O 81: Nanostructures at Surfaces I

Time: Thursday 10:30–12:45 Location: MA 042

O 81.1 Thu 10:30 MA 042

One-dimensional electronic structure of phosphorene chains — •Maxim Krivenkov[1], Maryam Sajedi[1], Dmitry Marchenko[1], Evangelos Golias[2], Oliver Rader[1], and Maxim Krivenkov[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]MAX IV Laboratory, Lund University, Fotongatan 2, 22484, Lund, Sweden

Phosphorene, a 2D allotrope of phosphorus, is very appealing to electronic technology due to its semiconducting properties with narrow band gap. Further reduction of dimensionality could give rise to exotic properties of its electronic structure. Using angle-resolved photoemission we studied P atomic wires self-assembled on Ag(111) substrate. Dispersion of the P band measured along and perpendicular to the wires, reveals pronounced electronic confinement in a 1D band, dispersionless in perpendicular direction to the wire. Our density functional calculations, apart from precise reproduction of the 1D band for the P/Ag(111), predict a 1D to 2D metallic transition in the electronic structure upon increasing density of the nanowire array.

O 81.2 Thu 10:45 MA 042

Perturbations in quantum corrals — •Fabian Stilp, Marco Weiss, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

The surface state of Cu (111), a quasi-2-dimensional electron gas, is trapped to a small surface area of about 15 x 15 nm^2 by placing 48 CO-molecules in a circular shape on the surface via atomic manipulation. By doing so, one creates a quantum corral with discrete electronic states forming an artificial atom. This structure can be described reasonably well by an infinitely high circular potential well leading to corral states with Bessel-type radial functions and an angular momentum normal to the surface. To investigate the influence of single atom or molecule perturbations on quantum corrals we bring Fe atoms and CO molecules inside the corral and measure the response of the corral states.

Thanks to the large corral diameter, one can study the structure of the wave functions within that artificial atom by AFM and STM showing an angular dependence of the corral states after placing the perturbations inside the corral. This change of the wave functions leads to an energy shift of a few meV. By investigating the change of the corral states due to the perturbation, one can draw conclusion about the interaction between this artificial atom and a natural atom. Here we expand the interpretation of the adatom acting repulsively on the corral states as stated by Stilp et al. [1].

[1] F. Stilp, A. Bereczuk, J. Berwanger, N. Mundigl, K. Richter, F.J. Giessibl, Science **372**, 1196-1200 (2021).

O 81.3 Thu 11:00 MA 042

Intermediate metal-insulator phases of individual VO_2 nanocrystals for multilevel memory — Peter Kepič, Michal Horák, Jiří Kabát, Filip Ligmajer, Andrea Konečná, and •Vlastimil Křápek — Brno University of Technology, Czechia

Vanadium dioxide (VO_2) is a strongly correlated material that exhibits metal-insulator transition (MIT) around 340 K [1]. A broad conductivity hysteresis of VO_2 is vital for its applications as memory or memristor devices. In our contribution, we study the hysteresis of temperature-induced MIT in individual high-density VO_2 nanocrystals using analytical electron microscopy. We utilize low-loss and core-loss electron energy loss spectroscopy (EELS) combined with in-situ heating to analyze the metal-insulator transition [2] in more than 40 nanocrystals. We retrieve the parameters of the hysteresis loop and demonstrate their dependence on the size of the nanocrystals. Interestingly, some nanocrystals exhibit switching from the insulating to the metallic phase by parts, with the intermediate phases allowing to design multilevel memory. We also show by correlating the image contrast with EELS that signatures of MIT are observable simply and efficiently using annular dark-field imaging.

[1] P. Kepič *et al.*, ACS Photonics **8**, 1048 (2021).

[2] J. Krpenský, M. Horák *et al.*, arXiv 2309.11980.

O 81.4 Thu 11:15 MA 042

Nanoflower-like VSx@NC as a promising anode for stable potassium-ion storage — •Vincent Hartmann, Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, Germany

Potassium-ion batteries (PIBs) are promising candidates for large-scale energy storage due to their low cost and abundant potassium content in the earth's crust. However, owing to the large radius of K+ ions, the electrode material structure is easily damaged during the potassiation/depotassiation process, hindering their further applications. VSx has become a new PIB anode material due to its low cost, high theoretical capacity, and unique structure, which can provide sites for potassium storage. Here, constructing a flower-like VSx covered by nitrogen-doped carbon as an anode electrode for PIBs can effectively enhance electrical and mechanical properties and provide abundant active sites for pseudocapacitive behavior to achieve fast kinetics. As a result, it exhibits excellent cycling stability with a special capacity of 249.3 mAh g-1 at 100 mA g-1 after 1000 cycles with an initial discharge capacity of 293.8 mAh g-1. The strategy in this work provides inspiration for the rational design of advanced nanostructured electrode materials to develop PIB anodes with long cycle life.

