O 88: Electronic Structure of Surfaces II

Time: Thursday 15:00–17:45 Location: H26

O 88.1 Thu 15:00 H26

Probing the Surface States in β-Bi2Pd through YSR excitations — •Javier Zaldívar[1], Carmen Rubio-Verdú[1], Rubén Ibarrondo[1], Edwin Herrera[2], Isabel Guillamón[2], Hermann Suderow[2], and José Ignacio Pascual[1,3] — [1]CIC nanoGUNE, San Sebastián, Spain — [2]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

β-Bi2Pd in its bulk form is a topological semimetal with spin-polarized surface states which has drawn attention on the possibility of hosting spin-triplet components in the superconducting phase [1][2]. Previous works relied on quasi-particle interference for the detection of the spin-polarized surface states in the normal state [3]. In this work, we propose an alternative route based on the analysis of the periodicities of the Yu-Shiba-Rusinov (YSR) wavefunction [4]. Using this procedure we have been able to identify the spin-polarized surface states in the superconducting condensate. Our results open the possibility of studying spin-triplet components in mixed singlet and triplet systems through magnetic impurities.

1. M. Sakano et al, Nat. Commun. 6, 8595(2015) 2. J. Kačmarčík et al, Phys. Rev. B 93, 144502(2016) 3. K. Iwaya et al, Nat. Commun. 8, 976(2017) 4. B. Heinrich et al., Prog. Surf. Sci. 93, 1 (2018)

O 88.2 Thu 15:15 H26

Spin-polarized surface states of the SIC phase in Pb/Si(111) — •Christian Brand[1,2], Herbert Pfnür[1], Jan Hugo Dil[3,4], Stefan Muff[3,4], Michael C. Tringides[5], and Christoph Tegenkamp[1,6] — [1]Leibniz Universität Hannover, Germany — [2]Universität Duisburg-Essen, Germany — [3]Swiss Light Source, Villigen, Switzerland — [4]École Polytechnique Fédérale de Lausanne, Switzerland — [5]Ames Laboratory & Iowa State University, Ames, USA — [6]Technische Universität Chemnitz, Germany

Atomic monolayers (ML) of Pb/Si(111) have been found to be superconducting below $T_C \approx 1.8$ K [1], but the mechanism behind the evolution of these 2D states is not understood yet. In the so-called striped-incommensurate (SIC) phase close to 4/3 ML stripes with local H3- or T4-centered $(\sqrt{3} \times \sqrt{3})$-reconstruction are separated by $(\sqrt{7} \times \sqrt{3})$-domain walls. Here we present STM and (SR)-ARPES measurements at low T ($> T_C$) to evaluate the influence of the spin-orbit interaction on the Pb surface states. As it turns out the local adsorption geometry and symmetry of the atomic structure play important roles for the understanding of the measured spin-polarization by SR-ARPES showing strongly spin-polarized metallic surface states [2]. The experimental results are in very good agreement with DFT calculations [3] and reveal beside a complex spin-texture at E_F large Rashba-type and Zeeman-like spin-splittings of the Pb surface states. [1] Nature Phys. **6**, 104 (2010), [2] PRB **96**, 035432 (2017), [3] PRB **94**, 075436 (2016).

O 88.3 Thu 15:30 H26

In Situ Strain Tuning of the Dirac Surface States in Bi2Se3 Films — •David Flötotto[1,2], Yang Bai[2], Yang-Hao Chan[3], Peng Chen[2], Xiaoxiong Wang[4], Cai-Zhi Xu[2], Joseph A. Hlevyack[2], Mei-Yin Chou[3], James N. Eckstein[2], and Tai-Chang Chiang[2] — [1]Center for Soft Nanoscience, University of Münster, Germany — [2]University of Illinois at Urbana-Champaign, Urbana, USA — [3]Academia Sinica, Taipei, Taiwan — [4]Nanjing University of Science and Technology, Nanjing, China

A controlled manipulation of the bulk band gap and spin-polarized Dirac surface states of topological insulators is of great fundamental importance and relevant to novel device applications. A promising pathway involves the application of strain, which alters the interatomic lattice spacing thus induces corresponding changes in the electronic band structure. By performing angle-resolved photoemission spectroscopy and X-ray diffraction measurements during in situ tensile tests of ultrathin epitaxial Bi2Se3 films on flexible substrates we demonstrate that the band structure of the prototypical topological insulator Bi2Se3 can be reversibly tuned in situ by applying extrinsic elastic strain of up to 2.1%. In accordance with our first principle calculations, the Dirac point reversibly shifts to larger binding energies with increasing tensile strain as a result of the decreasing inter quintuple-layer distance. Our study is an important step forward towards using strain as an in-situ tool for tailoring of the functional properties of topological materials and opens new routes for a momentum-resolved quantification of strain-induced band-structure changes.

