KFM 24: New Methods and Developments: Spectroscopies, Diffraction and Others (joint session O/KFM)

Time: Thursday 10:30–12:30 Location: H6

Topical Talk KFM 24.1 Thu 10:30 H6

Element and Structure Analysis of Surfaces Using Positrons — •Christoph Hugenschmidt — Forschungs-Neutronenquelle Heinz Maier-Leibnitz (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

With the advent of bright low-energy positron beams novel analysis tools have been developed exploiting the unique properties of positron matter interaction such as repulsive crystal potential or positron trapping in surface states [1]. Positron annihilation is established for defect spectroscopy and the characterization of the free volume in amorphous matter. By applying a slow positron beam, however, defects near the surface can be specifically addressed, e.g. for the determination of the oxygen vacancy concentration in $YBa_2Cu_3O_{7-x}$ [2]. The positron counterparts of reflection high-energy electron diffraction (RHEED) and electron induced Auger-electron spectroscopy (AES) intrinsically exhibit superior surface sensitivity. In contrast to electrons, positrons show total reflection for small glancing angles. It was demonstrated that with reflection high-energy positron diffraction the structure of the topmost and the immediate subsurface atomic layer of surfaces are revealed with outstanding accuracy. The main advantages of positron annihilation induced AES are the missing secondary electron background and its topmost layer sensitivity for element analysis allowing, e.g. the *in-situ* observation of the Ni adatom migration from the Pd surface into the bulk [3]. [1] C. H.; Surf. Sci. Reports 71 (2016) 547; [2] M. Reiner et. al.; Phys. Rev. B 97 (2018) 144503; [3] S. Zimnik et. al.; Surf. Sci. 664 (2017) 61

KFM 24.2 Thu 11:00 H6

Active sample manipulation with electrostatic beams: a different way of bridging the high-voltage gap — •Francesco Guatieri, Kilian Brenner, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

Most electrostatic positron beams used to perform surface studies are accelerated to the desired implantation energy by floating the target to a high electrostatic potential relative to ground. The presence of tens on kilovolts of electric potential makes the use of instrumentation attached directly to the sample inconvenient. The conventional solution to this hurdle consists in wiring insulated connections from the sample to a high-voltage galvanic decoupling placed outside of the experimental chamber far away from the sample holder. This solution carries limitations on the kind and amount of electrical connections employed. We will present, instead, a novel approach to in-operando sample manipulation that we have developed to be used at the Doppler broadening spectrometer installed on the NEPOMUC positron source, which implements the galvanic insulation in situ and removes many of the limitations imposed by conventional solutions.

KFM 24.3 Thu 11:15 H6

Advanced Kernel-Based NMR Cryoporometry Characterization of Mesoporous Solids — •Henry R.N.B. Enninful, Daniel Schneider, Richard Kohns, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

NMR cryoporometry is a pore space characterization technique for industrial and natural materials such as catalysts, gas storage materials, cartilage, bones, rocks and many more. While gaining wide use, the fundamental phenomena underlying solid-liquid phase transitions in geometrically disordered porous materials is still not fully understood. This may lead to inaccurate pore size distributions from the NMR cryoporometry technique.

In this work, we have developed a new approach to NMR cryoporometry. Herein, it takes account of cooperativity effects in pores, the existence of a variable non-frozen layer (NFL) thickness between the frozen core and pore wall and the effect of curvature on thermal fluctuations in pores which hitherto are missing in the current approach. In the first place, we compile a family of transition curves characterizing the phase state in pores with different pore sizes, so called kernels. Thereafter, we apply a general framework for predicting phase equilibria in a collection of pores. Specifically, the proposed kernel-based approach is coupled with the serially-connected pore model (SCPM) to be able to predict phase behavior in independent pore systems as well as in pore networks. We demonstrate the new approach by applying it to ordered porous materials such as MCM-41 and SBA-15. Consequently, a more accurate pore size distribution (PSD) is obtained.

KFM 24.4 Thu 11:30 H6

Development of an electron spin resonance spectrometer in ultra-high vacuum for surface spins — •Juyoung Park[1,2], Franklin H. Cho[1,2], Jisoo Yu[1,2], Luciano Colazzo[1,2], Yejin Jeong[1,2], Junjie Liu[3], Arzhang Ardavan[3], Giovanni Boero[4], Andreas Heinrich[1,2], and Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]The Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, UK — [4]Ecole Polytechnique Fédérale de Lausanne, Laboratory for Microsystems, Lausanne, Switzerland

We present the development of an electron spin resonance (ESR) spectrometer operating in ultra-high vacuum (UHV) for studying surface-adsorbed molecular and atomic spin systems. Such surface spin systems are promising platforms for potential applications in quantum computing and information processing [Science 366, 509 (2019)]. Our spectrometer is capable of both continuous-wave and pulsed ESR measurement in the temperature range of 2.5 K to 300 K. The surface-sensitivity is attained using a surface-type microwave resonator with its resonance frequency in the X-band. The spectrometer is connected to a home-built in-situ preparation chamber which allows us to prepare and characterize surfaces with low-energy electron diffraction and Auger electron spectroscopy. We demonstrate that we are sensitive down to a monolayer of molecular film using organic radicals such as α,γ-Bisdiphenylene-β-phenylallyl, and metal phthalocyanine complexes such as vanadyl phthalocyanine.

