Nanoscience@Surfaces Summer School

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Poster Presentations

Hydrothermal Synthesis and Characterization of Nitrogen-Doped Carbon Quantum Dots (NCQDs) Derived from Waste PET Plastic

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The growing accumulation of post-consumer plastic waste, particularly polyethylene terephthalate (PET), represents a persistent environmental challenge that has driven interest in converting such waste into value-added carbon nanomaterials. In this study, nitrogen-doped carbon quantum dots (NCQDs) were synthesized from waste PET bottles via a one-pot hydrothermal carbonization route using urea as the nitrogen dopant source. PET waste was first chemically depolymerized under alkaline conditions to generate carbon-rich oligomeric precursors, which were subsequently carbonized hydrothermally at varying urea-to-precursor ratios and reaction temperatures. The resulting NCQDs exhibited a quasi-spherical, uniform morphology with an average particle size of ~4.2 nm, as confirmed by transmission electron microscopy (TEM). FTIR analysis confirmed successful nitrogen incorporation into the carbon framework, predominantly as pyridinic and graphitic species, alongside abundant oxygen-containing surface functional groups (–OH, –COOH, C=O) that enhanced aqueous colloidal stability. These findings establish a low-cost, scalable, and environmentally beneficial route for transforming hazardous plastic waste into structurally well-defined, highly fluorescent carbon nanomaterials, underscoring their broader potential for future use in optoelectronic, sensing, and bioimaging technologies.

Direct observation of hydrogen-driven surface evolution of HEA revealed by in situ XPS, NAP-XPS and NEXAFS from 1 mbar up to 1 bar

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The evolution of the surface electronic structure of High Entropy Alloy (HEA) ((Ti0.65Zr0.35)1.05MnCr0.8Fe0.2) was investigated using synchrotron-based X-ray Photoelectron Spectroscopy (XPS), Near-Ambient Pressure XPS (NAP-XPS), and Near-Edge X-ray Absorption Fine Structure (NEXAFS) under sequential activation conditions, involving high and moderate hydrogen pressures and various heating degrees. HEA was investigated using a connected off-line reactor; the near-ambient x-ray photoemission (NAP-XPS) cell is separated from the ultra-high vacuum (UHV) chamber and the high-pressure reactor (HPR) but connected via a vacuum transfer system. A reference sample was measured under Ultra High Vacuum (UHV) for comparison. The following samples were measured at moderate pressure in the NAP cell, high pressure in the HPR, and laser heating in the NAP. The findings show a selective reduction process on the HEA surface, where Fe is fully reduced to the metallic state. In contrast, Mn exhibits mixed oxidation states due to its multivalent nature, while Ti and Zr exhibit resistance to full reduction, maintaining partial oxide and suboxide states. This combination, created by hydrogen-induced electronic restructuring, is useful for hydrogen absorption and desorption, as the metallic states are efficient for hydrogen dissociation; meanwhile, the suboxide state facilitates hydrogen diffusion within the alloy.

Towards Arsenic in Germanium Quantum Devices: STM-Characterised δ-layer Fabrication

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Deterministically placed single dopant atoms in semiconductors are attractive candidates for qubits and other atomic-scale devices [1]. In these devices, the dopants and the nanoscale wires and gates that address them are patterned together in a single plane on the semiconductor surface, then encapsulated by molecular beam epitaxy (MBE). Phosphorus in silicon is by far the most studied donor-semiconductor combination, but recent work suggests that arsenic in germanium may be superior in several key respects [2].
Here we demonstrate the fabrication of atomically thin arsenic doping planes (δ-layers) in Ge(001), formed by dosing the surface with gas-phase arsine (AsH_3) and encapsulating with epitaxial Ge, entirely under ultra-high vacuum. Scanning tunnelling microscopy (STM) at every stage, from the clean Ge(001) and arsine-dosed surfaces through to the completed overgrowth, allows us to determine fabrication quality at the atomic scale. The δ-layers are patterned into Hall bars by conventional lithography and electrically contacted. Magnetotransport measurements will elucidate the electronic properties of the δ-layer's highly confined two-dimensional electron gas (2DEG), complemented by soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) of its band structure [3].
This work forms part of a close collaboration with the Paul Scherrer Institute (PSI) to develop large-scale donor devices in silicon and germanium using industry-compatible extreme-ultraviolet (EUV) lithography [4,5].

