell-nanowire interface [6,7].

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# Self-formation of heterogeneous nanostructures on transition metal oxide perovskite surfaces by thermal reduction and incongruent sublimation

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Transition metal oxide nanostructures are of great interest due to their wide-ranging applications in fields such as (photo)catalysis, optoelectronics and resistive switching. In order to facilitate the development of the real life applications, a dependable process for nanostructure formation has to be devised. Our newly developed method called Extremely Low Oxygen Partial Pressure (ELOP) is a bottom-up method used for the formation of oxide nanostructures on perovskite surfaces. It uses an oxygen getter to substantially lower the oxygen partial pressure during the thermal reduction. This leads to incongruent sublimation of a transition metal cation and the perovskite decomposition, resulting in the formation of crystalline oxide nanostructures, all in temperatures at which the perovskite is usually considered stable [1].

In the case of strontium titanate (SrTiO3(100)) the ELOP method leads to the formation of titanium monoxide (TiO) nanowires on its surface [2]. The nanowires are crystalline with an atomically sharp TiO/SrTiO3 interface. Their size can be controlled from nanometers to mesoscopic range by the reduction temperature. Moreover, they are characterized by a metallic conductivity, which remains after oxidation, unlike the work function which increases by not less than 0.5 eV. We show that further reduction leads to the formation of the thick porous layer of nonstoichiometric titanium oxides. We show that the ELOP mechanism is a phenomenon which may be employed also in the case of other oxides such as barium titanate (BaTiO3) and calcium titanate (CaTiO3).

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### Network based computation using molecular motors

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Non-deterministic polynomial time (NP) problems of a combinatorial nature require the exploration of a very large solution space which grows exponentially with the number of input objects, making traditional serial computation intractable, and parallel computation a necessity. These problems occur in a broad variety of applications including drug design, optimal network routing, artificial intelligence and cryptography.

Recently, a network based parallel computation technique (Nicolau et al, PNAS 113(10) 2016) based on active-transport molecular motors as discovery agents was demonstrated. The problems are encoded into physical structures of channels and junctions with each route representing a specific algorithm. Thus, by exploring the network, the agents solve the problem with a massively parallel approach, translating the exponential time-complexity into the number of possible paths and agents required. Due to the size of the motor systems, large networks fit into a very small area, using electron beam lithography to create nanostructures.

To improve this method for upscaling the mathematical complexity, we have developed a number of architectural enhancements. Here, we present progress in establishing the technical requirements for upscaling; high throughout processing by nanoimprint lithography (Lindberg et al, Mater. Res. Express. 6(2) 2019), material optimization (Lindberg et al, Langmuir 34(30) 2018), junction design for minimal errors, and sustainable network reuse by sample regeneration. Funding: EC-H2020 "Bio4Comp" Grant-No. 732482.

# Two-dimensional GaN grown on Si(111)7x7 with assisted hyperthermal nitrogen ions at low temperature

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We propose a new way of fabrication of 2D GaN on the Si(111)7x7 surface using post-nitridation of Ga droplets by hyperthermal (E < 50eV) nitrogen ions at low substrate temperatures (T < 220°C). Both deposition of Ga droplets and their post-nitridation is carried out using a special atom-ion beam source developed in our group. Such an approach brings well defined conditions of the growth of high purity GaN nanostructures. A well defined interface between the GaN nanostructure and the silicon substrate together with nanostructure elemental composition was observed by TEM. In addition, SEM, XPS, AFM, Auger microanalysis and measurement of photoluminescence response helped to elucidate unique characteristics of the fabricated nanostructures.

#### Neutrophil extracellular traps and nanoparticles

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Nanoparticles (NP) are used in many applications ranging from sunscreens to advanced sensors and targeting drug delivery agents. While NPs positive properties are being widely explored their eventual downsides does not draw the same attention. NPs come in a huge variation in terms of size, element composition, charge, functional groups etc and their interaction with the human body is often incompletely understood.

In the present study two types of nanoparticles, quantum dots (Qdots) and iron nanoparticles (FeNP), have been used as a model system to evaluate interactions with neutrophil granulocytes. Neutrophils are white blood cells involved in innate immunity. They scavenge the body for possible threats and their defense mechanisms include the process of phagocytosis, release of enzymes, production of reactive oxygen species, and more recently recognized the release and of neutrophil extracellular traps (NETs). During NET formation neutrophils unwrap its own DNA and throw/shot it out to physically entrap the invader.

Our results show that Qdots trigger NET release and that they are also trapped and incorporated into the web like structures (Fig 1). Not all neutrophils internalize NPs, some are filled with NPs and/or undergo NETosis and others are mostly unaffected which indicates a delicate cooperation between the cells to handle the threat.

We also show possibilities to manipulate NETs. By using FeNP with the same size and functionalization as the Qdots we are able to guide NET formation towards a magnet.

Refinement of these model systems will lead to a deeper knowledge in NP induced inflammatory responses.

## Electrodeless method for carrier-resolved mobility of nano-channel

Particle beam irradiation in to the sample has long been basic methodology for characterizing the emerging materials. Here, in contrast to the general belief, we show that the portion of primary beam current effectively interacting with the target material is sensitively dependent on the transport properties of the sample and demonstrate that the estimated effective primary current allows to probe in-situ evolution of the charge carrier mobility of nanometer length materials without metal electrode formation. Using this method, we show first experimental verification of unresolved intriguing prediction of the contrastive behavior between electron and hole mobility depending on the order of crystallinity of P3HT, veiled in prevailed side effects raised by impurity, uneven grains, defects and forcing field required in conventional method. This novel method opens up new opportunity for in-situ analysis of charge transport properties of nanoscale materials across the electrical critical point by means of the absence of interface and forcing field effects.

# Dark and Photo-Induced Charge Transport Across Boundaries in CsPbBr3-CdSe Hybrid Nanoparticles

Hagai Cohen, Miri Kazes, Swayandipta Dey, Iddo Pinkas, Dan Oron

Variable interface characteristics are demonstrated at the nanoscale, using two types of semiconducting nanoparticles with nearly identical optical band gaps, CsPbBr3 nanocrystals and CdSe nanoplatelets, capped with molecular linkers. By exploiting chemical recognition of the capping molecules, the two types of nanoparticles are brought into mutual contact, thus initiating spontaneous charge transfer and the formation of a strong junction field. Depending on the choice of capping molecules, the magnitude of the latter field is shown to vary in a broad range, corresponding to an interface potential step of 0.1-1.1 eV. The band diagram of the system, as well as the emergence of photo-induced charge transfer processes across the interface are studied here by means of optical and photoelectron based spectroscopies. Our results propose an interesting template for generating and harnessing internal built-in fields in heterogeneous nanocrystal solids.

## Enhancing Fluorescence Detection with Lightguiding Nanowires

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Semiconductor nanowires (NWs) can act as nanoscale optical fibers, collecting and guiding light emitted by surface-bound fluorophores [1]. Fluorescent emission couples into the free-standing NWs due to near-field interactions and it is guided to its tip independently of the emitters' position along the NW length. NWs can then be used as fluorescence signal integrators, enabling higher signal-to-noise ratio. Insights into this phenomenon, i.e. its dependence on NW geometry and fluorophore wavelength, are critical for the successful design of optical biosensors based on NWs.

We used confocal microscopy to investigate the lightguiding efficiency in gallium phosphide (GaP) NWs of various diameters for fluorophores with varying emission wavelength. Employing a combination of finite-difference time-domain simulations and analytical approaches, we identify the role of multiple waveguide modes and show how to predict the lightguiding ability of the NWs, as a function of diameter and fluorescence wavelength, by calculating the normalized frequency parameter [2].

As a proof-of-concept in the context of bioanalytical sensing, we characterize the diffusion of cholera toxin-decorated GM1 gangliosides in a supported lipid bilayer formed on silica-coated NWs. Diffusion of GM1 on a NW was detected via epifluorescence microscopy down to single-molecule level, and the simultaneous observation of hundreds of NWs provided significant statistics in short measurement times (~10 s). The temporal evolution of the number of bright NWs was fitted with an analytical model to determine both GM1 concentration and diffusivity. This highly parallel approach works optimally at low GM1 concentrations (< 1  $\mu$ m-2) and can be corrected for photobleaching.

#### On the role of recycling in high power impulse magnetron sputtering discharges

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In the high power impulse magnetron sputtering (HiPIMS) discharge a high density plasma is created by applying high power pulses at low frequency and low duty cycle to a magnetron sputtering device. We discuss the origin of the large discharge currents observed in HiPIMS discharges. We explore the current composition and the role of self-sputter (SS-) recycling and working gas recycling within the discharge. We demonstrate that above a critical current density Jcrit  $\approx$  0.2 A/cm2, a combination of self-sputter recycling and working gas-recycling is the general case [1]. For high self-sputtering yields, above YSS  $\approx$  1, the discharge become dominated by SS-recycling, and consequently only a few hot secondary electrons are accelerated across the cathode sheath and the effective electron temperature is low. Here, stable plateau values of the discharge current develops during long pulses, and the plateau values increase monotonically with the applied voltage. For low self-sputtering yields, below YSS  $\approx$  0.2, the discharges operated above Jcrit are dominated by working gas recycling, where acceleration of secondary electrons has a significant role and the effective electron temperature is higher, while the current evolution is generally less stable. For intermediate values of YSS the discharge character gradually shifts between these two types. In addition, these new insights on ion recycling have been applied to a series of selected sputter materials. When operating at high voltages and high discharge currents a discharge with Al target develops almost pure self-sputter recycling, while a discharge with Ti target exhibits close to a 50/50 combination of self-sputter recycling and working gas-recycling [2]. However, if the Ti target is operated in a reactive Ar/O2 gas mixture, it is found that working gas-recycling is dominating [1] and that the Ar +-ions contribute almost solely to the discharge current [3].

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#### Plasmon phase imaging by near-field digital holography

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We propose a novel method for the measurement of phase distribution of the near electric field of surface plasmon polaritons based on the principles of phase-shifting digital holography [1]. In contrast to previous methods the holographic interference occurs already in the near field and the phase distribution can be determined purely from the scanning near-field optical microscopy measurements without the need for additional far-field interferometric methods (e.g. the heterodyne methods). We demonstrate the capabilities of the proposed method by reconstruction of the phase difference between interfering surface plasmon waves and by imaging the phase of a single surface plasmon wave. We also demonstrate a selectivity of the method towards individual components of the field. The core of the proposed method is an on chip interferometer with a signal near field and a reference near field excited by a common far field (in our case a plane wave) on slits to ensure their coherence. The phase of the reference field is controlled by a Spatial Light Modulator (SLM) implemented in the illumination path of a collecting-type Scanning Near-Field Optical Microscope (c-SNOM), allowing phase-controlled excitation of the near field. We have used two specific implementation techniques of the on-chip interferometer: a circular slit forming a standing SPP wave and a V-shaped slit forming a propagating SPP wave.

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## Determining the mechanisms of Fe intercalation underneath epitaxial graphene on Ru(0001)

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Epitaxial graphene (EG) can be grown on Ru(0001) single crystal support by thermal decomposition of ethylene (C2H4) [1]. The graphene layer strongly interacts with the ruthenium substrate, which is manifested by the formation of a Moiré superstructure and modification of EG's electronic properties [2]. It was shown that the EG layer can be decoupled from the substrate by metal intercalation [3], however, the mechanisms of this process are still a topic of intense scientific debate. We used scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and density functional theory (DFT) to study the mechanisms of Fe intercalation underneath EG on Ru(0001). The results reveal two possible intercalation scenarios, which may be valid also for graphene grown on other single-crystalline substrates.

## Acknowledgement

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# Plasmons in atomic Au wires: tunability by selective chemisorption

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Gold-induced atomic wires on stepped Si surfaces provide a peculiar playground to study fundamental low-dimensional physics, but can also serve as test systems for ultimate limits of electronic circuits. Their interaction with a substrate causes deviations from pure one-dimensionality but also introduces tunability. Hybridization between Si surface states and Au related electronic bands turned out to largely determine the properties of the bandstructure close to EF, which can be modified by chemisorption.

Here we employ plasmon spectroscopy and atomistic DFT simulations to study the interplay between structural motifs of the Au chains and the Si(557) and Si(553) substrates in presence of chemisorbed atoms. By adsorbing atomic hydrogen and oxygen we show that these do not only act as donors or acceptors of charge. On Si(553)-Au hydrogen triggers band gap opening above the EF resulting in a reduction of metallicity, whereas oxygen has only a small effect on plasmon dispersion, but rather introduces disorder. On the other hand, the presence of additional chains of adatoms and rest-atom chains on Si(557)-Au increases chemical reactivity and induces further hybridization that results in site-specific and non-monotonic shifts of plasmon frequency upon oxidization. Hydrogenation of this system leads to a band-gap opening above EF and to a leveling off the plasmon dispersion at high k||. Nonetheless, since all chemical reactions mainly involve Si atoms and affect the Au chains only indirectly, even high exposures although modifying bandstructures, do not introduce metal-insulator transitions.

# Cerium oxide nanoparticles with antioxidant capabilities and gadolinium integration for MRI contrast enhancement

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The medical treatment is evolving towards the concept of individualized patient-based target medicine, the new generation of medical treatments combine therapeutic and diagnostic properties into one theranostic agent. Reactive Oxygen Species (ROS) are natural byproducts of normal metabolism but during environmental stress the ROS levels can increase radically resulting in a harmful condition, oxidative stress. Oxidative stress can cause critical damage to cell structures and the condition is related to several diseases such as chronic inflammation, cancer and neurodegenerative diseases. Antioxidants are substances that scavenge ROS and thereby regulate the ROS concentration levels.

In this study we have designed antioxidative cerium oxide nanoparticles (CeNPs) with precise fractions of MRI-active gadolinium atoms (Gd). CeNPs antioxidative properties originates from CeNPs' capability to switch between oxidation states Ce3+ and Ce4+ in redox scavenging reactions with ROS. The Gd-CeNPs have been carefully characterized utilizing combined experimental and theoretical efforts to determine the particles' crystal structure and electronical configuration. The as-prepared Gd-CeNPs display superior MRI contrast enhancement properties (~3 times better than clinical MRI contrast agents) and we have shown significant antioxidative properties in vitro and in vivo. Our goal is to guide our developed Gd-CeNPs to a specific site at pathogenic tissue, visualize the targeting tissue and suppress the inflammation on site.

## SIMS investigation of OLED structures

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Organic Light Emitting Diodes (OLED) are gaining the importance and everyday's use in the present. The OLED fabrication process is much simpler as concerning the laboratory conditions for inorganic counterparts; but however the OLEDs need to be packaged well enough to prevent their degradation. The degradation may be caused mainly by the light, water, and oxygen. The degradation evaluation is often correlated to the lifetime, which is recently almost at values ~20.000 hours of operation [1]. One way of lifetime exploration is possible by constant voltage/current stress applied to the OLED structure and search for correlation of these results with SIMS depth profiling before and after the stress process. Our aim is to look for chemical reactions by comparison of the OLED structures without any cover layer or another prevention by SIMS depth profiling. The OLED structures were prepared on the model structure Ag/Ca/Alq3/alpha-NPD/ITO [2]. The contribution is discussing the OLED structures without any cover layer degradation under constant current stress applied and the approach with SIMS depth profile analysis. The shown examples are describing, which changes we can expect. Since the OLED structures were not packaged, the results only showing the trends, which will be further analyzed.

The research leading to these results has received funding from the projects of APVV 17-0501 and VEGA 1/0929/17.

