

## O 37: Poster: Electronic Structure of Surfaces and Spectroscopy of Surface States

Time: Tuesday 18:00–20:00

Location: Poster D

O 37.1 Tue 18:00 Poster D

**iMott - imaging spin detector based on Mott scattering for SARPES** — ●DMITRY A. USANOV<sup>1</sup>, J. HUGO DIL<sup>1,2</sup>, and VLADIMIR N. STROCOV<sup>1</sup> — <sup>1</sup>Spectroscopy of Quantum Materials group, Paul Scherrer Institut, Villigen CH-5232, Switzerland — <sup>2</sup>Institut de Physique, École Polytechnique Fédérale de Lausanne, Lausanne CH-1015, Switzerland

The electron spin is the crucial parameter of modern spintronics and therefore its determination in energy structures of solids is highly important. In order to boost spin-resolved ARPES' efficiency and accessibility, a prototype of a new imaging-type multichannel spin detector for electrons based on Mott scattering (nicknamed iMott) is being developed. The presentation will be focused on two main aspects: first, high stability and excellent image transfer will be demonstrated; second, the algorithms of signal acquisition and processing will be discussed. Two possible operation regimes, namely, the accumulating and single-electron counting modes, will be compared in conjunction with intensity and signal-to-noise ratio requirements, which determine reliable detection of spin asymmetry. The energy resolution of the multichannel detectors and the whole polarimeter will be shown and discussed. Further development directions will be outlined.

O 37.2 Tue 18:00 Poster D

**A New Setup for the Measurement of the Angular Correlation of Annihilation Radiation** — ●KILIAN BRENNER, FRANCESCO GUATIERI, and CHRISTOPH HUGENSCHMIDT — Lichtenbergstr. 1 85748 Garching

The measurement of the Angular Correlation of positron Annihilation Radiation (ACAR) provides an elegant solution to investigate Fermi-surfaces. The present ACAR spectrometer at TUM uses Anger cameras basically comprising large NaI(TL) crystals read out by an array of 61 photomultiplier tubes. In our new setup, we employ pixelated LYSO scintillation crystals in combination with state-of-the-art Multi-Photon-Pixel-Counters (MPPCs), drastically improving momentum resolution and count rate by capitalizing on the smaller detector-element size and faster readout. We present the new setup, its capabilities and preliminary measurements.

O 37.3 Tue 18:00 Poster D

**Two-photon photoemission on Ag(111) with time-of-flight momentum microscope** — ●YU-CHAN LIN<sup>1</sup>, CHIEH-I CHEN<sup>1,2,3</sup>, MUKESH SINGH<sup>1</sup>, PRABESH BISTA<sup>1,2,4</sup>, and CHENG-TIEN CHIANG<sup>1,2,5</sup> — <sup>1</sup>Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan — <sup>2</sup>Molecular Science and Technology Program, Taiwan International Graduate Program, Academia Sinica, Taipei, Taiwan — <sup>3</sup>Department of Chemistry, National Tsing Hua University — <sup>4</sup>Department of Physics, National Central University — <sup>5</sup>Department of Physics, National Taiwan University, Taipei, Taiwan

This study explores two-photon resonances in the electronic structure of Ag(111) through the application of two-photon photoemission. The light source is based on third harmonic generation via nonlinear optical crystals, transforming 1.2 eV, 300 fs laser pulses to 3.6 eV. By employing time-of-flight photoelectron momentum microscope, the electronic states of both occupied and unoccupied regions of the Ag sp bands can be observed via resonant two-photon absorption. By measuring the angular and time-of-flight distributions of the photoelectrons, the energy-momentum dispersion relation of these bands can be retrieved. These results are analyzed in detail and compared with earlier literature at different photon energies.