O 88.4 Thu 15:45 H26

Growth and electronic properties of Fe on Nb(110) studied by STM and STS — •Johannes Jung, Niclas Schmidt, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany

Superconductivity and ferromagnetism with the underlying singlett and triplett pairing mechanisms, respectively, are often considered two antagonistic phenomena. Here we report on the investigation of the growth and the electronic properties of Fe on the Nb(110) surface, which exhibits the highest $T_c = 9.2$ K of all elements. In the submonolayer range we observe three kinds of Fe–islands which exhibit different surface patterns. Spatially resolved data taken at the boundary between the superconductor and the ferromagnet show a narrow transition region with a width $w_{sc-fm} = 1.5 \pm 0.5$ nm. On Fe monolayer islands a small but finite conductance dip with a 10-20% reduction remains visible in normalized STS data, indicating that the superconducting wave function has a non-zero probability amplitude at the tip position. We will present date on the dependence of surface superconductivity of Nb(110) on Fe coverage and discuss implications in the context of topological superconductivity and Majorana fermions.

O 88.5 Thu 16:00 H26

Determination of the superconducting gap of Ru(0001) and observation of a proximity-induced gap in 1ML Co/Ru(0001) — •Julian Skolaut[1], Loic Mougel[1], Marie Hervé[1], Timofey Balashov[1], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut, Karlsruhe Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany

The proximity effect at the interface between a superconductor and a ferromagnet is of great interest since it can, in combination with specific spin textures in the ferromagnet, potentially be used as a platform to study majorana modes.

We used a scanning tunneling microscope (STM) mounted on a dilution cryostat to investigate the superconducting gap of Ru(0001) and its dependence on the temperature.

Furthermore, Cobalt islands were grown on Ru(0001) to investigate the the proximity-induced superconducting gap on the Cobalt islands. Even though significantly reduced in intensity, the gap was observed on both substrate and islands.

O 88.6 Thu 16:15 H26

Adsorption of atomic Fe-clusters on superconducting Pb — •Carl Drechsel, Rémy Pawlak, Philipp d'Astolfo, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Due to their potential use as topological qubits in quantum computers, Majorana bound states (MBS) have attracted a large interest in Physics. Recent experiments at low temperature (< 5 K) have shown that iron chains grown on lead surfaces exhibit zero-bias conductance peaks at their ends [1,2,3,4], which can be interpreted as signature for a MBS [5].

Here, we investigate the internal structure and adsorption sites of small iron clusters evaporated on lead surfaces. Combining scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS) and atomic force microscopy (AFM), we characterize the structural and electronic properties at the atomic scale. This can be used as fundamentals for fabrication methods of iron chains on lead with atom-by-atom manipulation.

[1] Nadj-Perge, S. et al.; Science 346, 602 (2014) [2] Ruby, M. et al.; Phys. Rev. Lett. 115, 197-204 (2015) [3] Pawlak, R. et al.; npj Quantum Information, 16035 (2016) [4] Feldmann, B.E. et al.; Nature Physics 13, 286-291 (2017) [5] Mourik, V. et al.; Science 336, 1003 (2012)

O 88.7 Thu 16:30 H26

Electronic structure of the LaB_6 (001)-surface — •Florian Sohn[1,2], Philipp Buchsteiner[3], Jan Voigt[3], Martin

Wenderoth[3], and Peter E. Blöchl[1,2] — [1]Institut für theoretische Physik, Technische Universität Clausthal — [2]Institut für theoretische Physik, Universität Göttingen — [3]IV. Physikalisches Institut, Universität Göttingen

Lanthanum hexaboride (LaB_6) is the first compound among the rare earth hexaborides. Due to its low work function and high melting point, LaB_6 is widely used for thermionic electron emission. Recently, the LaB_6 (001)-cleavage plane has been investigated with scanning tunneling microscopy (STM) and spectroscopy (STS). Our data shows a mainly 2×1 reconstructed surface. We rationalize the constant current topographies and differential conductance spectra by simulations based on density functional theory (DFT). Our simulations of a LaB_6 (001)-surface, terminated by chains of lanthanum ions, show, that in STM measurements with positive bias voltage the *d*-orbitals of the topmost lanthanum ions are addressed. In contrast, at small negative bias voltages, a broad feature in the local density of states below the Fermi energy could be successfully resolved by both STS and DFT and is traced back to surface boron orbitals. Our study shows the necessity of surface calculations in order to understand the experimental data in detail and can be applied to various model systems.

O 88.8 Thu 16:45 H26

STM investigation of scattering phase shifts of single non-magnetic impurity atoms buried in Cu — •Thomas Kotzott[1], Mohammed Bouhassoune[2], Henning Prüser[1], Samir Lounis[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

Impurities in nanostructures can be crucial for the functionality of the devices. Hence, scattering properties of impurity atoms in metals have been thoroughly investigated in the past by theoretical calculations and experimental measurements of the bulk. Here, we present a study to characterize the scattering phase of single, non-magnetic atoms buried in Cu by means of scanning tunneling microscopy (STM) and density functional theory. Using the electron focusing effect we visualize single Ge and Ag atoms several layers below the Cu surface. Experiments have been performed with a home-built low-temperature UHV-STM operating at 6K. Dilute alloys were grown by co-deposition of Cu and Ag or Ge, respectively, onto a clean Cu(100) surface. Ab-initio calculations and a plane-wave toy model are compared to the data.