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# Growth of dislocation-free and atomically flat III-nitride micro-prisms

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III-Nitride materials are considered as building blocks of electronic and optoelectronic devices. They still suffer from poor quality, especially due to the presence of dislocations. We present a novel technique to grow micron-sized, completely dislocation-free and atomically flat GaN hexagonal prisms. The growth sequence starts with blocking dislocations from the substrate prior to nanowire (NW) growth by optimizing the SiN mask hole diameter, in which nanowires (NWs) are grown. The NWs are used as nuclei to grow GaN radially, followed by in-situ reformation of the structures. Presence of NH3, a high temperature and a high pressure are three key elements to reshape the GaN structures. Before the reformation, the GaN structure is dominated by pyramidal s-facets. The reformation creates flat-top hexagonal prisms, dominated by an about 1 µm wide c-facet, consistent with equilibrium Wulff construction calculations. TEM, AFM, and CL data confirm the absence of dislocations in the GaN prisms. The c-facet extension can be increased and the pyramidal-shaped tip can be avoided, greatly reducing optical diffraction losses. To show the potential of these GaN prisms in one of many applications, we have included them in vertical optical cavities. This was done by sandwiching the GaN prisms between two dielectric distributed Bragg reflectors. The fabricated vertical GaN prism cavities were electron-beam pumped to measure the quality (Q) factors of the cavity. Experiments and simulations of the cavity Q factors are in good agreement and highlight the importance of large prism diameters to achieve high quality optical microcavities.

# Conducting polymer coatings on plasma-processed polymeric substrates: Towards bio-inspired self-cleaning touch screen applications

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Polymeric materials such as poly(methyl methacrylate) (PMMA), polycarbonate (PC), poly(ethylene terephthalate) (PET), and highdensity polyethylene (HDPE), which are normally used in making pressure sensors and touch screens/panels, were treated with oxygen plasma produced from a P300 plasma device (Alliance Concept, France) to provide surface cleaning, surface structuration, and surface functionalization. The plasma-processed polymers are then coated with different conducting polymers such as polypyrrole, polyaniline, and polythiophene that were polymerized by chemical oxidative techniques. The conducting polymer coatings would serve as the polymer backbone for grafting short fluorinated chains that provides self-cleaning properties like those exhibited by different plants (e.g., Asparagus setaceus, Nuphar luteum, Viola tricolor, and Strelitzia reginae) and insects (e.g., Hydrometra stagnorum, Aquarius remigis, and Dolomedes triton). This study examined the role of the plasma treatment on the adhesion or anti-adhesion of the conducting polymers on the substrates. The surface effects of the plasma treatments were characterized by contact angle measurements, scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Fourier transform infrared spectroscopy (FTIR), and optical profilometry. Changes in the chemistry, presence of nanostructures and surface etching, and increase in roughness on the substrates. Wettability studies were also performed both on the plasma-treated polymeric materials and after they are coated with the conducting polymers.

## Theoretical study on surface structures of S/Ni(110)

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It is well known that surface structures strongly depend on the adsorbate coverage. S atoms on Ni(110) surface form c(2x2), c(2x8) or p(2x3) surface depending on its coverage: their surface coverage correspond to 0.5, .0.625, and 0.667, respectively [1]. In the recent STM observation, it was found that Ni(110) doped with S and C atoms shows the interesting surface structures after annealing, i.e. high S density lines, which run along [1-10] and [001] directions, formed in the c(2x2) surface [2]. We theoretically investigate the structures and the stabilities of the lines by using the PHASE/0 code [3], which is based on the density functional theory and the pseudo potential scheme with the plane wave basis set. We found that the high S density lines are the arrays of p (3x2) units formed in the c(2x2) surface. The formation energy of a one-unit kink in a p(3x2) line is calculated to be only 0.1 eV and that for a two-unit kink is 0.2 eV. This result explains the experimental observation that the lines have some kinks well. We also found that two parallel lines prefer to be separated than to be adjacent to each other, which is consistent with the experimental observation.

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## Novel UV-curable Materials for High-Resolution Intermediate Polymer Nanoimprint Stamps

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Nanoimprint lithography patterning is used nowadays for a wafer-large definition of sub-200 nm Au dot arrays for epitaxial growth of III-V nanowires [1]. The imprint technique is implemented using a modified process with a single-use intermediate polymer stamp (IPS), replicated from a master stamp. The pattern is transfered by a double-layer lift-off process with TU7 and LOR resists. The standard process, based on a proprietary IPS-polymer (Obducat AB, Sweden), does not provide sufficient reproducibility when pitch in the array exceeds 1 µm due to mechanical bending of the IPS features, in particular when the required feature size is below 100 nm. In the current work we present a systematic comparison of four IPS materials, the standard IPS-plastic, OrmoStamp [2] (Micro-Resist Technology, Germany) and two novel polymers GMN72 and GMN92 (OpTool, Sweden). The new polymers are based on acrylated silane and offer high Young's modulus of 4800 MPa to provide good mechanical stability during the imprint process of well-separated structures. Besides, as opposed to the standard IPS-plastic and the OrmoStamp resin, the GMN72 and GMN 92 polymers do not require antisticking treatment and showed a resolution <30 nm. Our investigation is focused on reproducibility of the imprint step for making seeds for III-V nanowires and the resolution limits of these novel polymers.

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## High resolution coherent X-ray Imaging

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For the last 20 years synchrotron sources have produced brighter and more coherent X-ray beams. This has allowed the development of Coherent X-ray Imaging techniques which yield a resolution which is neither limited by the X-ray beam size, nor by the pixel size on the detector. A variety of techniques are currently available: phase contrast, coherent diffraction imaging, ptychography, allowing the study of materials with different sizes (from a few 100 of nanometers to millimeters) and a resolution down to about 10 nm.

These techniques can be applied in the small angle regime, yielding the object's electronic density, and thus giving a unique threedimensional view of a wide range of samples, with applications from biology to electrochemistry or electronics.

In the case of crystalline materials, measurements can also be performed in the Bragg geometry to give access to quantitative strain maps at the nanoscale, from bio-engineered minerals to catalysts or semi-conductor nano-structures.

Lastly we will discuss the development of improved X-ray sources: beyond the advent of X-ray Free Electron Lasers, synchrotron users facilities are being upgraded, with two orders of magnitude more coherent photons per second, ultimately leading to a combination of higher spatial resolution and faster dynamical studies.

# Engineering intracellular access to primary blood cells using nanostraws

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Nanostraws are hollow metal-oxide nanotubes that can be made to form stable, healthy pipelines into living cells. Nanostraws protrude from a track-etched polymer membrane that connect to a fluidic environment beneath the membrane. Placing exogenous molecules such as RNA, DNA, or proteins, beneath the membrane allow for diffusive transport into cells cultured on the nanostraws. By adding a low voltage electric field across the membrane, the molecular transport can be electrokinetically enhanced. Nanostraws have been shown to provide intracellular access to a wide variety of adherent cell types ranging from cell lines to primary derived neurons and cardiomyocytes. This has been utilized to deliver molecules to cells as well as to repeatedly sample out cytosolic contents. Non-adherent cells, such as blood cells in suspension, have so far not been possible to use with nanostraws since the intracellular access has relied on the cells pushing themselves on the straws.

Coupling the nanostraws with an external force enables intracellular access also to suspended blood cells. In here, we exemplify this in a sensitive, and clinically relevant, cell type: primary human hematopoietic stem cells. We show that by centrifuging the cells down on the nanostraws and adding a low-voltage electric field, we can achieve high efficiency and high viability delivery of transiently expressed mRNA. We also show that the nanostraws can perform stable genetic modifications using a CRISPR/Cas system. Our results show that nanostraws provide a high efficiency, high viability, easy-to-use, and scalable platform for genetic modifications of primary cells in suspension.

# The growth of gold thin film on cellulose surface: a model case of fabricating an electrode of paper electronics

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The advance of flexible electronics does not only call for the higher efficiency, long lifetime and good mechanical robustness, but also raise the demand to be environmental-friendly. Despite the vastly used petroleum-based polymer substrate in organic electronics, papers made of cellulose fibres becomes an alternative with good biodegradability, excellent mechanical properties and tuneable optical transparency. The so-call paper electronics has emerged as a frontline of technological development. In any electronic devices, different functional component need connecting with electrode, which should be mechanically compatible with substrate. However, paper itself is a fibre-network with inherent porous structure on the surface. The complex connection on the paper surface may have interesting impacts or challenges for electrode fabrication. In this work, we try to study a model case of the electrode of paper electronics by growing Au thin film on paper via sputter deposition. We used grazing incidence small angle X-ray scattering (GISAXS) to follow the Au thin film morphology during preparation. In combine with atomic force microscopy (AFM), we observed a direct correlation between the substrate porous structure and the thin film growth kinetics. Nevertheless, Au thin film follows islands-growth model in all cases and experience three-stage growth with nucleation, coarsening and coalescence. The results in this work could help us understand nanostructure development on porous surfaces in a broader sense.

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# Integrated on-chip system for DNA purification and surface stretching

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DNA analysis can be a powerful tool for diagnosis of disease at the point of care. However, available tools are often cumbersome to use, requiring advanced sample preparation using bulky equipment. Here we present a concept where important steps in the sample preparation takes place in an integrated lab on a chip device.

We have developed a microfluidic platform that can purify DNA and subsequently label and stretch it on a surface. We have successfully extracted DNA from a gel-filled microfluidic channel using electrophoresis and subsequently stretched the DNA linearly by absorption to either a hydrophobic or a positively-charged surface. To our knowledge, DNA has not previously been stretched on to a surface while being moved using an electric field in this way. We have also labelled DNA after stretching with intercalating dyes. This lays the ground for optical mapping of bacterial genomes for ultrafast diagnosis of infectious disease.

## Rotational state distribution of molecularly chemisorbed H2 on Pd(210)

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On a flat metal surface, hydrogen typically chemisorbs dissociatively. On the other hand, it is known that hydrogen can molecularly chemisorbs on stepped surfaces, such as Ni(510)[1] and Pd(210)[2], in which the potential is expected to be highly anharmonic, unlike the case of physisorption. The anisotropic potential would modify the rotational state of H2 and promote ortho-para (o-p) conversion. For the system of H2/Pd(210), a previous study with rotational-state-selective temperature programmed desorption indicated the occurrence of fast o-p conversion [3].

In this study, to further probe the rotational state and conversion of molecularly chemisorbed H2, a combination of photo-stimulated desorption and resonance-enhanced multiphoton ionization techniques is used. It is found that photo-desorbed H2 consists of a variety of rotational states from J=0 to J=5 with an anisotropic angular distribution. Observed rotational state distribution of H2 and desorption process will be discussed.

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# Cell sorting using Electrokinetic Deterministic Lateral Displacement

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Conventional cell and particle sorting schemes use intricate labeling schemes to identify different subpopulations. Here instead we report how electrokinetics can be used together with Deterministic Lateral Displacement (DLD) to create a label-free sorting scheme that fractionates based on the dielectric properties of the particles. We demonstrate how polystyrene particles are sorted by the difference in their surface charge. As a proof of principle of a biomedical application we also demonstrate that this type of device can sort viable from non-viable yeast cells and viable from non-viable E. coli bacteria. In particular for the case of E. coli, a 50/50 ratio of viable/non-viable cells population can be separated into different reservoirs with more than 90% purity. This lay important groundwork for devices that can be used for precise selection of antibiotics with strong relevance in light of the growing threat of antibiotic resistance.

## Targetable dual-color nanoprobe for sensing a wide range of pH in cells

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Cells are smallest structural and functional of living organisms. The cellular compartments require proper conditions to perform their normal functions. Intracellular pH is an essential factor that regulates much cellular behaviour, including proliferation and apoptosis, as well as enzyme activity and protein degradation. Disruptive variation in the pH may lead to dysfunction of the organelles. Abnormal pH is a hallmark of many common diseases such as cancer, stroke, and Alzheimer's disease. Therefore, accurate monitoring of pH variations inside cells is important for the early diagnosis of diseases and prior to the treatments. Fluorescence spectroscopy for quantitative measurement of intracellular pH is a direct and useful tool for cellular diagnosis because of its non-invasiveness, high sensitivity and specificity, and high signal-to-noise ratio. Towards this end, great efforts have been made to fabricate fluorescent pH probes. However, there are always obstacles such as the limited emission spectra shifts, limited working pH ranges, poor photostability and poor solubility under physiological conditions. Therefore, by using new conceptions and platforms, more novel versatile pH fluorescent probes are being generated, which allow the accurate pH monitoring in vivo and in vitro. Herein, newly-fabricated nanoprobe can monitor a wide range of pH in cells by means of the doped dual-responsive components (RhB and Flu) (Fig. 1). In addition, modifications of the terminated group of nanoprobe endow the nanoprobe with additional accessible functionalities such as specific labeling and targeting, which can allow a signal-on report of the cellular processes via determining pH fluctuations.

## Updates on European Spallation Source TARGET monolith Vacuum

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The European Spallation Source (ESS) is a multi-disciplinary research infrastructure neutron source facility based on a 2GeV -5MW linear accelerator. The goal of ESS is to be the brightest neutron facility and to enable novel science in many fields such as biology research, environmental technologies and fundamental physics. The facility includes Super-conductive Radio-frequency cavities (SRF) to accelerator a proton beam to produce neutron by spallation process on a helium-cooled tungsten wheel, possibility to host 42 neutron instruments and a supercomputing data management and software development center.

The LINAC will deliver 5 MW of power to the target at 2000 MeV. ESS is a long pulse superconducting LINAC that accelerates protons long pulse stream with a repetition rate of 14 Hz at a 4 % duty cycle providing an average beam power of 5 MW. The stream of protons is intercepted by a helium cooled tungsten target wheel. The moderators and reflectors maximize the yield directing the flow of neutrons to a suite of neutron instruments through neutron guides.

The Target Monolith Vessel (TMV) is a vacuum vessel nominally 6m in diameter x 9m high fabricated of 304L stainless steel running in a pressure < 100 Pa following high vacuum standards, nuclear and pressure codes. The major equipment located within this vessel are the helium cooled target wheel, 42 neutron inserts that provides the first optical neutron guides, actively cooled moderators and reflector plugs and water-cooled radiation shielding blocks. The TMV is designed to operate either under a helium atmosphere, normally at 1 bar pressure, or under high vacuum and is directly connected to the accelerator beam-line through that operates under ultra high vacuum conditions. A proton beam window (PBW) physically separates the two environments when the monolith is under a vacuum or helium atmosphere. In the vacuum mode the PBW is possible to remove and the two vacuum environments are directly connected.

The presentation reviews the various aspects of the Vacuum Design of the Target Monolith System including material selection, surface finishes and construction issues, equipment sizing and selection and the development of a Strategic Installation and Test Strategy in order to minimize project risk.

# Dielectrophoretic Deterministic Lateral Displacement for tunable particle sorting

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Cell and particle separation is an essential tool in biomedicine both for research and for clinical applications. An important challenge is to sort small particles on the nanoscale. Often nanofluidic devices must be made that present challenges in terms of nanoscale fabrication and limitations in terms of low throughput and high probability of clogging. Here we demonstrate a novel scheme for label-free sorting using on a unique architecture based on metalized obstacle arrays in microfluidic channels. We make a device based on Deterministic Lateral Displacement (DLD) where the posts can be electrically connected, enabling local application of strong electrical fields with modest applied voltages.

The result is a combination of electrokinetics and DLD that allows us not only to tune the separation but also to obtain separation of particles on size scales that are more than 20 times less than without any applied electric fields. With no need for advanced nanofabrication techniques we can now make DLD device using standard microfabrication technology, with a threshold size of 5µm to sort particles on the scale of a few hundred nanometers. The large channels ensure that throughput is improved and clogging minimized in relation to nanoscale devices. Proof of principle has been demonstrated using polystyrene microspheres. Future work will focus on fractionation and enrichment of a wide range of biorelevant nanoparticles.