O 37.4 Tue 18:00 Poster D

**Efficient Data Acquisition in Multi-Dimensional Photoemission Spectroscopy using denoising** — ●MUHAMMAD ZAIN SOHAIL<sup>1,2</sup>, DMYTRO KUTNYAKHOV<sup>2,3</sup>, and KAI ROSSNAGEL<sup>2,3</sup> — <sup>1</sup>RWTH Aachen University, 52066 Aachen, Germany — <sup>2</sup>Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — <sup>3</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

In the realm of photoemission spectroscopy, the exploration of large multi-dimensional phase spaces necessitates time-intensive data acquisition to ensure statistical robustness. Despite the unparalleled capabilities of free-electron lasers (FELs), in peak brightness and ultra-

short pulsed X-rays, the limitations of low repetition rates prolong the data acquisition process. This impedes the agility of decision making that could otherwise enhance experimental results in the limited and valuable beamtime. By employing denoising strategies to mitigate noise while preserving intrinsic information, our proposed approach aims to streamline the data acquisition process, and effectively manage the escalating size and complexity of multi-dimensional photoemission data.

O 37.5 Tue 18:00 Poster D

**Soft X-ray momentum-resolved photoelectron spectroscopy with a momentum microscope at Diamond Light Source** — ●DEEPNARAYAN BISWAS<sup>1</sup>, MATTHIAS SCHMITT<sup>1,2</sup>, JIEYI LIU<sup>1</sup>, OLENA TKACH<sup>3</sup>, RALPH CLAESSEN<sup>2</sup>, GERD SCHÖNHENSE<sup>3</sup>, and TIEN-LIN LEE<sup>1</sup> — <sup>1</sup>Diamond Light Source Ltd., UK — <sup>2</sup>University of Würzburg, Germany — <sup>3</sup>University of Mainz, Germany

Angle-resolved photoelectron spectroscopy (ARPES) experiments are usually performed with excitation energies below ~100 eV to harness the higher photoionisation cross-sections and better energy and (in-plane) momentum resolutions. However, the very short electron mean free paths at low energies severely limit the bulk sensitivity. It is therefore desirable to extend ARPES to the soft x-ray (SX) range, which opens up the opportunity for probing unconventional electronic structures at buried interfaces, studying 3D electronic systems etc.

We are currently commissioning a SX-ARPES end-station at Beamline I09 at DLS, equipped with a state-of-the-art momentum microscope (MM). MMs preserve the momentum view and resolution irrespective of the excitation energy, which is advantageous to ARPES performed at high energies. In addition, MMs enable selective studies of micron/sub-micron-sized sample areas using field apertures. Our MM is uniquely designed to use a single hemispherical analyser followed by a time-of-flight section fitted with a fast delay-line detector as a combined energy filter, resulting in highly efficient data collection. In this poster, we will present current progress and the potential applications of this new facility to quantum materials research.

O 37.6 Tue 18:00 Poster D

**Influence of optical orbital angular momentum on the circular dichroism of Rashba system surface states** — ●JANNIS LESSMEISTER<sup>1</sup>, TOBIAS EUL<sup>2</sup>, BENJAMIN STADTMÜLLER<sup>1</sup>, and MARTIN AESCHLIMANN<sup>1</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Germany — <sup>2</sup>Institute of Experimental and Applied Physics, University of Kiel, Germany

Since its discovery in 1992 [1], twisted light has found its way into a wide variety of research areas and applications. Recently the interaction between its intrinsic orbital angular momentum (OAM) and condensed matter has become a steadily growing field of research [2].

In our research we employ momentum microscopy to gain new insights into the interaction of twisted light with metallic surfaces. Using a circularly polarized light beam carrying OAM we investigate the circular dichroism of the Au(111) Shockley surface state. We particularly focus on the influence of the photonic OAM on the dichroism signal of materials with different atomic spin-orbit strengths.

[1] Allen et al., Phys. Rev. A 45 (1992)

[2] Quinterio Rosen et al., Rev. Mod. Phys 94 (2022)

O 37.7 Tue 18:00 Poster D

**Substrate doping and defect influence on P-rich InP(001):H surface properties** — RACHELE SCIOTTO, ●ISAAC AZAHEL RUIZ ALVARADO, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, Paderborn, Germany

Density-functional theory calculations on P-rich InP(001):H surfaces are presented. Depending on temperature, pressure and substrate doping, hydrogen desorption will occur and influence the surface electronic properties. For p-doped samples, the charge transition levels of the P dangling bond defects resulting from H desorption will lead to Fermi level pinning in the lower half of the band gap. This explains recent experimental data. For n-doped substrates, H-deficient surfaces are the ground-state structure. This will lead to Fermi level pinning below the bulk conduction band minimum. Surface defects resulting from the adsorption of additional hydrogen can be expected as well but affect the surface electronic properties less than H desorption.

