

O 85: Electronic Structure of Surfaces II

Time: Thursday 15:00–17:45

Location: REC C 213

O 85.1 Thu 15:00 REC C 213

Electronic structure of transition metal oxide surfaces from coincident electron spectroscopy — ●DANILO KÜHN¹, SWARNSHIKHA SINHA^{1,2}, ARTUR BORN^{1,2}, FREDRIK O. L. JOHANSSON³, RUSLAN OVSYANNIKOV¹, NILS MÄRTENSSON³, and ALEXANDER FÖHLISCH^{1,2} — ¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany — ²Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebkecht-Strasse 24-25, 14476 Potsdam, Germany — ³Department of Physics and Astronomy, Uppsala University, P.O. Box 256, 751 05, Uppsala, Sweden

Transition metal oxides are a much studied class of materials with a wide range of applications, e.g. solar cells, batteries, magnetic storage devices, sensors or pigments. Varying charge localizations in the s,p and d valence shells and coupling between subsystems invoke complex electronic, magnetic and optical phases as high Tc superconductivity. Here, results from the new COESCA station for coincident electron spectroscopy at the BESSY II synchrotron will be presented [Leitner, T. et al. J. El. Spec. 250, 147075 (2021)]. Combining the high transmission and energy resolution of ARTOF time-of-flight spectrometers with the tailored time structure of BESSY II, Auger- Photoelectron coincidence spectroscopy (APECS) is possible with unprecedented information rate in the soft x-ray regime. Exploiting enhanced chemical selectivity and surface sensitivity, we gain insight into the excitation-decay dynamics and electron correlation effects in Ni, Cu and their oxides [Born, A. et al. Sci Rep 11, 16596 (2021)]

O 85.2 Thu 15:15 REC C 213

Black Phosphorus and the Free-Electron Final-State Assumption in Photoemission Spectroscopy — ●CHARLOTTE SANDERS¹, KLARA VOLCKAERT², DEEPNARAYAN BISWAS³, MARCO BIANCHI², PHILIP HOFMANN², and IRENE AGUILERA⁴ — ¹Central Laser Facility, STFC Rutherford Appleton Lab, Research Complex @ Harwell, OX11 0QX, UK — ²Dept. of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus-C, DK — ³Diamond Light Source, Division of Science, Didcot, OX11 0DE, UK — ⁴Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, NL

In the photoemission process, the in-plane component (k_x, k_y) of the electron wave vector is conserved; but the k_z component is not, due to breaking of out-of-plane symmetry at the surface. This fact complicates analysis of photoemission spectra from k_z -dispersing states.

Bulk black phosphorus has a k_z -dispersing state that has been the subject of several studies wherein photoemission intensity close to the Fermi level resists interpretation on the basis of simple free-electron-like final-state assumptions. Experimental spectra have been interpreted in terms of surface resonances, or of complexities in the final state that go beyond the free-electron assumption. Here we present experimental and theoretical results concerning the latter interpretation; and, we consider the fundamental meaning of the free-electron-like final-state.

O 85.3 Thu 15:30 REC C 213

Direct observation of antiferromagnetic parity violation in the electronic structure of Mn₂Au — ●YARYNA LYTUVYENKO^{1,2}, OLENA FEDCHENKO¹, LIBOR ŠMEJKAL^{1,3}, MICHAEL KALLMAYER⁴, KATERINA MEDJANIK¹, SERGEY BABENKOV¹, DMITRY VASILYEV¹, MATHIAS KLÄUI¹, JURE DEMSAR¹, GERD SCHÖNHENSE¹, MARTIN JOURDAN¹, JAIRO SINOVA^{1,3}, and HANS-JOACHIM ELMERS¹ — ¹Institute of Physics, JGU Mainz — ²Institute of Magnetism of the NAS and MES of Ukraine — ³Institute of Physics Academy of Sciences of the Czech Republic — ⁴Surface Concept GmbH