## C60 adsorption on a two-dimensional oxide quasicrystal

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When approaching the two-dimensional limit, oxides are known to exhibit strong variations in their structures and properties as compared to the respective bulk materials [1]. One extreme example are two-dimensional oxide quasicrystals (OQCs), which have been discovered for monolayers of reduced BaTiO3 and SrTiO3 on Pt(111) [2,3]. These quasicrystals are forming self-similar tilings containing squares, triangles, and rhombs of equal side length. Inherent to the structure is the absence of translational symmetry.

Here we report the first adsorption studies on the BaTiO3-derived OQC using C60 molecules. Their van-der-Waals diameter of 10 Å matches roughly the distance between two neighboring squares in the dodecagonal tiling. By depositing the C60 at 150 K, the diffusion of individual C60 molecules is strongly suppressed and small C60 islands are formed on the OQC template as determined by STM. Besides local hexagonal C60 arrangements, we find C60 molecules forming quadratic arrangements. The latter also being combined into local square-triangle tilings which have been analyzed with respect to dodecagonal versus hexagonal alignment. From the comparison of the local C60 configuration with a periodic square-triangle approximant, we conclude, that the presence of rhombs in the OQC tiling hinders the formation of extended patches of C60 on the OQC template.

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### Studying the impact of salt on the structural properties of bread by means of Neutron and X-ray tomography

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Today we consume more salt than needed, by eating pre-prepared food, e.g. meat, bread and cheese products. Too much salt can lead to health issues, e.g. heart attack, heart failure, stroke and kidney damage [1]. WHO aims to reduce the global population's intake of salt by 30% by 2025 [2]. By reducing the salt consumption to recommended levels an estimated 2.5 billion lives can be saved [2]. The salt thus needs to be reduced, while maintaining the taste, quality, and processability, as required by both the consumers and producers. By exchanging many fine-grained salts with fewer layer-distributed coarser-grained salt, one can even obtain an increased sense of saltiness. In this work, we studied the impact of fine-grained and coarse-grained salt on the structural properties of bread using X-ray microtomography and Neutron tomography, whereas the latter is a sensitive technique to detect salt in bread and the former provides a high-resolution image of the bread structure. The tomographic data sets were used to extract a set of quantitative 3D descriptors about the bread, e.g pore size, the thickness of the beams and crust and connectivity index. By quantifying the microstructure of food products, it is possible to optimize the processing parameters and thereby obtain an improved food quality [3]. We also verified our findings with classical light microscopy. A better understanding of the 3D distribution of salt and its impact on the structural properties of bread, and consequently also the tastiness and quality, will help to develop healthier food products with reduced total salt content.

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# Simulation of pressure distribution and efficiency of ion transport in vacuum chambers of accelerator complexes

Alexander Tikhomirov, Georgy Gulbekyan, Boris Gikal, Igor Kalagin, Maxim Khabarov

The methods of numerical simulation of pressure distribution in vacuum chambers are applied by computer programs GENAP and VACLOS for designing and optimizing the vacuum systems for accelerator complexes to maximize the efficiency of accelerated ion beams. These computer codes have been developed and tested on the basis of experiments on four heavy ion cyclotrons at the Flerov Laboratory of Nuclear Reactions. The simulation programs estimate ion beam losses based on the pressure distribution simulation in vacuum chambers of any arbitrary geometry as well as on calculation of cross sections for a recharge of ions during acceleration in exchange reactions by electrons with molecules of the residual gas. The simulation results are in good agreement with experimental measurements. These simulation programs were used to design vacuum systems for a number of new cyclotron complexes, such as the DC-72 (Slovak Republic), the CYTREC cyclotron complex (Dubna), the DC-60 (Astana University in the Republic of Kazakhstan), the DC-110 (Dubna Centre of Nano & Nuclear Technology) and the DC-280 heavy ion cyclotron complex as the Super Heavy Element factory, which was launched at JINR FLNR in December 2018.

#### Investigation of the reproducibility of commercial hot cathode ionization gauges after different treatments

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In the framework of the EURAMET EMPIR project "16NRM5-ion gauge" we investigated the reproducibility of sensitivity of hot cathode ionization gauges after selected treatments, which are often applied before the gauge is used either for vacuum measurements or in the process of calibration of the gauge.

Two types of ionization gauges were selected for the study: IE514 Extractor gauge from Leybold and Bayard-Alpert STABIL-ION gauge from MKS-Granville-Phillips. These two types are often used as reference gauges or transfer standards because they are known to have better stability compared to other commercial types of hot cathode gauges.

We will present the results of reproducibility of sensitivity for gases N2 and H2 at a pressure of  $1 \cdot 10-5$  Pa after 5 times repetition of the following treatments: (i) bake-out at 150 °C for 24 h, (ii) degassing at 100 °C for 10 min, (iii) bombardment of ion collector with Ar ions at a pressure of  $9 \cdot 10-3$  Pa for 1 h, (iv) venting to the atmosphere, and (v) exchanging the filaments.

# Ultra-Rapid Microlfuidic Genotyping: From DNA Forensics to Post-Transplant Monitoring

James Landers

Over the last decade, we have explored the development of number of different microfluidic platforms for sample-to-result systems for genetic analysis. In 2006, we developed a crude glass microchip for the detection of B. anthracis in mouse blood and B. pertussis in a human nasal mucous in a fully-integrated microfluidic system. We extrapolated this technology to create a 'Rapid DNA' system initially for military deployment and criminal justice use, but with the potential for widespread adoption in the civilian sector. Here, we discuss the development of the next generation of technology with CD-sized microfluidics, a 30 minute sample-to-result time with autofluidics in a 5 kg instrument that carries out a 31-step process to generate a genetic profile. Highlight characteristics include single step DNA extraction, ultrafast PCR, and high resolution electrophoresis with multicolor fluorescence. We not only show application to forensic DNA analysis for human identification, but describe how this technology could be used for home testing by organ transplant patients to monitor organ acceptance or identify signs of rejection.

# Salophene on graphene, on-surface chemistry and spin polarization

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Graphene as an inert substrate which is easy to modify via intercalation is ideal for studies of single adsorbed molecules. When grown on Ir(111) and intercalated with Co or Fe it provides a very rare inert ferromagnetic substrate. Such a combination proved to be ideal to study the magnetic properties of metalorganic complexes. Dibromo-5,5'-metal-salophene is one of the more interesting metalorganic complexes due to its Ullmann coupling capabilities and coupling of metal spin with the ligand. Not all metal-salophenes are stable in ambient conditions, therefore, an in situ synthesis is desired.

In this presentation, I will show our recent results on the on –surface chemistry forming Fe and Cr salophenes directly on a substrate. Moreover, I will present an Ullmann like coupling on top of graphene. Finally, I will present some first spin-polarized scanning tunneling microscopy data unraveling the magnetic coupling of these complexes with the magnetic substrate.

#### The Magnetic Properties of Individual Atoms/Molecules on Solid Surfaces

Haiming Guo

Control over charge and spin states at the single atom and molecule level is crucial not only for a fundmental understanding of charge and spin interactions but also represents a prerequisite for development of spin tronics. Recently, we demonstrate that the Kondo resonance of manganese phthalocyanine (MnPc) molecules can be reversibly switched via a robust route through chemical absorption and desorption of a single hydrogen atom, and further the site-dependent g factor mapping was revealed within a dehydrogenated-MnPc molecule within intramolecular resolution. The modulation of magnetic properties and Kondo effect of magnetic adatoms on graphene layer was also studied, and we show the first discovery of a Kondo effect caused from a magnetic impurities doped in graphene layer in experiment. Finally I will present the investigation of different inter-atomic spin interactions of artificial Mn nanolusters registered on graphene with magnetic field dependent inelastic spin excitation spectroscopy. All the dimers observed exhibit an antiferromagnetic singlet ground state and spin transitions from singlet to triplet states, but their AFM coupling strength shows unique dependence on their site registration on the graphene template. More intriguing spin coupling can be found in graphene mediated non-collinear Mn trimer. The exchange energies cannot be understood by direct spin exchange mechanism, but suggesting the non-local Ruderman-Kittel-Kasuya-Yosida (RKKY) indirect spin exchange mechanism through substrate modulation, which has not yet been achieved in graphene so far. The works open up new opportunities to access local spin properties and quantum states at the ultimate molecular limit.

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# Light-Emitting Diodes with a Patterned Top Electrode

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In light-emitting diodes (LEDs) with light extraction via top surface most of the generated light is shielded by a top metal electrode. Enhancement of light extraction from such LEDs is still a challenging task. One of the possible approaches to cope with this problem is to pattern the LED's top metal p-electrode as a mesh. Mechanism of the observed performance enhancement is related to the potential profile created by the designed electrode along the active region. At properly chosen mesh pitch, the current can be injected into the uncovered portions of the active region. Light, which is generated in this area, can be efficiently extracted via the mesh windows. Implementation of the mesh-like electrode in the LEDs with two sets of InGaN/GaN quantum wells for blue and green emission results in broad electroluminescence (EL) spectra with blue and green peaks separated by shallow trough. In dual-wavelength LEDs the designed electrode can be attributed to the spatially nonuniform compensation of piezoelectric field in the InGaN QWs. In this paper we report on fabrication and characterization of single- and dual-wavelength blue-green LEDs with top mesh metal p-electrode as well as the the results of our analytical study.
#### The ITER rough pumping system design

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The ITER vacuum system will consist of a number of large volume systems including: the Cryostat (~ 8500 m3), the Torus (~1330 m3), the Neutral Beam injectors (~180 m3 each) and a number of lower volume systems. The Roughing Pumping System, pumps all gases originating from these vacuum volumes.

The Roughing Pump System contains many novel features to facilitate demanding but differing pumping duties and the safe confinement of tritium inventories. The pumping duties have been split into 10 modules which work together to provide the complete functionality so as to utilize conventional technologies where possible.

Roughing pumps will initially evacuate systems from atmospheric pressure to pressures at which the cryogenic and other high vacuum pumps can operate on the tokamak. During plasma operations, the most demanding duty is to pump the mixture of gasses originating from the regenerations of torus and neutral beam cryo-pumps, at rate of around 200Pa/m3/s. To pump the gas streams which will be dominated by hydrogen isotopes, the design utilizes 3 identical pumping modules each within a cell containing 2 cryogenic viscous flow compressors (CVC). The CVCs cryogenically condense hydrogen isotope mixtures and function in combination with a roots mechanical pumping set which compresses helium ash originating from the fusion process. The configuration requires just one type of mechanical pump (an all metal scroll) for the high tritium pumping duty.

In this paper an overview of the ITER roughing pumping systems design is presented and the validation progress for ITER operations given.

# Carbon-Based Functional Nanomaterials in 2D Confinement: On-Surface Synthesis, Aromaticity, and Molecular Topology

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On-surface synthesis of carbon-based nanostructures has attracted considerable attention as a versatile approach for the functionalization of interfaces and the preparation of new functional materials. In this lecture, examples for the on-surface synthesis and atomic-scale characterization of novel conjugated hydrocarbon and nitrogen-doped materials, organometallic compounds, and metal complexes with cyclic and open-chain topology will be discussed. A wide range of experimental techniques, including XPS, UPS, TPD, STM and nc-AFM are used to obtain a comprehensive understanding of the nanostructures. Unusual regionselectivity of C-C coupling reactions achieved by monoselective C-H bond activation will be explained based on the relevant reaction mechanisms.[1] Using aromatic precursors with non-alternant topology, it is shown that 2D confinement enables thermodynamic control over the important competition between macrocycle and chain formation.[2] In this context, the substantial effects of the molecular Hückel topology on the metal-organic interaction at the interface will be demonstrated.[3] Furthermore, it will be shown that naphthalocyanines and their expanded homologs can be prepared by template-directed on-surface synthesis from dinitrile precursors. This approach also gives first-time access to the linear open-chain counterparts of naphthalocyanines. Structure, electronic properties and reactivities of these nanosystems will be discussed based on extensive experimental results and theoretical modelling.

# Bragg Coherent Diffraction Imaging of Metal Diffusion in Nanocrystals

Ian Robinson<sup>1</sup>

### <sup>1</sup> London Centre for Nanotechnology

The Bragg Coherent Diffraction Imaging (BCDI) method will be introduced for its abilities for in-situ X-ray imaging in materials science. BCDI's greatest strength is to reveal 3D phase-contrast images of the interiors of crystals with image resolution in the 30nm range. It achieves this through the projection of lattice displacements onto the diffraction Q-vector, showing up as a phase shift on a very sensitive scale: one lattice constant results in a phase shift of  $2\pi$ . Using this new channel of information about the detailed structures of crystals, we have found striking patterns of phase nano-domains within otherwise solid-looking crystals up to one micron in dimension. Since almost all materials are made up of microcrystals, this method has wide application in materials science and engineering and lies at the heart of a case for new X-ray beamline at Max-IV, NSLS-II and elsewhere.

This invited presentation will describe the BCDI method and illustrate it with our work on Au nanocrystals. The shapes of nanocrystals are strongly influenced by the presence of internal strain which can be imaged in 3D. This leads to highly inhomogeneous structures during mixing following UHV deposition of metals because of the important role of strain. I will show the result of in-situ Cu and Fe diffusion into Au nanocrystals.

Atomic Diffusion within Individual Au Nano-crystal Gang Xiong, Jesse N. Clark, Chris Nicklin, Jonathan Rawle and Ian K. Robinson, Scientific Reports 4 6765 (2013)

Bragg Coherent Diffraction Imaging of Iron Diffusion into Gold Nanocrystals, Ana Katrina C. Estandarte, Christopher Lynch, Marianne Monteforte, Jonathan Rawle, Chris Nicklin and Ian Robinson, New Journal of Physics 20 113026 (2018)

# The Vacuum System Design Of A New FEL Test Facility (CLARA) at Daresbury Laboratory

Keith Middleman

Recent UK government funding has facilitated the construction of Phase 1 of a unique FEL accelerator test facility (CLARA – Compact Linear Accelerator for Research Applications). This test facility will allow the UK to research a variety of FEL operating modes to establish a roadmap for the UK and its plan to build a UK FEL user facility.

This paper will look specifically at the vacuum system design of this unique accelerator detailing the challenging design of the photoinjector, the FEL section and the possible use of NEG coating and the requirement for implementing a differential pumping scheme to separate two vacuum systems with 3 orders of magnitude pressure difference over 50 cm. Many other aspects of the accelerator design will be described and data showing the 'real' performance of the accelerator presented.

# Daresbury Laboratory's vacuum contribution to the European Spallation Source (ESS)

Keith Middleman

The European Spallation Source (ESS) relies on 60% of it's funding coming from European countries other than Sweden and Denmark, as part of this funding the UK agreed to a £165 million pound contribution to the project. Daresbury Laboratory in the UK has forged close links with various groups at ESS and is responsible for delivering £50 million pounds worth of UK contributions to the project.

This talk will highlight 2 main areas of contribution, firstly the delivery of over 70% of the ESS beam transport system, secondly the role Daresbury is playing in the delivery of the ESS High Beta Superconducting Cavities. The talk will look specifically at the vacuum system design and specifications, the cleaning and particle control procedures employed and the important role our ISO 9001 quality control system has in the overall process.