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Characterization of superconducting niobium nitride thin films grown by thermal Atomic Layer Deposition

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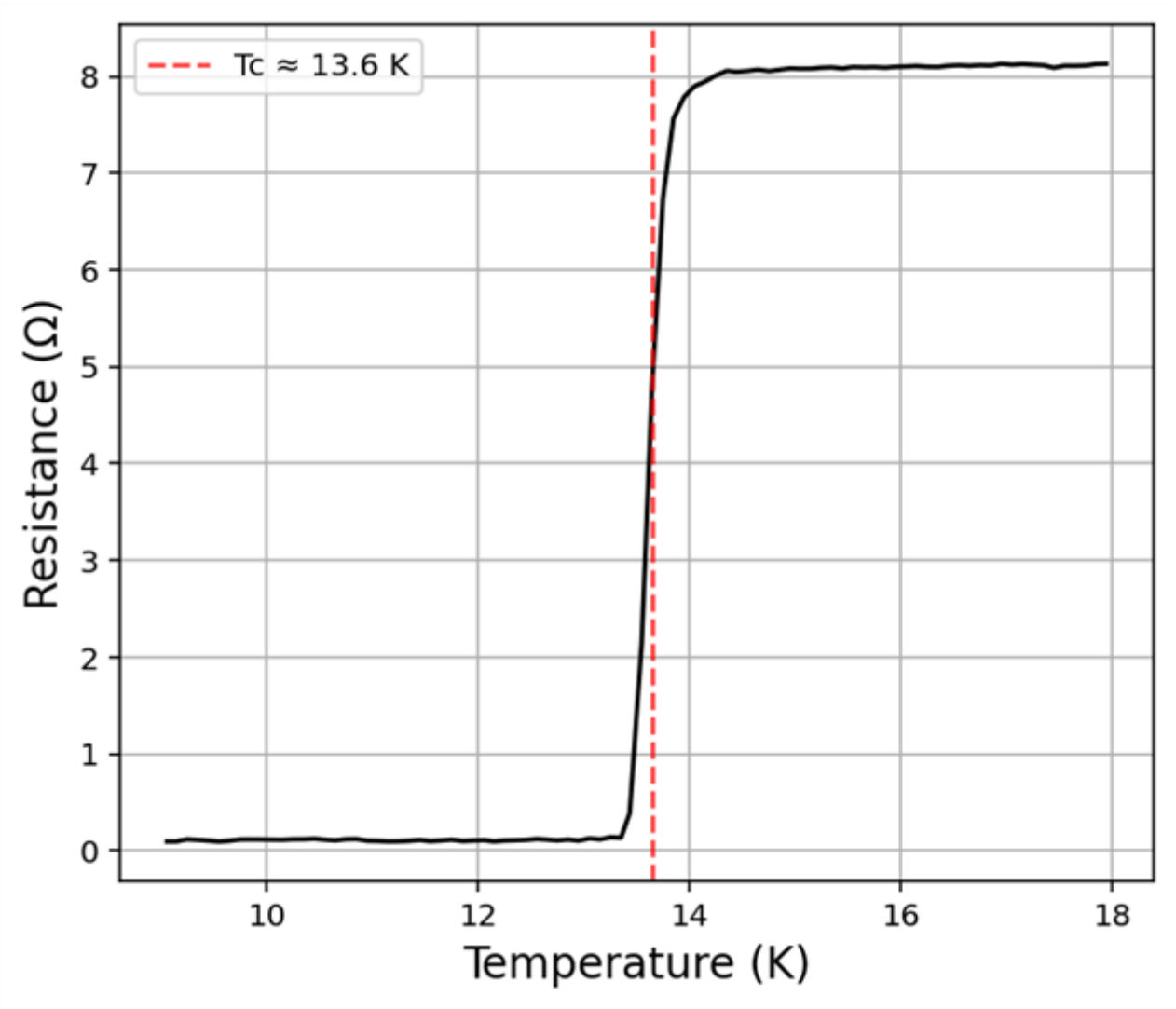
Metal nitrides are a promising group of superconducting materials for a wide range of quantum technologies and advanced electronic applications. The quality of superconducting thin film is very critical for its properties and achieving high-quality films requires precise thickness control and high conformality. These demands are met when growing the films with Atomic Layer Deposition (ALD). Among metal nitrides, niobium nitride (NbN) is especially interesting due to its relatively high theoretical critical temperature (17 K) and compatibility with thermal ALD processes.