O 37.8 Tue 18:00 Poster D

**Implementation of a fiber-based cathodoluminescence detector system for an ultrafast scanning electron microscope** — ●FILIP MAJSTOROVIC<sup>1</sup>, PAUL H. BITTORF<sup>1</sup>, and NAHID TALEBI<sup>1,2</sup> — <sup>1</sup>Institute for Experimental and Applied Physics, Kiel University, Leibnizstraße 19, D-24118 Kiel, Germany — <sup>2</sup>Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, Christian-Albrechts-Platz 4, D-24118 Kiel, Germany

When high-energy electron beams interact with materials, light can be emitted by the excited sample. This radiation is known as coherent or incoherent cathodoluminescence (CL), depending on the underlying interaction mechanism, and gained a major interest in the study of minerals, semiconductors and plasmonic resonances in nanoparticles, where both spectral and temporal statistics can be unraveled. Due to the high spatial resolution and large spectral excitation bandwidth of the electron beams inside an SEM, electrons locally probe photonic modes, resulting in the capability to image their spatial near-field distribution via CL spectroscopy. Here, we report on the construction of a fiber-based CL detector for an SEM. We present first measurements to prove the ability for raster scanning the samples CL emission using fibers. Additionally, this detector is implemented inside an ultrafast SEM (USEM) setup for realizing a time-resolved electron-light pump-probe measurement configuration, where the luminescence of a sample, coming from the excitation either with electron or laser pulses, will be spatially resolved. This will be used to improve the USEM setup and analyze the dynamics of electron-light-matter interaction.

O 37.9 Tue 18:00 Poster D

**Electronic structure study of intercalated transition metal dichalcogenide** — ●JYOTI KASWAN<sup>1</sup>, LAURENT NICOLAÏ<sup>1</sup>, MICHAL PROCHÁZKA<sup>1</sup>, SARATH SASI<sup>1</sup>, SUNIL W DSOUZA<sup>1</sup>, VERONICA VAVRUŇKOVÁ<sup>1</sup>, ROSTISLAV MEDLÍN<sup>1</sup>, ZDENĚK SOFER<sup>2</sup>, STEFANIE GÄRTNER<sup>3</sup>, and JAN MINÁR<sup>1</sup> — <sup>1</sup>University of West Bohemia, Plzeň, Czech Rep. — <sup>2</sup>University of chemistry and technology Prague, Czech Rep. — <sup>3</sup>University of Regensburg, Germany

Intercalated transition metal dichalcogenide (TMDs) has recently attracted attention of condensed matter community owing to the exhibition of the exotic phenomena depending upon the intercalate transition metal [1]. We explore the electronic structure of V-intercalated TMDs V1/3NbS<sub>2</sub> using spin and angle resolved photoemission spectroscopy (SARPES) in combination with one step model of photoemission as implemented in the SPR-KKR package [2], our calculations can combine temperature- and phonon energy-dependent effects via inclusion of both bulk and surface phonons. Raman spectroscopy has been employed to determine the spin-phonon interaction along with the in-plane metal-metal distance and out of plane interlayer distance. For determining bulk as well as surface lattice structure of the V1/3NbS<sub>2</sub> monocrystals, we have utilized multiple characterizations techniques Low electron energy diffraction (LEED), Transmission electron microscopy (TEM) and single crystal X-ray diffraction. [1] B. Edwards et al, Nature Materials 22, 459 (2023) [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011)

O 37.10 Tue 18:00 Poster D

**Model for Linear and Circular Dichroism in Angle-Resolved Photoemission Spectroscopy** — ●MAXIMILIAN ÜNZELMANN<sup>1</sup>, NOAH ENDRES<sup>1</sup>, BEGMUHAMMET GELDIYEV<sup>1</sup>, JAKUB SCHUSSER<sup>1</sup>, HENDRIK BENTMANN<sup>2</sup>, and FRIEDRICH REINERT<sup>1</sup> — <sup>1</sup>Experimentelle Physik 7 and Würzburg-DresdenCluster of Excellence ct.qmat, Universität Würzburg — <sup>2</sup>Center for Quantum Spintronics, Department of Physics, NTNU, Norway