Using time-of-flight momentum microscopy with a sub- μm spatial resolution (sub- $\mu\text{-ToFMM}$), allowing for momentum-resolved photoemission on individual antiferromagnetic domains, we observe an asymmetry in the electronic band structure, $E(\mathbf{k}) \neq E(-\mathbf{k})$, in Mn₂Au. This broken band structure parity originates from the combined time and parity symmetry, PT, of the antiferromagnetic order of the Mn moments, in connection with spin-orbit coupling [1,2]. The spin-orbit interaction couples the broken parity to the Néel order parameter direction. We demonstrate a novel tool to image the Néel vector direction by combining spatially resolved momentum microscopy with ab-initio

calculations that correlate the broken parity with the Néel vector [3].
References

1. L. Smejkal et al., Phys. Rev. Lett. 118, 106402 (2017)
2. H.-J. Elmers et al., ACS Nano 14, 17554-64 (2020)
3. O. Fedchenko et al., J. Phys.: Condens. Matter 34, 425501 (2022)

O 85.4 Thu 15:45 REC C 213

Impact of atomic defects in the electronic states of FeSe_{1-x}S_x superconducting crystals — ●YANINA FASANO^{1,2}, JAZMIN ARAGON SANCHEZ¹, MARIA LOURDES AMIGO¹, ESTEBAN GAYONE¹, and GLADYS NIEVA¹ — ¹Instituto Balseiro and Centro Atómico Bariloche, UnCuyo-CNEA, Argentina — ²Leibniz Institute for Solid State and Materials Research, Dresden, Germany

The electronic properties of Fe-based superconductors are drastically affected by deformations on their crystal structure introduced by doping and pressure. Here we study single crystals of FeSe_{1-x}S_x and reveal that local crystal deformations such as atomic-scale defects impact the spectral shape of the electronic core level states of the material. By means of scanning tunneling microscopy we image S-doping induced defects as well as diluted dumbbell defects associated with Fe vacancies. We have access to the electronic structure of the samples by means of x-ray photoemission spectroscopy (XPS) and show that the spectral shape of the Se core levels can only be adequately described by considering a principal plus a minor component of the electronic states. We find this result for both pure and S-doped samples, irrespective that in the latter case the material presents extra crystal defects associated to doping with S atoms. We argue that the second component in our XPS spectra is associated with the ubiquitous dumbbell defects in FeSe that are known to entail a significant modification of the electronic clouds of surrounding atoms.

O 85.5 Thu 16:00 REC C 213

Double Photoemission Spectroscopy of C₆₀ on SrTiO₃(001) with Laser VUV radiation — ●KATHRIN PLASS¹, ROBIN KAMRLA¹, FRANK O. SCHUMANN², and WOLF WIDDRA¹ — ¹Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — ²Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Via photoelectron spectroscopy, important insights into the electronic structure of solids were obtained. However, correlation effects can only be addressed indirectly. With double photoemission spectroscopy (DPE), such phenomena can be observed directly by detecting pairs of correlated photoelectrons emitted upon absorption of a single photon [1]. C₆₀ is classified as a strongly correlated material with a highly structured valence band spectrum. Moreover, theory predicts the possibility of plasmon-mediated pair emission in C₆₀ [2]. In this contribution we present DPE data for C₆₀ thin films on SrTiO₃(001), obtained by a laboratory high-order harmonic (HHG) light source, operating at an energy range from 14 to 40 eV and MHz repetition rates [3]. We analyze the 2D energy maps and compare the data to the SPE spectrum. In addition, we discuss plasmon-mediated DPE in fullerenes.