In this work superconducting NbN thin films were grown by thermal ALD at 400–500 °C using NbCl5 and NH3 as precursors. Film thicknesses varied between 16.9 nm and 128 nm and the depositions were done on Si, SiN and sapphire substrates. The effects of film thickness, deposition temperature, substrate choice, and post-deposition annealing (700–1000 °C) on the superconducting and structural properties were investigated. Film characterization was carried out using electrical resistivity and critical temperature measurements, Atomic Force Microscopy (AFM), X-Ray Diffraction (XRD), and Time-of-Flight Elastic Recoil Detection Analysis (ToF-ERDA).

Deposited films exhibited promising superconducting properties with critical temperatures up to 13.6 K after annealing at 850 °C and 14.1 K after annealing at 1000 °C. As-deposited films exhibited resistivities down to 524 μΩcm and after annealing resistivities decreased even further to 54 μΩcm. As-deposited films were slightly nitrogen rich and contained low concentrations of impurities such as O (< 3.2 at.%), Cl (< 3.4 at.%), C (< 0.26 at.%) and H (< 0.45 at.%). After annealing nitrogen content of the films decreased and films became more niobium rich. Superconducting critical temperature was dependent on the film thickness but even the thinnest films (16.9 nm) had a transition temperature of 11.35 K. These results highlight thermal ALD as a viable method for producing high-quality superconducting NbN thin films.


Tc ≈ 13.6 K
Resistance (Ω)
Temperature (K)
0
1
2
3
4
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6
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12
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16
18

Nanostructure and Stability of Perovskite Solar Cells

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Perovskite solar cells (PSCs) have achieved power conversion efficiencies exceeding 26%, making them one of the most promising emerging photovoltaic technologies. However, their long-term stability remains limited by interfacial degradation, defect formation, and environmental exposure. Ionic liquid (IL) additives and IL-based interfacial layers have recently attracted considerable attention as effective strategies for controlling perovskite crystallisation, passivating defects, and improving charge transport at buried interfaces. Despite these promising advances, the chemical interactions between ILs and electron transport layers (ETLs) remain insufficiently understood.

This project investigates the influence of ionic liquid additives and IL interfacial layers on SnO_2 electron transport layers using advanced synchrotron-based photoelectron spectroscopy. Thin-film samples were prepared on titanium (Ti) foil substrates using the spin-coating method. For half of the samples, a SnO_2 layer was spin-coated onto the Ti substrates, while for the remaining samples, a NiO_x layer was deposited using the same technique. Subsequently, various ionic liquids, including $BMIMBF_4$, BMIMCl, $C_1C_{14}ImBr$, and C_4C_8ImBr, were spin-coated onto the SnO_2 and NiO_x coated Ti substrates. A MAPbI3-xClx perovskite layer was then deposited over these substrates by spin coating. In addition, samples were prepared by incorporating the ionic liquids as additives into the perovskite precursor ink. The resulting ionic liquid-containing perovskite inks were spin-coated onto both SnO_2 and NiO_x coated Ti substrates. By correlating interfacial chemistry with photovoltaic performance, the work aims to establish structure, property relationships that underpin enhanced device stability.

Measurements were carried out at beamline MATline at ASTRID2 synchrotron in Aarhus University, where X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) spectroscopy measurements were employed to investigate the elemental composition, chemical bonding and electronic structure. Together, these complementary techniques provide detailed insight into surface passivation mechanisms, oxygen vacancy modification, and the formation of chemically stable interfacial layers.

By combining advanced spectroscopy with materials engineering, this work seeks to improve understanding of the interfacial processes governing charge extraction and degradation in perovskite solar cells.