KFM 24.5 Thu 11:45 H6

Unsupervised machine learning-assisted analysis of multidimensional ARPES data — •Steinn Ymir Agustsson[1], Mohammad Ahsanul Haque[2], Fatemeh Zardbani[2], Davide Mottin[2], Panagiotis Karras[2], and Philip Hofmann[1] — [1]Institute of Physics and Astronomy, Aarhus University, Denmark — [2]Institute of Computer Science, Aarhus University, Denmark

In recent years, the size and complexity of experimental data sets has been dramatically growing in many fields of science. For photoemission spectroscopy, the development of novel detectors and multidimensional measurement modes (e.g., including a time dependence or spatial dependence), has lead to orders of magnitude more data being produced. Even after a necessary upgrade of the data management system, it remains highly challenging to visualize and superficially interpret the data fast enough to feed back into decisions about what to measure in an ongoing experimental run. A promising approach to address this is the application of machine learning tools. These have shown promising results when applied to data reduction and feature detection tasks in many fields of science. We have developed an unsupervised clustering method which is able to distinguish differences between ARPES spectra obtained from different spatial locations in nanoARPES measurements. This enables quick and automatic identification and classification of regions with different spectral features, allowing to invest more time in the collection of significant data.

KFM 24.6 Thu 12:00 H6

ViPErLEED: A modern all-in-one LEED I(V) package — •Alexander M. Imre[1], Florian Kraushofer[1,2], Florian Doerr[1], Tilman Kisslinger[3], Michael Schmid[1], Ulrike Diebold[1], Lutz Hammer[3], and Michele Riva[1] — [1]TU Wien, Vienna, Austria — [2]TU Munich, Munich, Germany — [3]FAU Erlangen-Nürnberg, Erlangen, Germany

Many surface science groups use Low-Energy Electron Diffraction (LEED) for quick, qualitative analysis of surface periodicity. Analysis of the beam intensities as a function of electron energy [LEED $I(V)$] is sensitive to surface atom positions at the picometer scale. Thus, comparison with calculated intensities can verify or reject structural models. Despite this, LEED $I(V)$ is currently rather unpopular, largely because the available software solutions are not sufficiently user-friendly. To greatly lower the barrier of entry into the field, we present

the Vienna Package for TensErLEED (ViPErLEED) which provides a truly all-in-one package for LEED $I(V)$. ViPErLEED includes a freely available design for electronics that enable upgrading existing LEED setups for LEED $I(V)$ use. With sophisticated image acquisition and processing methods, as well as an automated spot-tracking tool for curve extraction, we greatly simplify the most tedious parts of the experiment. For the calculation of intensities, the package includes a user-friendly front-end and an extensive overhaul to the established TensErLEED package that only requires a few standardized input files. We further describe automated symmetry detection, improvements to the structure search algorithm, and a Python API.

KFM 24.7 Thu 12:15 H6

On-surface GNR fabrication via electrospray deposition of monomers and polymers from solution — •Felix Baier[1], Christoph Dobner[1], Michael Beckstein[1], Mamun Sarker[2], Alexander Sinitskii[2], and Axel Enders[1] — [1]Universität Bayreuth — [2]University of Nebraska - Lincoln, USA

Strategies for depositing large organic molecules such as proteins, DNA or graphene nanoribbons (GNRs) are urgently needed because the conventional method of evaporation is impossible due to the size of the molecules. GNRs prepared in solution are of particular interest because they are longer compared to those synthesized on the surface and can be produced in large quantities. Since GNRs form crystallites, they cannot be brought onto the surface by direct contact printing and characterized using STM. Therefore, a new electrospray setup was developed for the deposition of GNR precursor molecules, large precursor polymers, and GNR from a solution. The instrument consists of a heatable stainless steel capillary to which a high voltage in the range -8 to 8 kV, with respect to the sample can be applied. The assembly is placed in a glovebox which ensures the cleanliness of the working process. The characterization of the deposits was done with STM under ultra high vacuum after sample transfer. The deposition of TPTP monomers from solution onto Au(111) brought comparable results as other, established approaches were cGNR were formed after direct contact printing in UHV. Larger polymers were also deposited and completely cyclized on the surface after deposition, forming promising GNRs that have not been studied anywhere before.