- [1] J. Berakdar et al., Phys. Rev. Lett. **81**, 3535 (1998)
- [2] Y. Pavlyukh et al., Phys. Rev. B **91**, 155116 (2015)
- [3] A. Trüttschler et al., Phys. Rev. Lett. **118**, 136401 (2017)

O 85.6 Thu 16:15 REC C 213

Electronic structure at the "interface" of spin-orbit and exchange interaction: Ultrathin ferromagnetic films on W(110) — ●PASCAL JONA GRENZ¹, PETER KRÜGER¹, MARCEL HOLTSMANN¹, KOJI MIYAMOTO², SHIV KUMAR², TAICHI OKUDA², and MARKUS DONATH¹ — ¹WWU, Münster, Germany — ²HISOR, Hiroshima, Japan

Ultrathin ferromagnetic layers on W(110) provide a suitable platform for investigating spin phenomena originating from the interplay of spin-orbit coupling (SOC) and exchange interaction (XC). First, we focus on the influence of ferromagnetic adlayers on the SOC-induced topologically non-trivial surface state (TSS) hosted by the W(110) surface [1,2]. Our systematic angle-resolved photoemission study of thin Ni, Co, and Fe films and their influence on the TSS will be presented and discussed in view of conflicting literature results [3]. Second, the unoccupied electronic structure of thin Ni films on W(110) is surveyed by spin- and angle-resolved inverse photoemission. By carefully choosing

the Ni film's thickness, we tune the relative strength of SOC and XC. In such a way, SOC induces a degeneracy of Ni-related exchange-split states. Based on density functional theory, the strong interplay of SOC and XC is traced back to the hybridization of W and Ni states.

- [1] K. Miyamoto *et al.*, *Phys. Rev. Lett.* **108**, 066808 (2012)
 [2] P.J. Grenz *et al.*, *J. Phys.: Condens. Matter* **33**, 285504 (2021)
 [3] K. Honma *et al.*, *Phys. Rev. Lett.* **115**, 266401 (2015)

O 85.7 Thu 16:30 REC C 213

Circular dichroism in angle-resolved photoemission from core-level emission of W(110) — •TRUNG PHUC VO¹, OLENA TKACH^{2,3}, KATERINA MEDJANIK², OLENA FEDCHENKO², HANS-JOACHIM ELMERS², GERD SCHÖNHENSE², and JÁN MINÁR¹ — ¹New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic — ²Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, D-55128 Mainz, Germany — ³Sumy State University, Rymski-Korsakov 2, 40007 Sumy, Ukraine

Angle-resolved photoemission spectroscopy (ARPES) is a driving experimental technique for examining the electronic structure of quantum materials. There is another technique called X-ray photoelectron diffraction (XPD) which is considered to be the same thing as ARPES from an elementary point of see, specifically the angular distribution of photoelectrons emitted from a crystal surface. Nevertheless, the angular distribution of emitted electrons represents the momentum of initial states in ARPES meanwhile it reveals the interference of photoelectron waves from final states in XPD. At high photon energies, photoelectron diffraction (PED) effects are found in ARPES measurements beside other obstacles (e.g. non-negligible phonon scattering). Here, to disentangle these diffraction influences, we present a PED implement for SPRKKR package which makes use of multiple scattering theory and one-step model in photoemission process. For the sake of applications, we have calculated the circular dichroism in angular distributions (CDAD) associated with of 4f and 3d states from W(110). Photoelectrons are excited by hard X-rays (6000 eV).

O 85.8 Thu 16:45 REC C 213

Automatic Quantification of Transitional Metal X-ray Photoelectron Spectra using Convolutional Neural Networks — •LUKAS PIELSTICKER, WALID HETABA, and MARK GREINER — Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany

In X-ray photoelectron spectroscopy (XPS), quantitative analysis of the nature and composition of surface chemical species is typically performed manually through empirical curve fitting by expert spectroscopists. However, recent advancements in the ease-of-use and reliability of XPS instruments have led to ever more (novice) users creating increasingly large data sets that are becoming harder to analyze by hand. Reflecting this development, more automated analysis techniques are desirable to aid these users with the analysis of big XPS datasets. Here we show that by training convolutional neural networks (CNN) on artificially generated XP spectra with known quantifications (i.e., for each spectrum, the concentration of each chemical species is known), it is possible to obtain models for auto-quantification of transition metal XP spectra. CNNs are shown to be capable of quantitatively determining the presence of metallic and oxide phases, achieving competitive accuracy as more conventional data analysis methods. The proposed networks are flexible enough to accommodate spectra containing multiple chemical elements and measured with different experimental settings. The use of dropout variational inference for the determination of quantification uncertainty is discussed.

