O 51: Poster Electronic Structure of Surfaces: Spectroscopy, Surface States

Time: Tuesday 18:00–20:00 Location: P2

O 51.1 Tue 18:00 P2

Visualizing quantum states in fluorene-based organometallic quantum corrals — •Longfeng Huang[1], Wenchao Zhao[1], Ignacio Piquero-Zulaica[1], Johannes Barth[1], and Biao Yang[1,2] — [1]Physics Department E20, Technical University of Munich, 85748 Garching, Germany — [2]Institute of Functional Nano and Soft Materials (FUNSOM), Soochow University, 215123 Suzhou, China

Constructing well-defined and controllable quantum states holds promise for applications in quantum technology. As an exemplary quantum architecture, quantum corrals (QCs) which are considered as artificial atoms attract enormous attention.1, 2 Common strategies for manufacturing QCs have mainly involved atomic and molecular manipulations, molecular assembly, and on-surface synthesis.3-5 However, fabricating robust QCs simultaneously with a high yield and specific size still remains elusive. In this work, we realize stable QCs with a well-defined size via organometallic bonding between fluorine-based molecules and intrinsic Ag adatoms on Ag(111). In particular, we observe spatial quantum resonance states inside the QCs, which arise from the scattered two-dimensional electron gas. Additionally, stadium-shaped and triangular QCs exhibit intriguingly specific orbital-like quantum states in differential conductance maps. In addition, we tune the QCs by replacing the F to H atoms and tip manipulation. Our study provides new means to fabricate controllable exotic quantum states with atomically precise QCs, aiding in a rational design strategy towards materials with tailored electronic properties.

O 51.2 Tue 18:00 P2

Termination-dependent ARPES maps from novel magnetic Kagome metals GdV_6Sn_6 and $GdMn_6Sn_6$ — •Robin P. Forster[1], Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Yishui Zhou[2], Yixi Su[2], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]JCNS Forschungszentrum-Jülich

The magnetic Kagome metals GdV_6Sn_6 and $GdMn_6Sn_6$ combine in a single material phenomena such as flat Kagome bands [1,2], local moments of the 4f electrons of Gd, and itinerant Mn or V 3d electrons [3], providing a platform to study their complex magentic and electronic interactions. We have performed termination-dependent micro-ARPES measurements with 20 μm real-space resolution at 20 K of paramagnetic GdV_6Sn_6 [4] and ferrimagnetic $GdMn_6Sn_6$ [5]. Surface and bulk states could be distinguished in the series of scans made over a range of photon energies. We have chosen $h\nu$ of 80 and 130 eV for GdV_6Sn_6 and 80, 112, 140, and 200 eV for $GdMn_6Sn_6$ for detailed ARPES scans. In addition, XPS measurements were conducted, which provide an insight into the measured terminations. Preliminary circular-dirchroic ARPES maps exhibit multiple sign inversions that stem from a combination of initial state orbital angular momenta and photoemission final state scattering [6]. [1] PRL 127, 266401 (2021) [2] PRB 104, 15122 (2021) [3] JPSJ 90, 124704 (2021) [4] JMMM 202, 519 (1999) [5] PRB 104, 235139 (2021) [6] *arXiv:2410.19652 (2024).

O 51.3 Tue 18:00 P2

Structural fingerprints in the reflectance anisotropy of P-rich and In-rich AlInP(001) — •Isaac Azahel Ruiz Alvarado[1], Mohammad Amin Zare Pour[2], Thomas Hannappel[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn, Germany — [2]Grundlagen von Energiematerialien, Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The surface optical anisotropy of AlInP(001) surfaces is investigated through experimental and theoretical approaches. Comparison is made between spectra calculated for energetically favored AlInP(001) surface structures with data measured on epitaxially grown $Al_{0.52}In_{0.48}P(001)$ epilayers lattice-matched to GaAs samples. The anisotropies for photon energies below 3 eV provide clear fingerprints for the structure of the outermost surface atomics layers. The negative anisotropies for P-rich AlInP(001) surfaces are related to transitions involving surface states located at the top P-dimers. In contrast, In-rich AlInP(001) surfaces show anisotropies related to surface states localized on the In atoms of the In dimers of the second row. The spectral features at higher energies provide insight into the near surface bulk ordering of AlInP. In particular, optical anisotropies at the AlInP critical point energies are found to be related to the CuPt ordering in the material.

O 51.4 Tue 18:00 P2

Next-Gen ARPES: AI-controlled beam polarization through Graphene — •Ridha Eddhib[1], Balasubramanian Thiagarajan[2], and Jan Minar[1] — [1]New Technologies-Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic — [2]MAX IV Laboratory, Lund University, Lund, 22100, Sweden

Angle-Resolved Photoemission Spectroscopy (ARPES) stands as a cornerstone technique in condensed matter physics, offering deep insights into electronic structures and quantum states. However, the precision of ARPES measurements critically depends on the exact calibration of the photon beam polarization, a challenge that often confronts experimentalists. This study introduces an innovative application of artificial intelligence (AI) to revolutionize ARPES experiments by enabling precise calibration and tuning of photon beam polarization through graphene ARPES cross section, aiming for the ideal of 100% circular polarization. At the heart of our methodology is a neural network model, meticulously trained on datasets generated by the sophisticated one-step model of the SPRKKR [1] (Spin-Polarized Relativistic Korringa-Kohn-Rostoker) code, renowned for its accurate ARPES simulation capabilities. This study leverages the ase2sprkkr package for streamlined interfacing with SPRKKR, enriching our AI model training data with high-fidelity simulations. By implementing this AI-driven methodology, researchers can dynamically adjust their ARPES setups, ensuring that each measurement is conducted under optimal polarization conditions. [1] Ebert, H., Koedderitzsch, D., & Minar, J. (2011). 74(9), 096501.

O 51.5 Tue 18:00 P2

The CD-ARPES study of intercalated transition metal dichalcogenide V1/3NbS2 — •Jyoti Kaswan[1], Laurent Nicolaï[1], Raphaël Salazar[1], Aki Ismo Olavi Pulkkinen[1], Sunil W Dsouza[1], Zdeněk Sofer[2], and Jan Minár[1] — [1]University of West Bohemia, Plzeň, Czech Republic — [2]University of chemistry and technology Prague, Czech Republic

Intercalated transition metal dichalcogenides (TMDCs) have recently garnered significant attention from the condensed matter community due to the demonstration of exotic phenomena that depend on the intercalated transition metal [1]. We investigate the electronic structure of V-intercalated TMDC, V1/3NbS2, using Circular Dichroic Angle-Resolved Photoemission Spectroscopy (CD-ARPES) in combination with the one-step model of photoemission as implemented in the SPR-KKR package [2].The intensity asymmetry in CD contains a well-known dichroism component related to the measurement geometry, as well as a component associated with magnetic ordering, complicating the extraction of spin information from CD-ARPES data. To address this challenge, our group has developed a model of dichroism based on the one-step model of photoemission (SPR-KKR code). By incorporating the measurement geometry, the ab initio calculations enable the separation of geometric and spin contributions to the CD signal [3,4]. [1] B. Edwards et al, Nature Materials 22, 459*465 (2023). [2] H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011) [3] O. Fedchenko et al., Sci. Adv. 10, eadj4883 (2024) [4] S. Beaulieu et al, Phys. Rev. Lett. 125, 216404 (2020)