# Plasmon induced excitation of doublet emission at the single molecule level

Alberto Martin-Jimenez<sup>1</sup>, Koen Lauwaet<sup>1</sup>, Pablo Merino<sup>2</sup>, Jose Ignacio Martinez<sup>2</sup>, Rodolfo Miranda<sup>1,3</sup>, Roberto Otero<sup>1,3</sup>

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In this contribution we report a careful investigation of the topographic, electronic, and opto-electronic properties of electronically decoupled C60 nanocrystals by means of Scanning Tunneling Microscopy (STM), Scanning Tunneling Spectroscopy (STS), STM induced Light Emission (STM-LE), and Density Functional Theory (DFT), at the single molecule level. We have observed that depending on the tunneling parameters, we are able to reversibly switch from a broad plasmonic spectrum to a series of very sharp molecular resonances of 10meV width. Based on our STS data and DFT calculations we have reached a model to explain the molecular light emission of the C60 nanocrystals. We demonstrate that the emission arises from the recombination of a doublet exciton of negatively charged molecules (anions). Our results will contribute to the general understanding of the physical mechanisms involved in the light emission of organic molecules. They may also be of importance for applications such as single photon emitters or quantum computing, since future devices may need to be able to switch chromaticity in a controlled fashion.

# Surface Adsorbates probed by XPS during catalytic CO2 and CO hydrogenation at 150-450 mbar

David Degerman<sup>1</sup>, Peter Amann<sup>1</sup>, Mikhail Shipilin<sup>1</sup>, Anders Nilsson<sup>1</sup>

#### <sup>1</sup> Stockholm University

The new synchrotron endstation POLARIS, built by the authors, allows for studies of hydrogenation reactions by X-ray Photoelectron Spectroscopy (XPS) at pressures that has never been available before. I will briefly present the build-up process and design of the instrument and give an overview of our first results.

High pressure XPS has since long been limited to a few mbar due to the short mean free path of an electron in gaseous media. Utilizing a new design for the front cone of an electron analyzer and advanced positioning systems we have optimized the geometry to reduce the travel path of the electron to ~10-20 micrometer in gaseous media and thus allow for higher pressure than ever before. In an inert He atmosphere we have acquired spectra of metal surfaces in up to 2 bar atmosphere.

Synchrotron beamtime experiments have also been performed at beamline P22, PETRA III, Hamburg, Germany using various reactant mixtures of CO, CO2 and H2 between 150 and 450 mbar on Rh(111), Rh(211), Rh-Fe alloy, Fe(110) and Cu(111). Even though we have yet to reach industrially relevant pressures (>10 bar), the acquired data show signs of chemistry occuring where the surface species exhibit chemical shift with temperature. The intensities of the peaks also indicate two different temperature regimes where the low temperature comprise accumulation of hydrocarbon from CO2/CO dissociation and the high temperature regime have fast desorption of the adsorbates as they are produced.

# Synthesis of hard and super hard tribological coatings made by chemical vapor deposition

Mats Boman<sup>1</sup>, Linus von Fieandt<sup>2</sup>, Axel Forslund<sup>3</sup>, Henrik Larsson<sup>3</sup>, Mats Halvarsson<sup>4</sup>, Olof Backe<sup>4</sup>, Ren Qui<sup>4</sup>, Erik Lindahl<sup>2</sup>

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- <sup>4</sup> Chalmers, Gothenburg, Sweden

In thermally activated chemical vapor deposition, the chemical identity of the precursors interacts with the processing parameters, and together they will define several of the properties of the final coating. During the deposition process, precursors undergo chemical reactions on or in the vicinity of the substrate surface, i.e. either heterogeneously and homogeneously. In both cases, such chemical reactions will influence the properties of the deposit.

In my talk I will give some recent examples of how the tribological properties of CVD-coatings can be deliberately affected by a proper choice of the deposition parameters. As an example, almost single crystalline thin films of super-hard Ti(C,N) will be shown as well as how this coating could be optimized by applying a proper combination of precursors and processing parameters. As a result, coatings with a better tribological performance were obtained.

The CVD coatings were characterized by HR-SEM, HR-TEM, ERDA, nano-indentation, several XRD-techniques and AFM. By complementing with various calculations, using methods as DFT, thermodynamic modeling and consideration of kinetics, the investigation gained a more in depth view of the how the coatings were formed.

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# Precise setting of VCSEL resonance wavelength by dry etching

Mehdi Jahed<sup>1</sup>, Johan Gustavsson<sup>1</sup>

<sup>1</sup> Chalmers University of Technology, Department of Microtechnology and Nanoscience, MC2, Photonics Laboratory, Gothenburg, Sweden

With an intra-cavity phase tuning technique, we demonstrate less than 2 nm precision in wavelength setting of vertical-cavity surface-emitting laser (VCSEL) micro-resonators in the wavelength range 1040-1070 nm using an Ar ion-beam etching process with sub-nm precision in etch depth. This post-growth fabrication technique for controlling the wavelength of individual VCSELs is promising for the development of monolithic multi-wavelength VCSEL arrays with precisely defined wavelengths for wavelength division multiplexed (WDM) optical interconnects and the assembly of compact and high-capacity WDM transmitters.

# PVD Ni-GDC anodic films for SOFCs via Fuzzy and Electrochemical Modelling

Waqas Hassan Tanveer<sup>1</sup>, John Andersen<sup>1</sup>, Maroto Valer Mercedes<sup>1</sup>, Suk Won Cha<sup>2</sup>

<sup>1</sup> Heriot Watt University

<sup>2</sup> Seoul National University

Nickel-Gadolinium Doped Ceria (Ni-CGO) anodic films of 300nm thickness (T1), were deposited on 50~300µm thick (T2) zirconia electrolyte supports, by radio frequency (RF) sputtering. The sputtering was done at 25°C and the RF power (P) was varied between 50~200W. Lanthanum Strontium Manganite (LSM/YSZ) cathodes were screen-printed on the other side of the supports. The solid oxide fuel cells (SOFCs) were tested for maximum power densities under the product fuel of CO2 electro-reduced via industrial waste carbon(IWC)1 at a temperature (C) range of 600°C ~ 800°C by voltage (V)-current (I)-power curves. The resistances of various cell components were measured by nyquist plots. From the results of these electrochemical measurements, a fuzzy model was built with T1, T2, P, C, & V as inputs and I as output. Then, the particle swarm optimization (PSO) algorithm was applied to obtain the optimal parameters of the SOFC, which maximizes its power density. Furthermore, high resolution scanning and transmission electron 2D images were used to build an electrochemical model to simulate the reaction kinetics of these optimized IWC-SOFCs. The results showed that the PVD Ni-CGO based IWC-SOFC's power density can be increased by 45% when using the PSO algorithm when compared with experimental results.

### Simulation of Diamond Surface Chemistry - Reactivity and Properties

Karin Larsson

The diamond material possesses very attractive properties, such as superior electronic properties, large electrochemical potential window, and a controllable surface termination. Boron-doped diamond surfaces are nowadays working as a new class of electrode materials. The boron-doped diamond electrode is a semiconducting material with very promising properties like i) a wider potential window in aqueous solution, ii) low background current, and iii) corrosion stability in aggressive environments. The phenomena of diamond surface termination have experimentally been observed to significantly influence the broad-band infrared reflectivity and conductivity. H- terminated diamond surfaces have been found to be hydrophobic, and to show unique p-type surface electronic conductivity. On the other hand, oxygen-terminated diamond surfaces generally show hydrophilic properties, but no electronic conductivity.

The surface reactivity of diamond is expected to affect both chemical processes at the surface and properties related to the surface electronic structure. Examples of factors with the capability to influence the surface reactivity are i) type of plane, ii) surface termination, and iii) doping. Theoretical modeling based predominantly on Density Functional Theory (DFT) has during the last decade proven to become highly valuable in the explanation and prediction of experimental results. The simulation and theoretical analysis of especially surface reactivities has been shown to aid important information.

At this presentation, the effect of surface plane, termination and doping (B, P, N) on diamond surface electronic properties, will be presented by showing our recent theoretical result in the field of photocatalytic conversion of CO2 to fine chemicals and fuels using visible light.

# SiGe(001) Thermal Oxidation Investigated Using Ambient Pressure X-ray Photoelectron Spectroscopy

Gregory Herman<sup>1</sup>, Shane Lorona<sup>1</sup>, Trey Diulus<sup>1</sup>, Rafik Addou<sup>1</sup>

<sup>1</sup> Oregon State University, Corvallis, OR, USA

Silicon germanium (SiGe) is an important technology to improve the functionality of metal-oxide-semiconductor field effect transistors (MOSFET) for current and next generation complementary circuits. SiGe has many useful properties including high carrier mobilities and compatibility with standard silicon based processing. However, controlling the semiconductor-dielectric interface for SiGe is more challenging than Si due to the different thermodynamic stabilities of SiO2, GeO2, and their alloys. In this study, we have performed laboratory-based ambient pressure X-ray photoelectron spectroscopy (AP-XPS) on SiGe(001) surfaces to better understand the initial thermal oxidation processes at the SiGe surface. Chemical state resolved AP-XPS was performed at temperatures up to 300 C and O2 pressures up to 1 mbar. We have found that both Si and Ge thermally oxidize with two distinct regions at 300 C and 1 mbar. First there is a rapid oxidation regime, which is then followed by a quasi-saturation regime with a much slower oxidation rate. We find that the Si4+/Si0 and Ge4+/Ge0 ratios have very similar rates in both the rapid and quasi-saturation regime, but that the Si4+/Si0 ratios are always larger than the Ge4+/Ge0 ratios. To evaluate preferential SiO2 growth we have also performed experiments at lower oxygen pressures at 300 C. We have found that we can decrease the Ge content in the mixed oxide by controlling the oxygen partial pressure, which should lead to improvements in the electronic properties of the oxide/SiGe interface. These studies indicate that AP-XPS provides valuable insight into processes relevant to the semiconductor industry.

# **Emerging Materials for Photovoltaics and Optoelectronics**

Vanja Blazinic<sup>1</sup>, Dargie Deribew<sup>1</sup>, Leif Ericsson<sup>1</sup>, Ellen Moons<sup>1</sup>

<sup>1</sup> Karlstad University

### Spin structure of K valleys in single-layer WS2 on Au(111)

Markus Donath<sup>1</sup>, Philipp Eickholt<sup>1</sup>, Lukas Musiol<sup>1</sup>, Charlotte Sanders<sup>2</sup>, Maciej Dendzik<sup>2</sup>, Luca Bignardi<sup>3</sup>, Daniel Lizzit<sup>3</sup>, Silvano Lizzit<sup>3</sup>, Albert Bruix<sup>2</sup>, Philip Hofmann<sup>2</sup>

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Since the discovery of graphene, two-dimensional materials have driven intense research effort due to their fascinating electronic and optical properties. With respect to optoelectronic applications, semiconducting materials such as W- and Mo-based transition metal dichalcogenides are especially appealing. These materials exhibit an indirect-to-direct band-gap transition upon reducing the thickness to a single layer.

The spin structure of the valence and conduction bands at the K and K' valleys of single-layer WS2 on Au(111) is determined by spin- and angle-resolved photoemission and inverse photoemission [1]. The bands confining the direct band gap of 1.98 eV are out-of-plane spin polarized with spin-dependent energy splittings of 417 meV in the valence band and 16 meV in the conduction band. The sequence of the spin-split bands is the same in the valence and in the conduction bands and opposite at the K and the K' high-symmetry points. The first observation explains "dark" excitons discussed in optical experiments; the latter points to coupled spin and valley physics in electron transport. The experimentally observed band dispersions are discussed along with band structure calculations for a freestanding single layer and for a single layer on Au(111). Furthermore, the data for a single layer are compared with data for the surface of bulk WS2.

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# Nanoscale frictional properties of ordered and disordered MoS2

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The present work aims to understand the sliding of ordered or disordered molybdenum disulfide (MoS2) coatings against each other by combination of nanoscale sliding experiments and atomistic simulations. Disordered (polycrystalline) thin films of MoS2 were prepared by using radio frequency magnetron sputtering technique with a 150 W power from a 99.99 % purity MoS2 target. The 1x1 cm2 Si(111) single crystal substrates were coated by 200 nm MoS2. Single crystal MoS2 substrate was also used for comparison. Tribological experiments were performed using lateral force microscopy with AFM cantilevers (force constant 3 N/m) coated by 100 nm thick MoS2 coating.

The tribological characterization was performed in contact mode forcing the tip to slide on a single 5 micrometer line with 1 micrometer/s scanning speed. We detected the friction force during a load-decreasing ramp, starting at approximately 1.5 micronewton load down to the pull-of-force. The average coefficient of friction obtained in nitrogen atmosphere is 0.41±0.05 for disordered (polycrystalline) coating and 0.0121±0.0017 for ordered MoS2 single crystal.

Nanoscale contact area between the MoS2-coated tips and MoS2 samples opened up the possibility for close comparison with classical molecular dynamics simulations. Our simulations replicated well the coefficient of friction obtained by experiments for various contact conditions and shed light on nanoscale sliding of both crystalline and amorphous MoS2.

Experimental sliding at humid environment demonstrated detrimental effect of water molecules on the increasing of the friction coefficient. Such increase may cause the degradation of MoS2 lubricating properties. This work may shed light on the reasons of the degradation of a MoS2 as a dry lubricant.

# In situ TEM observations of Cu redox dynamics

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### <sup>1</sup> ScopeM, ETH Zurich

Catalysts need to be investigated under relevant conditions since the active surface of catalysts tends to be metastable and adopts to the chemical potential of surrounding atmosphere. In situ transmission electron microscopy (TEM) has proven to be a powerful method for studying the atmosphere and temperature induced dynamic changes of catalysts at µm to Å scale. Herein, we present an in situ TEM study on the state of copper nanoparticles during the hydrogen oxidation at near ambient pressure. Through combination of real-time imaging with on-line mass spectrometry, we are able to build a relationship between the structural dynamics and the catalytic activity. We reveal that water formation correlates with a highly dynamic state of the copper catalyst. Co-feeding of hydrogen and oxygen results in the simultaneous presence of metallic copper and copper oxide. Structural dynamics such as particle sintering and splitting as well as the involvement of the bulk in the redox process are directly observed. Based on the present observations we can conclude that active sites are not static, but rather associated with transient states which are constantly generated in response to the chemical potential of the gas phase.

# **XUV Free Electron Laser based Nonlinear Optics**

Claudio Masciovecchio1

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The recent advent of Free Electron Lasers (FELs) allowed to push experimental techniques peculiar of table top pulsed laser towards much shorter wavelength allowing to probe dynamical processes with an unprecedented time-space resolution. Within the portfolio of FEL based experimental methods we will discuss the new opportunities offered by the extension of non-linear spectroscopies in the vacuum ultraviolet to soft X-ray energy range. Pioneering wave mixing experiments have been successfully carried out at the FERMI FEL, signifying that second harmonic generation and four wave mixing experiments are now possible at nanometer wavelength. These results pave the way to a new class of experiments like investigation of heat transfer at the nanoscale or energy transfer in light harvesting devices.

### Atom probe tomography: Analysis of soft matter, liquids and interfaces at the top of the tip

Guido Schmitz<sup>1</sup>, Patrick Stender

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Atom probe tomography is an exciting tool in the analysis of nano-structured materials, interfaces and surfaces. The method stands out by joining single-atom sensitivity with a volume reconstruction, that delivers three-dimensional maps of the atomic arrangement. Due to this direct 3D information, the method is especially suitable for the investigation of complex microstructures that comprise curved or rough interfaces. By extension with laser-assisted evaporation modes, the analysis of semiconductors and ceramics has become a substantial task. Nowadays, the method is about to break the barrier towards soft matter and liquids.

The talk provides an overview of the experimental technique. Modern concepts for improving the data processing and the tomographic volume reconstruction are described. Atom probe tomography is well established in the analysis of solid-state materials. The analysis performance is demonstrated with recent examples of nano-crystalline thin films and silicide formation.