Nanostructure and Stability of Perovskite Solar Cells (DTC Funded PhD Project 2025-2028)

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Introduction

Perovskite solar cells (PSCs) have emerged as a leading photovoltaic technology because of their exceptional power conversion efficiencies (PCE) and low fabrication costs. However, their large-scale production is limited due to lead toxicity, instability under ambient conditions, and the need for all-air fabrication environments. This PhD project aims to develop stable, non-toxic, and environmentally sustainable perovskite materials using ionic liquid additives, lead replacement strategies and interfacial optimisation.

Objectives

- To optimise the deposition of electron transport layers (ETLs) and perovskite films on NSG trademark glass substrates.
- To investigate the effect of ionic liquid/polymer additives in lead-based perovskites, lead-free perovskites and perovskites with partial lead replacement.
- To investigate different electron transport layer materials and how these affect interfacial properties in the device using various techniques such as using XPS, HAXPES, NAP-XPS, PL, and AFM.
- To assess the stability of fabricated perovskite layers under moisture, oxygen, heat, and illumination, and characterise decomposition pathways.
- To fabricate perovskite solar cell devices based on the most promising materials and test their efficiency.

Perovskite Cell Structure

- General Formula: ABX_3 (Eg: $MAPbI_3$)
- X is an anion (oxide or halide), B is a small divalent metal cation, and A is a larger monovalent cation (organic or inorganic).
- Six X anions octahedrally coordinate the B cation in this structure, creating corner-shared BX_6 octahedra inside a cubic lattice, with the A cation occupying the spaces between them (Seyisi et al., 2025).

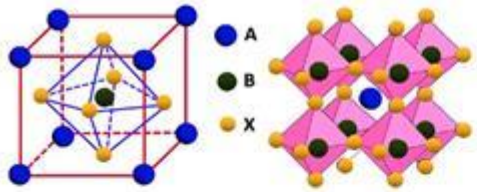

Fig.1. Structure of Perovskite (Aslam et al., 2021)

Methods

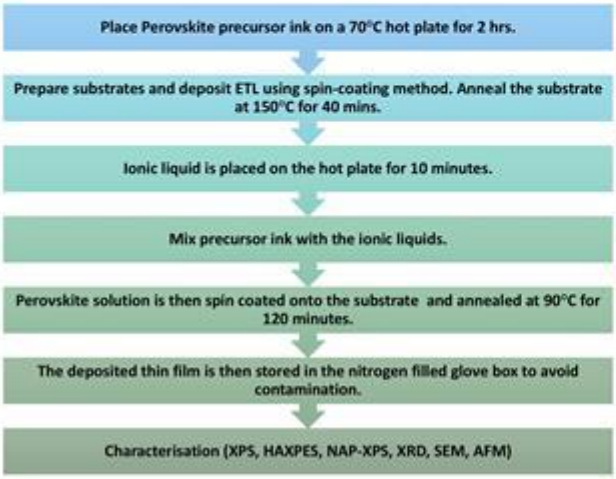

Fig.2. Flowchart depicting the Experimental Procedure of thin film deposition of Perovskite.

Design of Perovskite Solar Cell

- PSCs typically employ a multilayer thin-film architecture in which each functional layer contributes to light absorption, charge separation and selective extraction.
- In the conventional n-i-p layout, a transparent conducting oxide (TCO) such as fluorine-doped tin oxide (FTO) or indium tin oxide (ITO) is coated with an electron transport layer (ETL) such as SnO_2 or TiO_2.
- The perovskite absorber layer (ABX_3), which can include mixed A-site cations (FA/MA/Cs/Rb) and lead-reduced B-site compositions (Sn/Bi).
- Above this resides the hole transport layer (HTL), typically Spiro-OMeTAD or polymeric additives.
- The device is completed with a metallic back electrode such as Au, Ag or carbon.

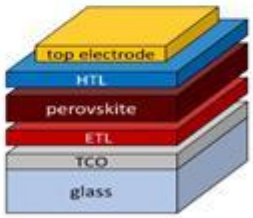

Fig.3. Device architecture of a perovskite solar cell device showing glass/TCO/ETL/perovskite/HTL/metal layers, with directional electron and hole transport pathways (Sławek et al., 2021)

Research Gaps

- Although, perovskites are highly efficient, they are not stable due to several factors such as moisture, oxygen, light, electric bias, heat, lattice stress, and ion migration.
- Replacements for Pb in perovskite materials are being investigated due to environmental and regulatory concerns
- Interfacial losses at the perovskite solar cells and their causes should be explored.