O 81.5 Thu 11:30 MA 042

Investigation of highly efficient black titania nanotube photocatalyst by soft-X-ray spectroscopy — •Hesham Ali Fahmy Abdalla Hamad — City of Scientific Research and Technological Applications (SRTA-City), Alexandria, Egypt

The recent discovery of black TiO2 nanoparticles with enhancing solar absorption, especially in the visible and near-infrared region will trigger an explosion of interest in the application of TiO2 in a diverse set of solar energy systems; but black TiO2 nanoparticles really remain a mystery. Here we elucidate more properties and try to understand the inner workings of black TiO2 nanotubes with hydrogenated disorders in a surface layer surrounding a crystalline core. In this work, TiO2 nanotubes (TNT) and its black hydrogenated TiO2 nanotubes (BTNT) were synthesized and investigated by characterization techniques. The merit of this project is to investigate the prepared synchrotron-based X-ray absorption fine structures (XAFS). It probed the unoccupied and occupied molecular orbitals of densities of states for O 2p and Ti 3d hybrid orbital characteristics, respectively. The reduction behavior and electronic and crystalline structure of a series of TNT and BTNT as photocatalysts will be investigated by using synchrotron-based XAFS. These techniques provide novel opportunities for tackling the structure and the dynamics of chemical and physical systems in solution.

O 81.6 Thu 11:45 MA 042

Diffusion studies on Pb islands and on the wetting layer in Pb/Si(111)-(7x7) — •Paul Philip Schmidt, Felix Hartmann, Lea Faber, and Regina Hoffmann-Vogel — University of Potsdam, Institute of Physics and Astronomy, Germany

Metallic structures on semiconductors offer a wide range of technical applications. This presentation will focus on the diffusion behavior of Pb/Si(111)-(7x7). It is known that Pb initially forms a wetting layer on Si, from which islands then form. Previous research has shown that this system exhibits explosive island growth and abnormally fast diffusion [1][2]. In our study, we focus on the wetting layer. After fabricating the 7x7 reconstruction on Si(111) under ultra-high vacuum conditions, we evaporate between 2 and 7 monolayers Pb at substrate temperatures between 120 and 300K. The diffusion was studied using non-contact cantilever scanning force microcopy (NC-SFM) and simultaneous Kelvin probe force microscopy (KPFM). While the topographical data of the NC-SFM essentially confirmed known data on the growth of the islands, the KPFM showed changes in the local contact potential difference (LCPD). In one experiment, a local imbalance was additionally generated on an island by manipulating a Pb island using the SFM-tip. Despite the low time resolution of an SFM measurement, it was possible in this way to determine the time scales of the mass transport. [1] M. Hupalo et. al. Phys. Rev. B, 23 (2007) [2] K. L. Man et al. Phys. Rev. Lett., 101 (2008)

Topical Talk O 81.7 Thu 12:00 MA 042

Trapping single atoms of noble gases in nanocages: from

fundamental studies to applications — •Jorge Anibal Boscoboinik — Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, USA

Confinement effects can result in exciting properties in the chemistry and physics of small molecules. In this talk, we will explore the trapping of noble gases in the confined space inside silicate nanocages and at the interface between these cages and their metal support. Understanding the fundamental aspects of these confinement effects can lead to designing new materials for specific applications. Based on the lessons from the fundamental studies for noble gas trapping in 2D-model systems, we are developing new nanoarchitectures that are potentially scalable and can be used for various applications related to producing and detecting noble gases.

O 81.8 Thu 12:30 MA 042

Automating measurements on the nanoscale: Artificial Intelligence versus classical analysis of SPM data — •Tim J. Seifert[1], Ziba Akbarian[1,2], Birka Lalkens[2], Ingo Busch[3], Harald Bosse[3], and Uta Schlickum[1,2] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig — [2]Laboratory for Emerging Nanometrology LENA, Braunschweig — [3]Physikalisch-Technische Bundesanstalt, Braunschweig

The continuous trend in research and technology towards structures on the nanometer scale drives the growing interest in imaging mechanisms using Scanning Probe Microscopes (SPM). As the experimental methods continue to evolve, the increasing output of data requires fast, reliable and accurate analysis methods avoiding the need for an experienced user. The automatization of image analysis procedures for SPM mainly consists of well-established routines using classical methods requiring laborious manual work. Artificial Intelligence (AI) based analysis techniques have recently attracted great interest hoping to provide true autonomous imaging and analysis procedures. While the accuracy of classical methods is often limited by noise, AI can overcome these challenges, albeit with the additional need for high amounts of labeled training data. Here we present a framework to analyze SPM data and extract distance information using AI-based methods trained on synthetic data, as well as classical alternatives, highlighting the benefits of each approach. The procedure is applied to measure a novel DNA-Origami based Single-Molecule length reference providing a fast, cheap and accurate way to calibrate SPMs on the nanoscale.