Atom probe analysis of soft matter is still a widely unexplored landscape. Well-controlled field-desorption of macromolecular materials has been confirmed by studies of self-assembling monolayers and polyelectrolyte coatings. An accurate volume reconstruction, however, would become possible only after having derived a detailed understanding of the complex evaporation sequences. For the analysis of liquids, the method is combined with cryo-preparation. For this purpose, at the University of Stuttgart, a dedicated atom probe has been attached to a cryo dual beam scanning microscope. The unique instrument has the potential of analysing liquid/liquid and solid/liquid interfaces. Exemplary analyses of sugar solution demonstrate the cutting-edge possibilities of the innovative instrument.

# Epitaxial semiconductor-superconductor hybrid materials for topological superconductivity

Thomas Kanne Nordqvist<sup>1</sup>, Dags Olsteins<sup>1</sup>, Mikelis Marnauza<sup>1</sup>, Lunjie Zeng<sup>2</sup>, Damon Carred<sup>1</sup>, Martin Bjergfelt<sup>1</sup>, Joachim Sestoft<sup>1</sup>, Erik Johnson<sup>1</sup>, Thomas Sand<sup>1</sup>, Eva Olsson<sup>2</sup>, Jesper Nygård<sup>1</sup>

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Semiconductor-superconductor hybrid materials with proposed one or two-dimensional topological classification is a new and interesting class of materials. The field is mainly driven by the search for materials hosting Majorana bound states, which is expected to become building blocks for topologically protected quantum computation.

In this study we present recent progress in finding new material combinations that eventually would allow for a broader parameter space when designing new quantum transport experiments.

Atomically sharp and aligned bi-crystal interfaces between nanoscale materials that individually possess unique physical properties are realized by state of the art molecular beam epitaxy growth techniques. We discuss what material combinations that are experimentally possible and determine the driving forces that play the defining role in the minimization of the superconducting grain excess energy. The superconducting films are, in this study, all deposited on highly defined type 1 or 2 faceted nanowires, but the general mechanisms would presumably also apply on two-dimensional thin films. We find that the contributions to the overall excess energy determines not only the bi-crystal interfacial domain match and overall grain size and morphology but also enable a theoretical prediction of which materials that possibly would yield a large grain hetero-epitaxial interface. Additionally, we discuss new mechanisms that promote increased flatness and a reduction of possible bi-crystal orientations. We show preliminary electrical measurements indicating that these materials would eventually become very promising for topological superconductivity and quantum transport experiments in general.

### Floating bilayers as planar models to study membrane-nanoparticle interactions and membrane protein function.

GIOVANNA FRAGNETO<sup>1</sup>

# <sup>1</sup> INSTITUT LAUE-LANGEVIN

Cells, the basic units of living organisms, are well delineated and separated from the external environment by membranes. Capable of both enclosing the cellular constituents and allowing exchanges with the outside world, these membranes are only a few nanometers thick. To study the dynamics and function of these amazing objects, physicists first seek to understand their structure. This involves experiments on model systems, simpler and better controlled than real membranes, and can profit from a probe that is able to access different scales of size and time: thermal neutrons.

Since the pioneering work in the seventies on cell membrane structure by neutron scattering, developments driven by constantly improving neutron instrumentation, coupled with development of measurement and analysis methods, have involved both the optimization of samples towards more biologically relevant model systems and include the use of more complex lipid mixtures up to natural extracts.

Recent developments in the study of the structure of membranes will be presented including:

- Neutron reflectometry experiments combined with atomistic and coarse-grained molecular dynamics simulations to study the interaction between cationic gold nanoparticles and model lipid membranes composed of floating lipid bilayers: understanding the molecular mechanisms governing nanoparticle-membrane interactions is of prime importance for drug delivery and biomedical applications.

- Neutron and x-ray reflectometry study of the out-of-equilibrium fluctuations of phospholipid membranes induced by the active transmembrane protein bacteriorhodopsin (BR). A detergent-mediated incorporation method was used to incorporate BR in model planar bilayers and structural modifications induced by light activation were measured.

# Coherent x-ray imaging of nano-structures

Ivan Vartaniants

Coherent X-ray Diffraction Imaging (CXDI) is presently rapidly developing technique that allows to determine electron density in the forward scattering experiments or deformation field in nano-crystals in the Bragg scattering geometry. CXDI is based on the phase retrieval of the coherently scattered intensity from the sample. Ptychography is a branch of CXDI that allows to perform coherent imaging of extended object by overlapping the probe positions. In my talk I will present few examples of application of CXDI and prychography to understanding of the structure of single colloidal grains [1], deformation field in single nanowires [2-4], and strain evolution in catalytic nano-particles in different environment.

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# **III-V Nanowire MOSFETs**

Lars-erik Wernersson

III-V nanowires are attractive for various device applications. The small nanowire footprint reduces the possibility for defects to propagate from the substrate opening a path for integration of high-quality III-V materials on Si. The advantageous transport properties find usage in transistor applications where the reduced scattering enhances the drive current. The realization of such devices, requires processing strategies for structures with 10 nm dimensions and detailed material characterization to avoid detrimental parasitic effects on the device performance. Besides, the direct band gap and the wide range of wave lengths addressable makes the material suitable for optoelectronic applications including light emitting diodes, solar cells, and long wave length photodetectors.

In this talk, III-V heterostructure nanowire MOSFETs and TunnelFETs will be presented and benchmarked towards Si MOSFETs. Devices with state-of-the-art performance in terms of transconductance (gm), drive current (lon), subthreshold swing (S), and offstate leakage current (loff) will be presented. In particular, we will focus on InAs/InGaAs heterostructure MOSFETs and InAs/InGaAsSb/GaSb TunnelFETs, where the nanowire growth technology allows for incorporation of materials with strong lattice mismatch into the transistor channel. These heterostructures are essential for the III-V device performance both in terms of reducing the off-state leakage currents and for expanding the useable voltage range.

# Atomic Switches and Beyond: Fusion of Digital and Analog in Nanoelectronic Devices

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The atomic switch, which was invented/developed by some of the present authors (MA, KT) and co-workers more than a decade ago [1-3], has recently been put to practical use as a field programmable gate array (FPGA) by NEC Corp. [4]. As compared to conventional FPGAs, NEC's new FPGA is characterized by nonvolatility, small size (~1/3), low power consumption (~1/10) and remarkable radiation tolerance (~100 times), so that it is going to be used in a wide variety of fields. In the present paper, we also focus on various novel devices derived from the atomic switch, i.e., an artificial synapse [5], an electric-dipole-layer transistor [6], an ionic decision maker [7], etc., which will make great contributions to ICT, IoT, and AI. A comprehensive list of papers related to the atomic switch (until 2017) is available at the end of the following booklet: https://www.nims.go.jp/mana/atomswitch2017/

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- [7] T. Tsuchiya et al., Science Advances 4 [9] (2018) eaau2057.

## Microfabricated organ-on-chip models

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Organ-on-chip is an emerging research field with the aim to combine microtechnology and biology to develop microphysiological model systems for biomedical research and drug development. In my research group, we focus on developing microfabricated and micropatterned hydrogel-based 3D cell culture scaffolds with the aim to provide in vivo like culture conditions for cells cultured as models of biological barriers.

We are specifically exploring biologically derived hydrogels as these initially contain necessary cell adhesion motifs. These polymers can also easily be functionalised with growth factors or chemical moieties for controlled cross-linking via different pathways such as heat or UV light. We are studying how the processing parameters affect the mechanical properties of the gels and how this in turn relates to the cell proliferation for 2D and 3D cultures using these culture scaffolds. Further, we are investigating additional schemes to control the chemical functionalisation of the scaffolds to achieve specific cell adhesion or incorporation of growth factors.

To be able to obtain direct read-out of the barrier integrity in our systems, we have developed integrated transparent electrodes fabricated in ITO and structured these in proximity to the cell culture site for optimal signal-to-noise ration by using transparent electrodes allows for a combined electrical and microscopy read-out which is beneficial.

# Measurement of surface diffusion at solid liquid interfaces using in situ linear optical diffraction

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### <sup>1</sup> CAU Kiel Germany

Surface diffusion at solids in liquid environment is a fundamental process in many interface reactions, but much less understood than surface diffusion under vacuum conditions. Because these processes occur at or near room temperature, the diffusion rates of most adsorbates are too high for direct microscopic measurements, e.g. by scanning probe microscopy. We present a novel in situ method to measure the surface diffusion rates in such systems. It is based on the linear optical diffraction technique, which has been used extensively for diffusion studies under vacuum conditions. Here, a density grating in an adsorbate layer is created by thermal desorption induced by the two interfering beams of a nanosecond Nd:YAG laser. The evolution of the grating is then probed by linear optical diffraction of a HeNe laser beam at the grating. From the exponential decrease of the diffraction intensity the surface diffusion coefficient can be extracted. The technique allows measurements of surface diffusion at solid-liquid interfaces over several orders of magnitude at variable coverages and electrode potentials, making it suitable for a wide range of adsorbate systems. In addition to the experimental setup, first experimental results for the surface diffusion of CO on Pt(111) electrodes are described.

#### Development of Sustainable, Smart, Secure, and Safe Society by Transformative Electronics

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Vacuum technology has been playing a key role in the establishment of smart systems. The role of vacuum technology will become even more important in the future for establishing a sustainable, secure, and safe society. In this presentation, I would like to discuss how to establish a future society through the Internet of Energy for connection of the electronics system at any time and any place. Because of ubiquitous energy transmission systems, one need not worry about a shortage of electric power. We can realize such a transmission system with high efficiency using GaN-based devices and modules. One of the most important items is electric vehicles (EVs). However, EVs can be driven only in a short range owing to insufficient battery capacity. The long charging time of EVs is another problem. To solve these problems, we are trying to establish a new wireless electricity transmission system. If an EV can be charged while driving, it will run like a tram, but with more freedom because it can be driven anywhere. Drones have the same problem as EVs, that is, they can fly only in a short range on a single charge. If drones can be charged while flying, we can expect drones to fly all day, increasing their applications such as in the inspection of old bridges, roads, and buildings. In such a way, we will no longer need to worry about electricity shortages, not only for EVs and drones, but also for any electronic system.

# Surface chemistry and degradation of Li2VO2F Li-rich disordered rock-salt cathodes

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Li-rich disordered rock-salts, are a new promising candidates for next-generation cathodes in Li-ion batteries. This is due to their ability to reversibly cycle more than one Li-ion per transition metal. Several new variations of these Li-rich materials have been developed with promising initial capacities. The road block is, however, capacity fade and voltage decay during cycling. These detrimental processes need to be understood to allow for the design of new materials where these reactions are mitigated. In this study the origin of the capacity fade in the Li-rich material Li2VO2F is investigated. Li2VO2F, consists of the multivalent V3+/V5+ redox couple with the incorporation of ideally two Li+ per TM. This gives a theoretical capacity of 462 mA h g-1. Not all of the lithium can be extracted from the structure due to stability constraints, but experimental capacities as high as 420 mA h g-1 (i.e. 1.8 Li+ per TM) can be obtained. Based on careful photoelectron spectroscopy studies using the advantage of tuning the photon-energy of the beam bombarding the sample depth profiles of the surface of the cathode particles can be obtained. The results show the degradation to begin at the particle surface and then spreading inwards with continued cycling. There is both a redox reaction of the vanadium taking place at the surface as well as the buildup of a surface layer. The presentation will compare these results with those from other lithium rich cathode materials.

# Towards Operando Photoelectron Spectroscopy on Lithium Ion Batteries

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The solid electrolyte interphase (SEI) which is formed as heterogeneous film on the negative electrode is considered one of the least understood parts in the lithium-ion battery. It is known that the SEI forms from decomposition products of the liquid battery electrolyte on the negative electrode at electrochemical potentials close to that of lithium. The exact formation mechanism of the SEI and how this influences the functionality of the battery is unclear It is both an electrode protection layer with Li-ion conductivity and a layer leading to irreversible loss of lithium. In this presentation, we will first discuss the challenges of SEI characterization and then present our approach to operando ambient pressure x-ray photoelectron spectroscopy (AP-XPS) on lithium ion battery systems. This technique can provide the key tool that has been missing so far to probe the functionality of the electrode/electrolyte interface in more realistic battery environments. We will show our results of AP-XPS characterizations of liquid carbonate-based battery electrolytes, battery electrodes such as thin films of lithium cobalt oxide with the liquid electrolyte present, and how the electrochemical reactions of a battery can be driven and followed inside a spectrometer.

# Assessing the Application Potential of Electronic Devices based on Graphene and related 2-dimensional Materials

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Graphene has been researched intensely over the past 15 years. Its intrinsic electronic and physical properties are unrivaled in many aspects. Hundreds of related two-dimensional (2D) materials with different properties have since been added to the "2D Zoo". Physicists, chemists, material scientists and engineers continue to report new highlights on a daily basis. Yet, there are no end-customer products on the market today where 2D materials are utilized as a active elements in in electronics, optoelectronics or sensing, because the process technology is not yet mature. In this talk, I will introduce promising applications, for which 2D materials clearly could make a difference, such as photodetectors [1], [2] and pressure sensors [3], [4]. I will further discuss the major bottlenecks towards integration of graphene and 2D materials into semiconductor processing lines.

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[2] C. Yim et al., "Wide Spectral Photoresponse of Layered Platinum Diselenide-Based Photodiodes," Nano Letters, vol. 18, no. 3, pp. 1794–1800, Mar. 2018.

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### Data Driven 4D X-ray Imaging of Nanoscale Dynamics

Mathew Cherukara

Observing the dynamic behavior of materials can reveal insights into the response of materials under non-equilibrium conditions of pressure, temperature and mechanical load. Such insights into materials response under non-equilibrium is essential to design novel materials for catalysis, low-dimensional heat management, piezoelectrics, and other energy applications. However, material response under such conditions is challenging to characterize especially at the nano to mesoscopic spatiotemporal scales. Time-resolved coherent diffraction imaging (CDI) is a unique technique that enables three-dimensional imaging of lattice structure and strain dynamically. In this talk I will present some examples of our recent work on imaging and modeling of phonon transport and lattice dynamics in nanomaterials under a variety of external stimuli. I will highlight the use of experimentally informed models that leverage large-scale computational resources. These experimentally informed models were used to provide information complementary to the imaging experiment, and at spatio-temporal scales inaccessible to the experiment.

With the upgrades to synchrotron sources around the world, it will become possible to image at similar resolution to what is attainable today with significantly shorter acquisition times, or conversely acquire significantly higher resolution data using the same acquisition times as today. Either route will create challenges associated with data/memory that will necessitate unconventional approaches to image recovery. I will describe our work in the use of deep generative neural networks (CDI NN) in accelerating the analysis of, and potentially increasing the robustness of image recovery from X-ray diffraction data. Once trained, CDI NN is thousands of times faster than traditional phase retrieval algorithms used for image reconstruction from coherent diffraction data, opening up the prospect of real-time 3D imaging at the nanoscale.

#### Deep UV lithography in a university owned nano-fabrication facility, benefits versus complexity and cost

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<sup>1</sup> DTU Nanolab

DTU Nanolab owns a 248 nm Canon FPA-3000 EX4 DUV stepper. The specified resolution limit is 250 nm, but we have successfully printed 140 nm structures. The tool can process 4, 6 and 8 inch wafers.

There is an increased need for sub-micron resolution in many research areas, such as optics and micromechanics. The DUV stepper fills the gap between UV and e-beam lithography. It is very fast (40 wafers per hour) and results are highly reproducible. Furthermore, it offers full scalability from R&D to production. To our best knowledge, our DUV stepper is the only university open-access DUV stepper in Europe.

The turn-around-time from submission of design file to printed structure is typically in the order of 2-3 weeks, including one week for fabrication of the reticle (mask). The cost of a DUV stepper reticle is roughly 5 times the cost of a UV contact mask. Most submicron patterns need simulation before exposure to help find the best process window. DTU Nanolab uses the Prolith software package from KLA-Tencor.