Upcoming Experiments

- Sample preparation using Perovskite precursor ink.
- Characterisation of samples in ASTRID2 Beamtime in Denmark.
- The stability of the samples while heating will be studied in the synchrotron facility, Denmark.
- Preparation of lead-free perovskites and characterise those samples.

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Thermoelectric properties of the high-quality nanocomposite alloy K0.005Cu1.95S

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Abstract: In this work, the compound K0.005Cu1.95S, belonging to the family of potassium-containing copper sulfides, was obtained and studied. K0.005Cu1.95S by low-temperature method in molten alkali metal hydroxides. According to X-ray phase analysis, the sample consists of a tetragonal Cu1.96S phase (72%), a monoclinic Cu2S phase (22%) and a KCu4S3 phase (6%). Electrical conductivity, Seebeck coefficient, heat capacity and thermal conductivity were studied in the range of 300–700 K. In the region of 550–610 K, anomalies in transport properties were revealed, accompanied by an increase in the Seebeck coefficient while maintaining low thermal conductivity at the level of 0.18–0.20 W m^{-1} K^{-1}. It has been established that the high thermoelectric efficiency of the material is due to a combination of structural heterogeneity, defectiveness of the copper sublattice, and the presence of interphase boundaries that ensure effective phonon scattering. The maximum value of the thermoelectric figure of merit reaches ZT = 3.2 at 700 K, which indicates that the K0.005Cu1.95S compound is promising for thermoelectric applications in the region of 500–700 K.

Keywords: copper sulfide; superionic conductor; thermal conductivity, Seebeck coefficient, electronic conductivity .

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Laser treatment of aluminium-doped Zinc Oxide thin films deposited via magnetron sputtering

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Transparent conductive oxides (TCOs) are a class of materials that are both electrically conductive and highly transparent in the visible spectrum. In many applications, indium tin oxide (ITO) is the industry standard due to its suitability for deposition on large surfaces and its excellent balance of conductivity and transparency. However, due to indium's toxicity, rising cost, and limited availability, there is a significant need for an alternative to ITO, and aluminium-doped zinc oxide (AZO) is one of the most promising candidates: it is cheap, non-toxic, and crystallizes spontaneously during magnetron sputtering. It is therefore important to improve the performance of this material, which depends heavily on intrinsic defects—such as vacancies and interstitials—as well as on crystal quality and microstructure [1]. Laser-assisted processing can lead to an increase in the mobility and/or density of charge carriers by improving dopant activation and/or reducing defect formation. In the linear and thermal regime, this change is associated with faster heating and cooling of the thin film, which leads to better control of chemical diffusion while allowing for recrystallization and grain growth [3], [4]. On the other hand, the use of ultrashort-pulse lasers (in the order of picoseconds and below) can induce nonlinear and nonthermal processes, such as multiphoton absorption and/or avalanche ionization phenomena, which may lead to profound changes in interatomic bonds [5]. In our studies, thin-film AZO samples with varying Al contents, deposited on glass and fused silica substrates via magnetron sputtering, are subjected to various laser treatment conditions, ranging from CW to sub-ps annealing.. Initial results obtained using a 1080 nm CW laser are promising, showing a reduction of the resistivity and a systematic improvement of the transmittance.

This work is part of the ANR-24-CE08-7917 project.

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Molecule Surface Energy Transfer in a Reactive System