We can extract the phase shift from the LDOS pattern above bulk impurities which is set by depth and species of the impurity. We find that the simple model of a Lorentzian scatterer is not sufficient for understanding all the characteristics on the local scale for a non-magnetic atom. This work was supported by DFG projects LO 1659/5-1 and WE 1889/8-1.

O 88.9 Thu 17:00 H26

Dielectric surface properties of $SrTiO_3$(001) surface studied by HREELS — •Jonas Pantzer[1], Florian Schumann[1], Manuel Bibes[2], and Wolf Widdra[1,3] — [1]Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Unité mixte de physique CNRS/Thales, 91767 Palaiseau, France — [3]Max Planck Institute for Microstructure Physics, 06120 Halle, Germany

$SrTiO_3$ is often considered as one of the most surprising materials in the complex oxides family [1]. The discovery of a two-dimensional electron gas (2DEG) at interfaces of SrTiO3 with $LaAlO_3$ [2] and the bare surface of $SrTiO_3$(001) [3] represents a milestone towards exploiting such properties in oxide devices.

Here we report on high-resolution electron energy loss spectroscopy (HREELS) studies of the $SrTiO_3$(001) surface for different preparation conditions, different doping levels, and upon adsorption of aluminum. From surface phonon-polariton and surface plasmon polariton line shapes, we extract the charge carrier contribution and the full complex surface dielectric response.

[1] Yun-Yi Pai et al., Rep. Prog. Phys. 81, 036503 (2018)
[2] Ohtomo et al., Nature 427, 423-426 (2004)
[3] W. Meevasana et al., Nat. Mater. 10, 114-118 (2011)

O 88.10 Thu 17:15 H26

Controlling fundamental electronic interactions in SrTiO3 thin films by Ni and Fe doping — •Fatima Alarab[1,2], Berengar Leikert[3], Laurent Nicolai[2], Lucie Prusakova[2], Pavol Sutta[2], Ralph Claessen[3], Jan Minar[2], and Karol Hricovini[1] — [1]Cergy-Pontoise University, Neuville, France — [2]University of West Bohemia, Plzen, Czech Republic — [3]University of Würzburg, Würzburg, Germany

Strontium titanate (SrTiO3) has been a subject of intensive discussion in recent years both experimentally as well as theoretically. Strontium titanate is an insolator with a large band gap (Eg=3.2 eV), but it can become conductive by doping with transition metals or oxygen vacancies [1]. Here we report the fabrication and electronic properties of Ni doped SrTiO3 polycrystalline and crystalline films. The polycrystalline films were prepared by reactive magnetron co-sputtering in a reactive magnetron units equipped by pure STO and Ni targets with different Ni concentration. Whereas the crystalline films were grown by pulsed laser deposition (PLD). In this experimental investigation, we used high energy ARPES, core level spectroscopy and XPD to perform the electronic properties of the films as a function of doping concentration. Our experimental results were supported by ab-initio calculations using SPR-KKR's one-step model of photoemission [2,3].

[1] F. Alarab et al., AIP Conference Proceedings 1996, 020001 (2018). [2] Braun, Rep. Prog. Phys. 59, 1267-1338 (1996). [3] H. Ebert, D. Kodderitzsch and J. Minar, Rep. on Prog. in Phys. 74, 096501 (2011).

O 88.11 Thu 17:30 H26

Investigation of Micro-stress at Si/SiO2 interface using Infrared spectroscopy — •Tahereh Mohammadi Hafshejani, Franz Königer, Jonas Wohlgemuth, Zhihua Fu, Meike Königedel, Matthias Schwotzer, and Peter Thissen — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Silicon is by far the most important semiconductor material in the microelectronic industry mostly due to the high quality of the Si/SiO2 interface. The potential use of silicon in microelectronic devices highly depends on the interface thermal properties of between (SiO2/Si). In this work, we study how the SiO2 layer changes the interfacial properties and has a direct effect on Kapitza resistance, which has not been experimentally investigated so far. Also, vibrational properties of the SiO2 thin films (the optical phonon bands) and contribution between its thickness with the amount of Si-O bonds are discussed in details using a combination of the spectrometer with a new self-made device, applying bending forces on samples and simultaneously performing IR measurements. The results of impedance measurements have shown that Kapitza resistance at SiO2/Si interface depends on both the interfacial coupling strength and thickness. Moreover, combining infrared measurements and bending forces provide a deep insight into the processes at atomic level when the samples are under different stresses, reveal their association with a thickness of SiO2 as well as interface properties.