The stepper has specially dedicated fully automated cassette-to-cassette coater and developer systems. Optical microscope and SEM are used for inspection and metrology. Apart from consumables like BARC and photoresist we also spend money on a service contract with Canon. The staffing on the stepper is 2 full time equivalents.

Several private companies are using the stepper to manufacture their devices, such as integrated optical waveguide devices for telecommunications, micro- and nanoprobes for resistivity mapping and submicron gratings for spectrometer applications.

## European XFEL - A new large scale X-ray Facility for basic Science

Robert Feidenhansl

Hard X-ray Free Electron (XFEL) lasers provide extremely and intense and ultra-short X-ray pulses that are ideal to investigate structural and dynamics of matter at very short time scales. X-ray free electron lasers have been in operation for 10 years now and have had wide range of areas of applications in physics, chemistry, materials and structural biology.

European XFEL is the most recent large scale research infra structure in Europe and was taken into user operation in September 2017. It is a hard X-ray free electron laser and provides a very powerful X-ray beam for research. European XFEL is an intergovernmental organization with 12 member states and is a facility that serves the European user community by providing the possibility for performing new classes of experiments to investigate the structure and dynamics of matter on the atomic length and time scales. The facility encompasses a 3.5 km long tunnel from DESY in Hamburg/Bahrenfeld to Schenefeld in Schleswig-Holstein where the experimental hall is placed. The tunnel encloses a 2 km long superconducting accelerator operated by DESY and undulator radiation sources. The first two experimental stations have been in operation doing user experiments for about one and a half years, one of them the SPB/SFX instruments for structural biology. Two more experimental stations were taken into operation end of last year. In total six instrumental stations will be in user operation by mid-2019. In the talk the basic principles of European X-FEL will be discussed and results of some of the first experiments will be shown.

# Metrological behaviors of ionization gauges with carbon nanotube cathodes

Yongjun Wang, Detian Li, Xiaoqiang Pei, Huzhong Zhang, Yongjun Cheng

In this work, an ionization gauge with carbon nanotube cathode was developed, and its vacuum metrological characteristics in different gases were studied in detailed. It is found that the developed ionization gauge exhibits excellent measurement linearity from 10-8 to 10-4 Pa in N2, H2, O2 and air, respectively, and the linear response region for He only lies in the range from 10-8 to 10-4 Pa. It is also found that the gauge sensitivities are highly dependent upon gas species and anode voltage, and a high sensitivity factor as high as 0.205 Pa-1 is acquired for N2 under an anode voltage of 300 V, which is the first reported carbon nanotube cathode ionization gauge whose sensitivity is higher than the parent hot cathode one. This novel cathode ionization gauge is very promising in space exploration applications.

# A field emission performance test device for continuous adjustment of the electrode spacing in the vacuum system

Xiaoqiang Pei, Yongjun Cheng, Detian Li, Wenjun Sun, Huzhong Zhang

This work presents a device that can adjust electrode spacing inside a vacuum system to evaluate the field emission characteristics of the carbon nanotube array cathode grown on a stainless steel (SS) substrate. It was made by coaxial connection of the rear end of a screw micrometer, which acts as the anode, with a stepper motor. The distance between the anode and the cathode was controlled by altering the pitch of the stepper motor with an angle precision of 1 degree. Therefore, the electrode separation can be tuned in the range of  $0 \sim 15$ mm at  $1.388 \mu$ m incremental steps. Comparing with devices with a fixed electrode spacing, the advantage is that this device allows continuous regulation of the electrode spacing after it is placed in a vacuum system to test the emission properties under various electrical parameters in one process thus avoiding repeated breaking of the vacuum environment. Therefore, test efficiency is improved, hence saving manpower, material resources, testing time and greatly reducing the cost of experimentation. This device is simple in structure and relatively easy to prepare.

# Controlling graphene functionalization and intercalation

Liv Hornekaer<sup>1</sup>

<sup>1</sup> Aarhus University

Extensive control of the electronic and chemical properties of graphene on Ir(111) is available through chemical functionalization and intercalation. Combined Scanning Tunneling Microscopy, (Standing Wave) X-ray Photoemission Spectroscopy and Density Functional Theory calculations show how on one hand, functionalization structures can be controlled via intercalation, while conversely, intercalation can be hindered via chemical functionalization. Hydrogen functionalization allows for extensive control of electronic properties for band gap engineering - a tunable band gap of up to at least 450 meV can be induced by nano-patterned functionalization templated by the moiré pattern. In addition, hydrogen functionalization enables control of the graphene-substrate interaction, providing proof-of-principle pathways to e.g. enhance the coating properties of graphene on metal surfaces. Furthermore, unique oxygen functionalization structures and molecular hydrogen dissociative adsorption pathways are available in this system.

# Factors Controlling Ion Uptake in Organic Electrochemical Transistors

David Ginger

Organic electrochemical transistors (OECT) are of interest for applications in biochemical sensing and signal transduction across the biological/digital divide. The excellent performance of conjugated polymers in these applications is due to the ability of the polymer to accommodate ionic countercharge throughout the transistor volume. The resulting volumetric capacitance allows for very large modulations of the charge density in the transistor channel and large transconductance values. Combining OECT measurements on different polymers with different counter ions, we study how polymer morphology, polymer structure, and the chemical nature of the counter ion all combine to affect ion uptake, and the coupling between ionic and electronic transport. Furthermore, we use electrochemical strain microscopy (ESM) to probe local swelling resulting from ion uptake, and photoinduced force microscopy (PiFM) to probe the IR fingerprints of ion injection. We correlate both methods to gain insight into how local polymer structure governs ion uptake, providing microscopic insight into these processes that lead us to propose new material design rules.
# Femtosecond electron-phonon lock-in via photoemission and x-ray free-electron laser (invited speaker)

Zhi-Xun Shen

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High-temperature superconductivity in cupper and iron based materials, with critical temperature well above what was anticipated by the conventional theory, remains a major unsolved physics problem today. The challenge of this problem is symbolized by a complex phase diagram consists of intertwined states with unusual properties in addition to unconventional superconductivity. These states are different manifestations of the same underlying physical system consists of multiple degrees of freedom, making an integrated understanding a necessity.

In this talk, we present experimental evidence for electron-spin and electron-phonon interactions in these superconductors. We then discuss a general theme of cooperative enhancement and positive feedback loop of different interactions exemplified by electron-electron and electron-phonon interactions [1-3]. In particular, we focus on the capabilities from newly developed ultrafast spectroscopy and diffraction capabilities from x-ray free electron laser (XFEL). In such multimodal experiments, the precision measurements of electron's energy, momentum and time dynamics provide evidence for cooperative interplay of different degrees of freedom as a route to increase the effective interactions, and the resulting superconducting properties. We will also provide some general outlook for the future application of ultrafast technique for condensed matter and materials physics research.

References:

[1] J.J. Lee et al., Nature 515 (2014)

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# Miniaturization, Hybrid Integration and Applications of GaN MicroLEDs

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Gallium Nitride light-emitting-diode technology has been the revolution in modern lighting. In the last decade, a huge global market of efficient, long-lasting and ubiquitous white light sources has developed around the inception of the Nobel-price-winning blue GaN LEDs. Today GaN optoelectronics is developing beyond lighting, leading to new and innovative devices, e.g. for microdisplays, being the core technology for future augmented reality and visualization, as well as point light sources for optical excitation in communications, imaging, and sensing. This explosion of applications is driven by two main directions: the ability to produce very small GaN LEDs (microLEDs and nanoLEDs) with high efficiency and across large areas, in combination with the possibility to merge optoelectronic-grade GaN microLEDs with silicon microelectronics in a fully hybrid approach. GaN LED technology today is even spreading into the realm of display technology, which has been occupied by organic LED (OLED) and liquid crystal display (LCD) for decades. In this talk, the exciting properties of GaN micro- and nanodevices beyond lighting will be discussed, including the growth and processing issues, with an up-to-date overview on the state of the art and a vision of what is yet to come.

# Vacuum technology for the Hyperloop - enabling new modes of transportation

There is no future vision of modern transportation, which has had more media coverage in the recent years, than Hyperloop. The idea of high speed pods shooting at high speed through vacuum pipes without any air friction, dates back to the last century. However, it was Elon Musk in 2012 who sparked unprecedented efforts to realize this idea. Nowadays, several companies and numerous groups at universities work on it. Hyperloop Transportation Technologies and Virgin Hyperloop One are the most advanced players for commercial systems. A famous Hyperloop pod competition by Space X aims at innovative solutions for the pod design by university student teams.

Vacuum technology is inherently needed for a Hyperloop. As a major vacuum supplier, the Leybold GmbH has carefully observed the rise of this new transportation technology. A lot of technical support has been invested in in advance. Publicity has been a major benefit for years. As of today, the first commercial orders for Hyperloop test systems have been already made.

# Metal borides - Improved control of the thin film synthesis and materials properties by integration of experimental and theoretical methods

Johanna Rosen<sup>1</sup>

#### <sup>1</sup> Linköping university

Formidable research has been invested over the past three decades in transition metal (TM) nitride, carbide, and oxide thin films. Recently, there has also been an increased interest in TM borides for, e.g., the next generation of hard and wear-resistant coatings. Using TiB2 as model system, I will in this presentation show pathways for controlled thin film synthesis by means of plasma tuning and choice of synthesis technique, including magnetron sputtering, high power impulse magnetron sputtering (HiPIMS), and cathodic arc. With optimized deposition processes and materials properties in mind, the correlation between plasma properties and the film composition and (micro-)structure has been investigated, including exploration of the effect of ion-to-neutral flux ratio on the coating microstructure. With an increased fundamental understanding of the synthesis process, the next step is identification of the optimal metal boride for further investigation, targeting relevant properties for various coating applications. Therefore, we have performed theoretical simulations based on Density Functional Theory (DFT) to identify novel ternary and/or quaternary TM borides for more detailed experimental as well as theoretical analysis. One such example will be presented, showing the possibility to go from a disordered solid solution to chemical ordering upon alloy formation. Effects thereof will also be discussed.

# Advanced molecular design from OLED to organic semiconductor lasers

Chihaya Adachi<sup>1</sup>

# <sup>1</sup> OPERA, Kyushu University

While the demonstration of the first OLED emitting thermally activated delayed fluorescence (TADF) in 2009 by our group gave a glimpse of TADF's potential, our successive report in 2012 of a TADF-based OLED with an internal quantum efficiency of nearly 100% grabbed the attention of researchers worldwide and established TADF as a truly promising technology. In this talk, recent progress on TADF OLEDs will be delivered from the aspect of exciton management, electroluminescence quantum efficiency, and device stability. Particularly, the progress of blue TADF-OLEDs and the advanced optoelectronic devices such as organic laser diodes will be mentioned.

# Inverted Atoms in SiC: Silicon Vacancies as Qubits

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## Abstract

We often make the natural assumption that a "perfectly structured" material is required to produce "perfect functioning" of a device, where the function may relate to precision sensing, or the storing or transmission of information. Recently, however, there has been excitement about the performance of defects in crystalline semiconductors such as diamond and SiC. The defects, such as vacancies or "missing atoms", are deviations from perfect, periodic crystalline order. Yet such defects can manifest optical emission at a variety of wavelengths, distinctively coupled to long spin coherence times. A more useful description might be that of an "inverted atom" where the defect forms an atomic-scale quantum mechanical bit (qubit) integrated within a high-bandgap protective environment (SiC). This talk will highlight our studies in 4H-SiC of defects (qubits), integrated within photonic amplifiers. This integrated system not only enhances the qubit signal, but also can serve as a "nanoscope" into the material, allowing us to learn about the details of their atomic environment.

## Bio

Evelyn Hu is the Tarr-Coyne Professor of Applied Physics and Electrical Engineering at the John A. Paulson School of Engineering and Applied Sciences at Harvard. Prior to Harvard, she was a faculty member at UCSB, in the Departments of Materials, and of Electrical and Computer Engineering. While at UCSB, she also served as the founding Scientific co-Director of the California NanoSystems Institute, a joint initiative between UCSB and UCLA. Before joining UCSB, she worked at Bell Labs in both Holmdel and Murray Hill. She is a member of the National Academy of Sciences, the National Academy of Engineering, the American Academy of Arts and Sciences, and the Academica Sinica of Taiwan. She is a recipient of an NSF Distinguished Teaching Fellow award, an AAAS Lifetime Mentor Award, and holds honorary Doctorates from the University of Glasgow, Heriot-Watt University, Hong Kong University of Science and Technology, and the University of Notre Dame.

#### III-V Semiconducting Nanostructures on Si. What are they good for?

For many years the semiconductor industry has been driven by decreasing the structural dimensions thus increasing the device density and boosting computing and memory performance. Today, true nanoscale dimensions are reached with, e.g., transistor finwidth of smaller than 10 nm in the current technology node. The semiconductor industry research agenda is no longer driven by exclusively scaling dimensions but by integrating new materials and devices offering additional functionality. In this regard, the integration of nanoscale, high quality crystalline materials with precise control of dimension and location on the silicon platform is crucial.

In this presentation I will review the Template-Assisted Selective Epitaxy (TASE) approach to monolithically integrate a broad range of III-V compound nanostructures on Si. We have developed this approach for a variety of III-V materials and applications in nanoelectronics and nanophotonics. Our investigations of the TASE materials as well as the fabricated nanoscale electronic and optical devices demonstrate the attractiveness of TASE to integrate nanoscale materials on silicon.

# A novel testing setup for speed of molecular pump

Huan Wang<sup>1,2</sup>, Yunning Dong<sup>1,2</sup>, Rui Yan<sup>1,2</sup>, Jing Qi<sup>1,3</sup>, Yaowen Lu<sup>1,2</sup>, Chuansen Yang<sup>1,2</sup>, Xiangchun Bai<sup>1,2</sup>, Mengmeng Wei<sup>1,2</sup>, Liangzhen Cha<sup>1,3</sup>

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As an effective tool to acquire ultra-high vacuum (UHV), molecular pump is broadly used in scientific research and advanced manufacturing, the performance testing of molecular pump is important to its quality evaluation and the design of UHV system. This paper will not only give a thorough introduction of a novel wide-range testing apparatus developed by Beijing Engineering Technology Research Center for Vacuum Metrology and Test, but also show the results of the testing program organized by CVS in 2017 to evaluate the molecular pumps used in Chinese vacuum industry.

For traditional dynamic conductance method, the pressure used for calculating pump speed is measured by two individual gauges, which introduces a conspicuous measured deviation. Additionally, its only in the region of molecular flow, the lowest limit can just reaches 10-6Pa.Comparing with other testing apparatuses, the newly-developed apparatus extends the measurement ranges in the following ways: I) a newly-developed combining standard gas flowmeter is applied and it can provide gas flow in the range of 10~10-12 Pam3/s, which makes sure that the pressure in the test dome can approach the range of 1~10-7 Pa in the testing process only by flowmeter method; II) the test dome module consists of a series of test domes with different sizes to meet the needs of various pumps; III) the test domes are special treated to the lower rate of outgassing.

The experimental results show that the testing apparatus provides a pumping speed measurement range of  $1\sim6000$ L/s with a combined standard uncertainty of  $1.6\%\sim5\%$ .

# A study on key technologies and characteristics of space simulation equipment for helicon plasma thruster

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Helicon plasma thruster is a novel electric propulsion system. This kind of electric propulsion system has a wide range of applications, such as deep space exploration and long-life satellites where reliable propulsion system is essential. To improve the adaptability and reliability, we carry out the study and develop the space environmental simulation equipment on ground for helicon plasma thruster. Especially under certain space simulation environment, we test its plume characteristics, interference effects, and other performance. In response to the above test characteristics, specific requirements are proposed on space simulation equipment on the ground for helicon plasma thruster. This article gives an overview of the working principle and system components of the space simulation equipment, with a focus on the configuration of the vacuum pumping system, inert gas inflation system, establishment of pumping methods, and other key technologies. We summarize the comprehensive application of the vacuum technology, which has the plume flow characteristics and was generated by ionization of a large flow of medium gas. We also study the characteristics of the gas flow during the test.