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Energy transfer between molecules and surfaces dictates fundamental surface chemistry processes, such as heterogeneous catalysis and gas-surface reactions. Traditional time-of-flight methods used to measure this energy transfer are fundamentally limited in their energy resolution by the velocity spread of the incident molecular beam [1]. Recent advances in molecular spin-echo interferometry have overcome this limitation, achieving ultra-high energy resolution to successfully measure surface phonons using a D2 beam scattered from a non-reactive Cu (111) surface [2]. Building upon this proof-of-concept, our current research extends the spin-echo technique to investigate molecule-surface energy transfer in a reactive system, specifically D2 scattering from a reactive Ni (111) surface, where energy transfer processes directly influence catalytic reaction pathways. D2 molecule scattering measurements have been performed to study molecular surface energy transfer close to specular at different incident energies. By analysing complex signals and applying a tilted projection of 1 where the magnetic fields in both arms of the spectrometer are scanned identically (B1= B2)-we aim to eliminate the intense diffuse elastic scattering peak from the spectrum. This technique helps us to resolve low inelastic energy transfer features close to the specular region. As a comparison, 3He spin-echo measurements were performed at three different nozzle temperatures. We observe the same phonon energy (ΔE) and momentum (ΔK) transfer features for both D2 and 3He, despite these different 3He beam conditions. To overcome instrumental limits and beam velocity spread, these experiments utilised optimised tilted projection angles by scanning the magnetic fields proportionally [3]. This eliminates beam broadening, enabling the ultra-high energy resolution required to resolve the closely spaced Rayleigh and longitudinal mode phonons [4]. Provisional analysis suggests that the ratio between the excitation of the longitudinal mode and the Rayleigh mode does not change as the incident kinetic energy changes. Ultimately, this work sets up the essential framework for future coherent control experiments with H2, aiming to directly quantify how a molecule's anisotropic rotational orientation—specifically helicopter versus cartwheel modes—governs inelastic scattering probabilities and energy dissipation during gas-surface collisions [5].

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Using the electrochemical-surface force balance (e-SFB) to study electrode-electrolyte interfaces

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The surface force balance (SFB) is the gold-standard technique for directly measuring surface forces.1 In an SFB experiment, white light interferometry is used to precisely determine the separation and interaction force between two atomically smooth mica surfaces separated by a medium of interest. The resulting force versus distance curves give us insight into the free energy of the interaction between the surfaces, as mediated by the liquid. Conventional SFB measurements have been used to better understand the interfacial structuring of battery electrolytes to date, however, the applicability of these results to understanding a real battery environment is somewhat limited by the electrically insulating nature of the mica surfaces used in the experiments.

The electrochemical-surface force balance (e-SFB) replaces one of the mica surfaces with a conductive metal surface, most commonly gold.2-3 The potential of this surface can then be controlled to act as an electrode, allowing surface forces to be measured at an interface with the range of applied potentials that an electrolyte would encounter in electrochemical applications. Force versus distance data from the e-SFB is analogous to electrochemical-atomic force microscopy but has the additional benefits of giving access to absolute, rather than relative, distances.

This poster will summarise new measurements of highly concentrated electrolytes, including ionic liquids and water-in-salt electrolytes, in contact with a gold electrode using the e-SFB technique. Measurements of ionic liquids reveal interfacial structuring that changes as the potential applied to the gold surface is varied. Additional measurements of lithium-based electrolytes where solid electrolyte interphases (SEIs) are grown in-situ on the gold electrode will also be presented.4

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Electrochemical and Atomic-Scale Evolution of Amorphous Ti–O Interfaces under Oxidative Conditions

Dr. Riya Thomas[1], Sana Khayyamifar[1], Johan Hektor[1], Philip Miguel Kofoed[1], Tautgirdas Ruzgas[1], Harald J. Wallander[1], Alexander Yaroslavtsev[2], Denis Music[1]
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Titanium implants are widely used in clinical practice due to their excellent corrosion resistance and biocompatibility, which rely on the stability of a nanoscale surface oxide layer. However, the integrity of this passive film under oxidative stress, particularly in the presence of reactive oxygen species such as hydrogen peroxide (H_2O_2), remains insufficiently understood. To address this, sputter-deposited Ti–O thin films were employed as model systems and exposed to phosphate-buffered saline solutions with and without H_2O_2. Electrochemical measurements revealed suppressed anodic currents and increased charge-transfer resistance upon H_2O_2 exposure, suggesting enhanced passivation. In contrast, high-resolution X-ray photoelectron spectroscopy performed at the MAX IV Laboratory identified subtle shifts in titanium oxidation states and oxygen species, indicating early-stage chemical modifications of the oxide layer. Complementary density functional theory simulations provided atomistic insights into H_2O_2 interactions with Ti–O surfaces, supporting the experimental findings. Together, this integrated electrochemical, spectroscopic, and theoretical approach uncovers early indicators of peroxide-induced surface modification and highlights the importance of engineered Ti–O nanofilms as robust platforms for evaluating implant durability under oxidative stress.

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