Angle-resolved photoemission spectroscopy (ARPES) in combination with linear and circular dichroism (LD and CD) has evolved as a powerful tool to study spin-split electronic states in solids including, e.g., Rashba systems [1,2] or Weyl semimetals [3]. In particular, the combination of spin-orbit coupling (SOC) and inversion symmetry breaking

(ISB) leads to the formation of spin- and orbital angular momentum (OAM) in the electronic wave functions. Here, we show – using a simple model for the photoemission matrix element – that both LD and CD are sensitive to the OAM in the initial state wave function. We apply our model to the eigenstates obtained from tight-binding band structure calculations. On this basis, the influence of (i) experimental parameters and (ii) properties of the initial state on the dichroic signal will be discussed. Finally, we show that those model calculations compare nicely with real experimental data on various types of material systems.

- [1] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017)  
 [2] M. Ünzelmann et al., Phys. Rev. Lett. 124, 176401 (2020)  
 [3] M. Ünzelmann et al., Nat. Commun., 12, 3650 (2021)

O 37.11 Tue 18:00 Poster D

**Surface preparation of topological insulator Bi<sub>2</sub>Te<sub>3</sub> and ferromagnet La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> for band structure measurements** — ●ØYVIND FINNSETH, DAMIAN BRZOZOWSKI, INGRID HALLSTEINSEN, and HENDRIK BENTMANN — Norwegian University of Science and Technology

The proximity coupling of topological insulators with magnetically ordered systems in heterostructure systems, wherein the magnetic order serves to break the time reversal symmetry of the topological insulator, have attracted much attention in later years. As components in such a system, we consider thin films of the topological insulator Bi<sub>2</sub>Te<sub>3</sub> and ferromagnetic La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (LSMO) grown by pulsed laser deposition. The signature of the topological state of Bi<sub>2</sub>Te<sub>3</sub> may be found in the electronic band structure of the surface state. In order to understand the effect of proximity coupling on the surface state in a heterostructure, a full understanding of the properties of its constituents is required. However, the surfaces of both Bi<sub>2</sub>Te<sub>3</sub> and LSMO degrade after exposure to air, rendering band structure measurements of surface states challenging. We therefore study surface preparation methods necessary for ARPES measurements on these materials. The studied methods include annealing with and without an oxygen atmosphere for LSMO, along with argon ion sputtering at different energies and duration for both samples. The suitability of each method is evaluated by XPS, yielding information on the presence of contaminants as well as the stoichiometry of the samples, while LEED serves to inspect the crystalline quality of the sample surface.

O 37.12 Tue 18:00 Poster D

**Sum-Frequency Generation Spectro-Microscopy in the Reststrahlen Band of Wurtzite-type Aluminum Nitride** — ●DOROTHÉE MADER, RICHARDA NIEMANN, MARTIN WOLF, SEBASTIAN MAEHRLEIN, and ALEXANDER PAARMANN — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Non-centrosymmetric materials including ferroics are commonly studied by second-harmonic imaging.<sup>1</sup> This method is highly sensitive to the material's symmetry, but is commonly employed non-resonantly. In contrast, infrared-visible (IR-VIS) sum-frequency generation (SFG) spectroscopy is employed resonantly to reveal vibrations, local structure and bonding of the material.<sup>2</sup> In SFG, the sample is excited at the IR-resonance and mixed with a non-resonant VIS beam leading to generation of sum-frequency light that is detected in the VIS. SFG benefits from the resonance but typically lacks spatial resolution. In this work, we combine the benefits of nonlinear optical imaging and SFG spectroscopy by employing SFG spectro-microscopy using the free electron laser of the Fritz Haber institute.<sup>3</sup> Specifically, we test the feasibility of our instrumentation for spectroscopy with m-plane wurtzite-type aluminum nitride as a model system. We find the experimental spectra to agree with our theoretical calculations. In the future, this method will provide spatially resolved spectroscopic information in inhomogeneous systems such as ferroics and their domains.

- [1] M. Fiebig et al., APL 66, 2906, (1995).  
 [2] W. Faust et al., PRL 17, 1265, (1966).  
 [3] R. Niemann et al., APL 120, 131102, (2022).