# 2D materials: Inorganic nanotubes and fullerene-like nanoparticles at the crossroad between materials science and nanotechnology and their applications

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After almost 100 years of research inorganic layered (2D) materials, like MoS2, are currently used as catalysts, lubricants, and perhaps most importantly in rechargeable Li- ion batteries. Much research is currently focused on monolayers (beyond graphene) of 2D materials and hybrids thereof in relation to their electronic and optoelectronics properties. After a short briefing on the history of 2D materials research, 1 the concepts which led to the first synthesis of hollow-cage nanostructures, including nanotubes (INT) and fullerene-like (IF) nanoparticles from 2D compounds, will be presented. The progress with the high-temperature synthesis and characterization of new inorganic nanotubes (INT) and fullerene-like (IF) nanoparticles (NP) will be presented. In particular, the synthesis and structure of nanotubes from the ternary and more recently quaternary "misfit" layered compounds (MLC), like LnS-TaS2 (Ln= La, Ce, Gd, etc), CaCoO-CoO2 and numerous other MLC will be discussed.

Major progress has been achieved in elucidating the structure of INT and IF using advanced microscopy techniques, like aberration corrected TEM and related techniques. Mechanical, electrical and optical measurements of individual WS2 nanotubes reveal their unique quasi-1D characteristics. This analyses demonstrate their altered behavior compared with the bulk phase, including quasi-1D superconductivity. Applications of the IF/INT as superior solid lubricants and reinforcing variety of polymers and light metal alloys was demonstrated. Some of this research resulted in commercial products (a few spin-off companies) which are exploited world-wide with rapidly expanding marketshare. Few recent studies indicate that this brand of nanoparticles is less toxic than most nanoparticles. With expanding product lines, manufacturing and sales, some of these nanomaterials are gradually becoming an industrial commodity.

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## Tuned electronic structure of a two-dimensional ErCu2 intermetallic compound monolayer

Chaoqiang Xu, Kejie Bao, Junyi Zhu, Xudong Xiao

Tuning the electronic structure of a two-dimensional (2D) material has recently attracted increasing interest owing particularly to its potential application in novel device fabrication. Here, using scanning tunneling microscopy/spectroscopy (STM/STS) and density functional theory (DFT) calculation, we found that the Moiré pattern originating from the lattice mismatch between the 2D rare earth/metal compound monolayer ErCu2 and underlying Cu(111) substrate provides a reliable approach to tune the electronic structure of the 2D material. The 2D ErCu2 surface intermetallic compound exhibiting intriguing Moiré pattern is formed after depositing Er atoms onto Cu(111) followed by annealing treatment. Atomically-resolved STM images determine the atomic structure of such 2D material, while STS measurements reveal the emergence of one characteristic energy states in the unoccupied region of ErCu2 monolayer (582 – 663 meV). The electronic structure of ErCu2 is found to be position-dependent because the Moiré structure provides a periodical modulation on the coupling interaction between the intermetallic compound layer and underlying Cu(111) surface, as suggested by the DFT calculation results. More strikingly, the calculated band structure of free standing ErCu2 monolayer presents exotic band structure, which definitely deserves further experimental exploring. These results provide perspectives for tuning the electronic structures in such atomically-thin layers.

## Ab initio kinetic Monte Carlo simulation analysis of methane dry reforming on stepped Ru and Ni Surfaces for cokingresistance-catalysts design

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The dry reforming of methane is one of the most employed processes in producing hydrogen. There is a general consensus from experiments that precious metals such as Ru, Rh, Pt, and Pd have high activity for this reaction, though Ni is most frequently used because of its lower cost despite its notorious activity towards carbon formation or "coking". Focusing on active stepped Ru and Ni surfaces, we investigate the reaction mechanism of methane dry reforming using density functional theory and kinetic Monte Carlo simulations. We found that Ru is selective toward methane decomposition to CH fragment, compared to Ni that favors methane decomposition to C[1-2]. The calculated minimum activation barrier path showed that the CH fragment on Ru undergoes oxidation via the CHO intermediate while on Ni, CH decomposes further into C. Kinetic simulations revealed that a small amount of C forms on Ru at the temperature range of only 500-700K. On Ni surface, a great amount of C forms because of the noted high activation barrier for CO formation from C. Focusing on addressing the carbon formation or "coking" on Ni, the implications of these results toward the rational design of coking-resistance catalysts will be discussed in the conference, suggesting a new approach to catalyst design for hydrocarbon reforming applications[3-4].

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# **Gravitational Waves from Detectors to Detection**

The experimental challenges to detect gravitational waves, the technical innovations that enabled the discovery and the initial science will all be discussed. New technologies, the prospects for upgrades to better sensitivity in LIGO, the options for next generation detectors and future science will all be explored.

# Laser treatment to reduce the secondary electron yield of copper

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In this paper, laser treatment was used on copper to change the surface topography and the SEY was obviously reduced. In this experiment, 355nm laser instrument was used. The repetition frequency is 40 kHz, and the spot size is 15 $\mu$ m when while the energy is reduced to 1/e^2 of the center energy. Using the motion of the mechanical platform, the sample surface is etched once every 10~30 $\mu$ m. After the laser treatment, the scanning electron microscopy and the X-ray photoelectron spectroscopy were used to characterize the topography and analysis the component. Then we used the secondary electron measurement instrument to test the secondary electron yield(SEY). After laser treatment, the maximum of secondary electron yield ( $\sigma$ max) of three materials are reduced to 0.9.

# Insights into the Surface Science, Storage Mechanism and Electrochemical Phase Evolution of MoS2/CNT Hybrid Electrodes for Supercapacitive Application

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## <sup>1</sup> Indian Institute Of Technology Roorkee

Direct growth of atomically thin hierarchal MoS2 nanoflakes on CVD grown carbon nanotubes has been achieved using DC magnetron sputtering technique for electrochemical storage application. The distinct physiochemical properties of these electrodes makes them extraordinarily robust and efficient in nature with high columbic efficiency as well as cyclic stability. The super capacitive measurements of the MoS2/CNT electrode shows high specific capacity of 337 mF cm-2 at 5 mV/s. The storage mechanism involves both the electrostatic ionic adsorption as well as Na+ intercalation into the MoS2/CNT matrix. Further, using Trassati and Dunn's methods we found that the ionic diffusion and the inner electrode material contributes majorly to the total stored charge. In order to study the phase evolution of electrode material upon several charging and discharging cycles, we employed surface sensitive XPS technique, which indicated shift in the binding energies of Mo as well as S towards lower values. This shift indicates partial transition of  $2H \rightarrow 1T$  phase due the transverse gliding of S plane upon the intercalation of electrolytic ions. The all solid state supercapacitor built using symmetric MoS2/CNT electrodes in 1M Na2SO4 electrolyte was found to have high areal and volumetric capacitance of 131 mF/cm2 and 2.9 F/cm2 respectively, with high cyclic stability of 97.6% after 2500 cycles. The robustness and high performance of this device may be attributed to specially engineered growth of ordered MoS2 structures wounded on the surface of CNTs which restrict the volumetric changes and support structural integrity of the electrode material.

# Determining surface structure: why and how.

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The axiom that structure determines function applies not only to bulk materials including biological material, but also to solid surfaces. The structural influence of the chemical reactivity of surfaces, the crucial ingredient of heterogeneous catalysis, is implicit in common references to 'the active site' in catalysis literature, while the functionality of essentially all electronic devices is strongly influenced by the structure of the hetero-interfaces that make up the device, such as those between a metal conductor and a semiconductor. The key conclusion is thus that it is important to determine the atomic-scale structure of surfaces with chemically and electronically significant precision, specifically less than ~ 0.1 Å.

During the 50 years or so of development of 'modern' ultra-high-vacuum surface science, a large number of different experimental methods have been developed that are not only sensitive to the presence of the outermost few atomic layers of a surface, but also provide information that is specific to this region, despite the presence of the vastly larger number of atoms in the underlying bulk. Amongst these are a number of techniques capable of obtaining quantitative structural data, although in general analysis of data from these experiments can be quite demanding. Somewhat more recently two other techniques have become widely used, namely scanning probe microscopy (especially scanning tunnelling microscopy - STM) experiments and density functional theory (DFT) calculations. Both STM and DFT have had a hugely positive impact on surface science studies in general, and as I will show, when used in combination with quantitative experimental structural data they can significantly aid structural studies. However, I will also show how structural investigations based only on these two techniques, as has become common in recent years, are far from ideal.

# Anisotropic Atomic Layer Etching of Chrome

Doo San Kim<sup>1</sup>, Won Oh Lee<sup>1</sup>, Ju Eun Kim<sup>1</sup>, You jung Gill<sup>1</sup>

## <sup>1</sup> Sungkyunkwan University

Two Cr atomic layer etching (ALE) methods which are composed of O radical adsorption followed by CI+ ion desorption (chemical anisotropic ALE) and CI/O radical adsorption followed by Ar+ ion desorption (physical anisotropic ALE) have been applied for the precise control of Cr etching and their effects on Cr etch characteristics were investigated. For both ALE methods, a saturated Cr etch depth/cycle of 1.1 Å/cycle for the chemical anisotropic ALE and 1.5 Å/cycle for the physical anisotropic ALE could be obtained while keeping near infinite etch selectivities with various Si-based materials such as silicon, silicon dioxide, and silicon nitride. The Cr etch depth could be controlled precisely with atomic precision by controlling etch cycles for both Cr ALE methods in addition to the infinite etch selectivities over Si-based materials. Also, the surface roughness and the chemical composition of Cr surface were maintained similar before and after the Cr ALE. It is believed that the ALE technique can be used to precisely control the thickness of materials including metals such as Cr without any damage on the surface.

## Label-free particle and cell sorting based on inherent physical properties

Jonas Tegenfeldt<sup>1</sup>

<sup>1</sup> Lund University

Cell sorting is a key tool in medicine and biology to find and characterize cells of interest. Whereas standard immune-labelling is a powerful technique combined with for example fluorescence activated cell sorting (FACS), it does require expensive and sensitive equipment and reagents. Relying instead on the inherent physical properties of cells, we do not need any labelling, and by implementing our sorting schemes on a microfluidics platforms we make the preparation and analysis of a sample simpler, more widely accessible and cheaper.

In our laboratory we pioneered morphology, density and deformability-based sorting using deterministic lateral displacement (DLD). We characterized the mechanical and morphological properties of different variants of red blood cells as well as cancer cells. Furthermore, we demonstrated the enrichment of parasites from blood by using their distinct shape which may form the basis for a simple tool for diagnosis of parasitic disease by mere observation of any parasites in a blood sample.

Our overall aim is to combine several functionalities on a microfluidics chip so that we can extract narrowly defined subpopulations of cells of interest in a multidimensional parameter space defined by the biophysics of the cell.

## Structure and phase transition of a dense monolayer phase of indium on Si(111)

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Dense monolayers of metals on semiconductor surfaces provide an ideal platform for investigating physical properties of twodimensional (2D) metals. However, only a few structures are known as a monolayer metal having 2D metallic electronic structure. Indium adsorbed Si(111) surfaces are one of the most extensively studied metal/semiconductor systems, but such a monolayer metal of In/Si(111) was not previously established. Recently, we succeeded in prepararing a dense monolayer phase of In/Si(111) with a long-range order and revealed that it has metallic electronic structure [1].

In this work, we have investigated the atomic structure of the monolayer phase of In/Si(111) and a temperature-driven phase transition. Although the phase was previously considered to have a commensurate (root7 x root3) structure [2], we show that it has an incommensurate structure with the indium overlayer uniaxially contracted by 2 percent from (root7 x root3) by means of low-energy electron diffraction (LEED) and scanning-tunneling microscopy (STM).

We also observed that the monolayer phase changes to a (root7 x root7) phase at 250-210 K upon cooling. Macroscopic fourpoint-probe conductivity measurements revealed that the transition induces a rapid decrease in electrical conductivity. This is consistent with the disappearance of metallic surface states measured by angle-resolved photoelectron spectroscopy (ARPES), indicating that the transition is an electronic metal-insulator transition.

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# Advanced Peo-Nanoporous Composite Electroyesfor Lithium-Ion Batteries

Jae Hyun Kim<sup>1</sup>, Anupriya Arul<sup>1</sup>

<sup>1</sup> DGIST

The challenging and critical issue with solid polymer electrolytes are to improve the ionic conductivity, interfacial contacts between electrodes and electrolytes and electrochemical stability window. In order to above requirements, recent research in PEO-based solid-state electrolytes (SSEs) has focused on the design of additive for solid polymer electrolytes (SPEs). The additives include ionic liquid, oxide particles, etc.

Porous nanoparticles may be a relatively effective additive to increase the ionic conductivity than the nonporous particles, which is mainly attributed to the pores creating more space charge regions to facilitate Li+ transport. The implanted materials with rich nanoporous structure can effectively promote the formation of an Li+ enrichment area through the adsorption effect.

In this study, we used 3-dimensional nanoporous structures(NPSs) to make composite solid electrolytes. The NPSs are characterized by three-dimensional structures with large, cage like cavities that can accommodate sodium, calcium, or other cations (positively charged atoms or atomic clusters), water molecules, and even small organic molecules. The choice of lithium salt also plays a crucial role in solid polymer electrolyte. The chosen lithium salt were LiOH and lithium bis(trifluoromethane sulfonyl)imide (LiTFSI). We changed the ratio of EO and Li. The best lithium ion conductivity was 4.5 x 10-4 S cm-1 at room temperatur, whigh is one of best in SPE.

# Oxidation Behavior of AI-Cr-Nb-Si-Zr Nitride Thin films

Fan-Yi Ouyang<sup>1</sup>, Jian-Jie Wang<sup>1</sup>, Shou-Yi Chang<sup>1</sup>

# <sup>1</sup> National Tsing Hua University

This study investigated high temperature oxidation behavior of high entropy alloy (HEAN) Al-Cr-Nb-Si-Zr nitride thin films. The HEAN films were first deposited on the Si substrate in Ar+N2 mixed atmospheres using radio frequency (RF) magnetron sputter system and then subject into the dry air atmosphere at 850 oC for different periods of time. The results show that the thickness of oxidation scale was about 234- 260 nm after test for 1 h, and it only increased to about 517-565 nm after 25 h, demonstrating that HEAN films possess good oxidation resistance at 850 oC. After oxidation process, triple scales, Al2O3/Cr2O3/Al2O3, were observed and the growth of inner  $\alpha$ -Al2O3 layer is predominant. The nano-crystallined ZrO2 was found to disperse in the oxide scales. Furthermore, XRD analysis indicate that the crystallinity of the HEAN films changed from amorphous-like to crystalline after test. To understand the the oxidation mechanism of HEAN films, Au nanoparticles was deposited at surface of films as diffusion markers. We found that markers were diffused to locate at Cr2O3/inner Al2O3 interface after oxidation test. The corresponding microstructural evolution of oxide and oxidation mechanism would be discussed in details in the talk.

# Ultrasensing optical spectroscopy of plasmonic nanocavity

HONGXING XU

Plasmonics is a rapidly emerging branch of photonics, which offers variable means to manipulate light using plasmon excitations on metal nanostructures. Most prominently, the huge electromagnetic enhancement of plasmonic nanocavity offers the physical basis of single-molecule SERS and many other plasmon related research fields, such as tip-enhanced spectroscopy, plasmonic antennas, plasmon hybridization, quantum plasmonics, nonlinear plasmonics, plasmonic optical forces, and plasmochemistry. In this talk, the discovery, mechanism and applications of plasmonic nanocavity are briefly introduced firstly. Then we will talk about our recent studies using plasmonic nanocavity for sub-picometer sensitivity of spatial changes, extremely high optical nonlinearity and strong coupling.