O 85.9 Thu 17:00 REC C 213

Revisiting the Strongly Correlated Si-terminated 3C-SiC(100)-p(2×1) Surface with Density- and Wave Function-Based Methods — •NIKLAS THOBEN and THORSTEN KLÜNER — Carl von Ossietzky Universität, Oldenburg, Germany

Silicon carbide is an environmentally friendly, abundant and chemically stable wide band gap semiconductor. From the numerous known polytypes, cubic silicon carbide (3C-SiC) shows the lowest band gap with 2.36 eV, which straddles the water redox potentials and thus making this material a possible candidate for photoelectrochemical water splitting [1]. 3C-SiC is generally obtained as thin films on Si(100) substrates [2], resulting in the 3C-SiC(100) surface being the most common surface. In the Si-terminated case, this surface can exhibit a p(2×1) reconstruction with symmetric Si-dimers [3]. In literature, this system has almost exclusively been described by periodic closed shell density functional theory (DFT) even though the symmetric dimers should be strongly correlated and thus show open shell and multi-configurational character to a certain extent. Consequentially, in this contribution we apply spin-polarized periodic hybrid DFT and multi-configurational wave function-based methods on the 3C-SiC(100)-p(2×1) surface.

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 [2] V. Jokubavicius *et al.*, *Cryst. Growth Des.* **2014**, *14*, 6514.
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O 85.10 Thu 17:15 REC C 213

Coulomb potential truncation in hybrid calculations — •KRISTIAN KACARS and ANDRIS GULANS — University of Latvia

Solving Poisson's equation is a fundamentally important part of electronic structure calculations. The long-range character of the Coulomb potential makes this task non-trivial in a range of applications. It leads to diverging Fock exchange and spurious interactions of periodic images of low-dimensional systems in supercell calculations. We address this problem in the context of linearized augmented plane waves(LAPW), considering two different approaches to extending Weinert's method. In the first of them, we employ a wavelet-based Poisson equation solver from the *psolver* library. In the second one, we use Coulomb potential truncation schemes. Both approaches are implemented and tested in the LAPW code *exciting*. We apply and compare these methods for bulk materials and low-dimensional systems in calculations with local and hybrid functionals.

O 85.11 Thu 17:30 REC C 213

Ultra-fast machine learning potentials for hydrogen under pressure — •THOMAS BISCHOFF¹, BASTIAN JÄCKL¹, and MATTHIAS RUPP^{1,2} — ¹Department of Computer and Information Science, University of Konstanz, Germany — ²Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Luxembourg

Hydrogen exhibits remarkably complex behavior at high pressures. Its rich phase space with multiple solid and liquid polymorphs is the subject of controversial scientific debate [1,2].

We apply ultra-fast potentials (UFPs) to model hydrogen under pressure. UFPs are recent robust interpretable machine-learning potentials that enable accurate simulations of large atomistic systems over long time scales [3].

We examine the accuracy of UFPs for training data from density functional theory and quantum Monte Carlo calculations. We also demonstrate the physical interpretability of UFPs for reference configurations composed of atomic and molecular hydrogen. With the obtained machine-learning potential, we investigate solid-liquid and liquid-liquid phase transitions for an extensive part of the phase diagram of dense hydrogen.

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 [2] A. Tirelli *et al.*, *Physical Review B* **106**(4): L041105, 2022.
 [3] S. R. Xie *et al.*, *arXiv 2110.00624*, 2021.