# Magnetic properties of the iron nitride monolayers tuned by the symmetry of the substrate

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Iron nitride has a great interest in their various electronic and magnetic properties which are dependent on the nitrogen content or interatomic distance between Fe and N. In the present study, we focus on the ferromagnetic Fe2N monolayer grown on the Cu substrate. Recently, we have observed a square Fe2N monolayer even on Cu(111) with a threefold symmetry by scanning tunneling spectroscopy. It has the same structure as on Cu(001). Changing the symmetry of the substrate would enable us to control the magnetic properties of the Fe2N monolayer. Here, we have investigated the electronic and magnetic properties of the Fe2N monolayers tuned by changing the symmetry of the substrates by using scanning tunnel spectroscopy(STS) and X-ray absorption spectroscopy/ magnetic circular dichroism (XAS/XMCD).

We have fabricated the Fe2N monolayer by N ion bombardment to the Cu substrate cleaned by repeating the cycle of the sputtering and annealing, Fe deposition in the ultra-high vacuum and subsequent annealing up to 580 K.

The magnetic moment of the Fe2N monolayer on Cu(111) obtained by the XMCD study was much lower than that on Cu(001). Our STS measurements revealed that the local density of states on Cu(001) was different form that on Cu(111). In addition, superstructure formed by the symmetry difference between the triangular Cu(111) substrate and square Fe2N monolayer causes the spatial modulation of density of states. The difference in hybridization of the Fe2N monolayer with the Cu substrate can tune the magnetic properties of the Fe2N monolayer.

# Simulation of the influence of stray magnetic fields on the operation of a Bayard-Alpert ionisation gauge

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Ionisation gauge is the only device for pressure measurement in high and ultrahigh vacuum ranges, which are of extreme significance for both science and industry. Gauge to gauge variations of these devices is typically ±15-30 %, while even successive calibrations introduce differences of typically 3-6 %. We have recently developed two approaches for modelling of ionisation gauges, based on well-known SIMION 8.1 software for charged particles optics calculations. In this work we use these models to explore the influence of external magnetic fields on the operation of ionisation gauges. For that purpose, the geometry of a Bayard Alpert ionisation gauge developed at CERN was investigated. Magnetic fields inside the ionization gauge can be caused by ion pumps or Penning gauges mounted on the same vacuum system. It appears that even uniform magnetic fields of the order of Earth magnetic field, influence electron trajectories inside the gauge. Depending on the field direction, constant magnetic inductions of few Gs can both increase or decrease the gauge sensitivity. Magnetic induction distribution measured along the axis along the Penning gauge (model IKR 251, Pfeiffer) confirmed that such field intensities are produced 20-40 cm away from the vacuum connection port. These results suggest that magnetic shielding of ionisation gauges is recommended for high precision and reliable pressure measurements using these devices.

#### Photostable and highly emissive organic nanoparticles exhibiting long lifetime emission

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#### <sup>1</sup> Kyushu University

For the bio-imaging, we have much variety of exogenous emitting probes, e.g. fluorescence materials, lanthanide complex, organic dots, and quantum dots. Recently, the probes having long lifetime emission attract the attention of researchers to do the time resolved imaging because it makes clear imaging by elimination of autofluorescence. Recently, the thermally activated delayed fluorescence (TADF) materials were developed for the highly efficient organic light emitting diode. That shows high emissivity with a long lifetime delayed emission without heavy metal. However, TADF materials having donor and acceptor conjugation show low PLQY in the polar solvent, i.e. water. In this presentation, we demonstrate novel organic dots, which are containing a TADF material (4CzIPN) and providing high photostability, high PLQY and long lifetime emission (3.1 µs) in aqueous medium.

We employed o/w emulsion method with the microwave processing to fabricate organic nano-particles which is in the glassy state. While the organic nano-particles prepared by the conventional aggregation method with sonication showed only 14% PLQY and red-shifted emission, the obtained particles in aqueous solution showed extremely high PLQY and similar emission properties to the toluene solution. In addition, the TADF dots showed high photostability (LT50 = 360 h) to UV irradiation (300–400 nm, 5 mW/cm) which was better than blue quantum dots (LT50 = 140 h). We also demonstrated cell imaging using developed TADF dots. The TADF particle can be traced over several weeks with less toxicity in HEK cells. The TADF materials light up a new way toward bio-applications.

# Effects of variable vacuum capacitors in the inductively coupled plasma discharge for the plasma uniformity control

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In this work, we focused the effect of variable vacuum capacitors in the antenna of an inductively coupled plasma discharges. For the large area substrates such as glass for the display devices, it is well known that the uniformity control is difficult. In the the semiconductor device manufacturing cases, the two-dimensional symmetry may be assumed, However, in the display device cases, the assumption cannot be applied that large size three dimension problem should be considered. We solved the complex modeling equations of electric circuit, electromagnetic field, plasma, gas flow, and heat simultaneously. By changing the capacitance in the antenna, we could find the effective change in the characteristics of the plasma. Although, this model have simplified parts such as fluid description of the plasma, and the capacitive field of the antenna is not considered. It is sufficient to focus the major role of the variable vacuum capacitors in the plasma discharge.

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# High performance electrical double layer capacitor electrodes in graphene nano walls synthesized by electron cyclotron resonance plasma

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Electron Cyclotron resonance (ECR) plasma source is promising method for not even large scale but rapid and efficient to synthesize vertical graphene nano walls. The aim of this research is to investigate capacitance and frequency response of vertically aligned graphene nano walls (GNW) grown in same ECR system. Grown GNWs on Ni substrates used as electrodes in electric double layer capacitor (EDLC).

Vertically aligned GNWs were synthesized and post-treated with nitrogen plasma in ECR system on various flow ratio and synthesis time.

GNWs synthesis process was carried out for two steps. For the first step to synthesize GNWs, H2 gas was injected into process chamber as carrier gas aiming to anneal the substrate, provide active defects, which promote graphene nucleation formation, and remove surface contaminations on substrate on surface. Reactive CH4 gas was then infused into processing chamber during discharging H2 plasma.

electrochemical properties measured in 1 M of Na2SO4 neutral electrolyte.

electrochemical experiments carried out cyclicvoltammetry (CV) in range of scan rate of 100mV/s to 1,000 mV/s and electrochemical impedance spectroscopy (EIS) and life cycle test was also conducted up to 1000 cycle charge-discharge, which presented outstanding results. in our experiments showed specific capacitance in range of 33 to 2.9 mF/cm2. Doping of nitrogen process was carried out as post-treatment method in same ECR plasma chamber. capacity of charge storage in pristine GNW and N-doped GNW was remarkably changed from 800 µF/cm2 in pristine GNW to 1.9 mF/cm2.

#### Zirconium-doped tungsten boride thin films deposited by magnetron sputtering combined with pulsed laser deposition

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Tungsten borides doped with transition metals (Ti, Cr, Mo, Ta etc) may have very wide range of applications in modern industry. Small addition of different dopants can result in increased thermal, oxidation, electrical properties when exhibiting high hardness.

In this work we present results of doping WB2 coating with zirconium by using magnetron sputtering combined with pulsed laser deposition. Tungsten boride target (atomic ratio B/W = 2.5:1) was sputtered by magnetron powered with radio frequency electrical supply. Doping was carried out by evaporation of zirconium or zirconium diboride target by nanosecond laser pulse at 1064 nm wavelength. The amount of dopant in final coating was controlled by adjusting the laser fluence.

Surface morphology and chemical composition was analysed with scanning electron microscopy with EDS. Investigation of phase composition was performed by using X-ray Diffraction, hardness was measured by nanoindentation tester equipped with Berkovich indenter.

Observations have shown that doping with pure zirconium targets leads to creation of more droplets and higher amount of dopant when using the same laser fluence compared to zirconium diboride target. X-ray Diffraction has revealed that crystallinity of tungsten boride films changes with amount of zirconium. The hardness of presented coatings is high, up to 25GPa.

# Adsorption site identification in single molecule junctions

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The geometry of the metal-molecule interface is of paramount importance in single-molecule junctions as it strongly determines its electron transport properties. This is particularly true for thiol-based junctions, where conductance can change by orders of magnitude. In this work, we present a series of density functional theory (DFT) based transport calculations, which in combination with surface enhanced Raman scattering and current-voltage characteristics experiments result in a powerful adsorption siteselectivity technique [1]. We illustrate the impact of this technique on prototypical junctions of aminobenzenethiol (ABT) and benzenedithiol (BDT) molecules, connected to Au electrodes. This methodology distinguishes multiple molecular adsorption sites, and uncovers the origin of conductance fluctuations, which had never been detected experimentally up to now. We are able to determine the adsorption site for each single-molecule junction by calculating the effect of the Au-tip motif. Previous studies on BDT junctions have reported reported multiple or continuous extended conductance state. For example, Tsutsui et al. showed two conductance states, arguing that they were caused by positions of the adsorbed [2]. Similarly, Leary et al. observed two conductance peaks, proposing he formation oligomeric units at the molecule-metal interface to explain such features [3]. However, even though these junctions have been thoroughly investigated, there are still large discrepancies in measured conductance peaks and their relation with the thiol adsorption site on the metallic electrode. In the present work, the observed results and the adsorption site assignment resolves these discrepancies. In the case of ABT and BDT single-molecule junctions, electrical conductance can vary by up to a factor 100, hampering the development of reproducible conductance signatures. This study unambiguously monitors changes in molecular adsorption geometry for the first time and demonstrates their significant role on junction conductance fluctuations.

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## Nanostructure Arrays for Nano-Bio Sensorics and Nano-Bio Interfaces

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#### <sup>1</sup> Yonsei University

Nanostructure arrays can provide unique characteristics such as enhancing optical signals, controlling cell-material interactions, and modulating surface wetting properties depending on their nanoscale and material properties. This can lead to many interesting applications including nano-bio sensorics and nano-bio interfaces that are described in this presentation.

For nano-bio sensorics, optical nanostructure arrays based on nanoplasmonics offer the enhancement of optical response by the localized surface plasmon resonance (LSPR), thus enabling highly sensitive biosensing platform for early stage detection. Recent studies indicate abnormal concentration of miRNAs in patient serum and plasma so they can be used as potential biomarkers for cancer diagnosis. Nanoplasmonic coupling hybridized by targeted miRNAs can shift the resonance characteristics for highly sensitive and selective colorimetric sensing.

For nano-bio interfaces, nanostructure arrays can be utilized to control cell-material interactions by mimicking the extracellular matrix, thus enabling artificial substrates for tissue engineering. This work will describe cellular response of adipose-derived stem cells (ASCs) on nanostructures correlating their properties with focal adhesion and cell spreading. High resolution studies of stem cell response to nanostructure arrays can allow us to understand further details on the stem cell regulation by surrounded environments.

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#### Cutoff probe modeling for precise electron density diagnostics

Plasma electron density is a primary plasma parameter to characterize the plasma and equipment properties in plasma processing industry such as semiconductor and LCD. In this paper, we introduce a diagnostic method called "cutoff probe" and its modeling technique which has been performed for recent year. This paper focus on the whole progress for the cutoff probe including how to start to develop the cutoff probe in the initial period, what idea has been included during the development, how to evolve it by means of our physical modeling.

The cutoff probe looking like double Langmuir probe but operated by very high frequency of GHz range and is the simplest structure among the plasma diagnostics tools. It was made by simple intuition for the cutoff phenomenon of the plasma wave but without test of validation of probe itself. Later, EM waver simulation supported the validation for the cutoff frequency determination. Recently, by supposing the circuit modeling, the physics behind for the cut off probe spectrum (S21) was revealed and the accuracy and the application window of the probe were established. Recently, as an extended version of the circuit model, we makes transmission line modeling to explain the cutoff spectrum in high density plasma as well as low density plasma. All other different versions of cutoff probe based on the different ideas and mathematical models would be presented through this talk

#### Designing bioinspired materials and other small challenges

This talk will provide an overview of our recent developments in the design and characterisation of nanoparticles and nanoneedles for applications in regenerative medicine, drug delivery and cell interfacing. I will show how we are exploiting materials characterisation techniques, including SEM, FIB-SEM and electron tomography, as well as chemical mapping techniques to investigate the biomaterial interface and tissue ultrastructure [1,2]. This analysis informs the design of effective materials-based approaches for applications in healthcare for example nanoparticle-based diagnostics [3] and nanoneedle platforms capable of interfacing with cells to inform multiplexed intracellular biosensing at sub-cellular resolution [4].

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# Suppression of acoustic streaming in inhomogeneous medium enables acoustofluidic bacteria separation from lysed blood

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In acoustophoresis induced by a standing-wave field, suspended microparticles in a microchannel are subject to both the acoustic radiation force and the Stokes drag force from the acoustic streaming. The relative magnitude of the two forces depends on the size of the microparticles and the material of the solvent. For the microparticles of which the acoustic contrast factor is slightly higher than that of water, theoretical studies have predicted a critical diameter of 2 µm for the cross-over in water at 2 MHz, where the two forces are equal. Acoustofluidic manipulation of the bio-particles smaller than the critical size is therefore challenging. We recently found that acoustic streaming can be greatly suppressed in fluids made inhomogeneous in density and compressibility by the addition of solute molecules, due to the competition between the boundary-induced streaming stress and the inhomogeneity-induced acoustic body force. In this talk, we will discuss the physics of streaming suppression in inhomogeneous medium, as well as the application of this novel phenomenon for separating bacteria (e.g. S. aureus) from lysed blood.

# Single nanoparticle analytics in medical diagnostics, drug discovery and drug delivery

Fredrik Höök

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Next generation drug-delivery vehicles aimed to carry biological drugs, such as proteins or nucleic acids, are often designed to mimic how natural biological nanoparticles, such as viruses and exosomes, transfer genetic information between cells in vivo. Due to the large heterogeneity of nanoparticles irrespective of whether they are of biological or artificial origin, it is crucially important to advance analytical instrumentation to complement ensemble averaging methods with single nanoparticle analytical approaches. A large set of tools with single-nanoparticle sensitivity is now available, to which we recently contributed a concept that enables simultaneous fluorescent and scattering-based label-free imaging of surface-bound biological nanoparticles. Examples will be shown that illustrate the use of this scattering microscopy concept i) to investigate supported lipid bilayer formation, ii) for label-free measurements of protein binding to individual liposomes, iii) to characterize DLVO-controlled non-specific interactions at cell-membrane mimics, and detergent free enrichment of pre-defined membrane proteins in crude cell membranes. By using a two dimensional fluid supported lipid bilayer, to which biological nanoparticles are directly anchored and imaged, we have also developed a new means to simultaneously determine both nanoparticle size and fluorescence / scattering intensity, which may potentially offer flow-cytometry-like sorting based on distinct features of individual nanoparticles. This 2D flow nanometry concept can also be used to quantify the valancy of nanoparticle binding to cell-membrane mimics. These new analytical possibilities will be discussed in the context of improved characterization of individual biological nanoparticles of diagnostic and therapeutic significance.

# Neutron Reflection and Scattering Studies of Mixed Layers with Lipids

Adrian Renne

# Uppsala University

Neutron techniques, particularly when used in combination with isotopic labelling of specific components, either whole molecules or parts of molecules, allows identification of the structure and composition of various model membranes that are of importance in biological and environmental sciences. The talk will describe the methodology and present new results that are related to oxidatively damaged lipids, penetration with preservative agents that are found in blood storage bags and by environmental contaminants