HL 16: Focus Session: Quantum Properties at Functional Oxide Interfaces (joint session DS/HL)

Time: Wednesday 9:30–11:00 Location: H17

Invited Talk HL 16.1 Wed 9:30 H17

Facet dependence of reconstructions at quantum material interfaces — •Eva Benckiser — Max Planck Institute for Solid State Research, Stuttgart, Germany

Oxide heterostructures promise a rational design of quantum materials with specific, functional properties such as magnetism and superconductivity. Our research aims to gain a fundamental understanding of spin, orbital, charge and lattice reconstructions at complex transition-metal oxide interfaces, mainly using x-ray spectroscopy.

In my talk, I will focus on implications of the choice of the crystallographic facet of the interface by showing examples of two prototypical correlated-electrons materials. In $NdNiO_3$ epitaxial thin films we observe modifications of the metal-insulator transition, which we explain by the facet dependence of the bond-order instability in the system [1]. The choice of a specific interface facet, in turn, allows to manipulate the complex spin order in ultrathin $NdNiO_3$ slabs [2]. In YVO_3 heterostructures, an artificial, layered orbital occupation pattern can be realized by the choice of the interface facet [3]. I have conducted the above-mentioned studies in collaboration with many scientists who are co-authors of the publications listed below.

[1] Y. E. Suyolcu, K. Fürsich *et al.*, Phys. Rev. Materials **5**, 045001 (2021). [2] M. Hepting *et al.*, Nature Physics **14**, 1097 (2018). [3] P. Radhakrishnan *et al.*, Phys. Rev. B **104**, L121102 (2021); Phys. Rev. B **105**, 165117 (2022).

HL 16.2 Wed 10:00 H17

A detailed interface and surface analysis of $BaSnO_3$ in $LaInO_3/BaSnO_3$ heterostructures — •Martina Zupancic[1], Wahib Aggoune[2], Daniel Pfützenreuter[1], Zbigniew Galazka[1], Houari Amari[1], Claudia Draxl[2], Jutta Schwarzkopf[1], and Martin Albrecht[1] — [1]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [2]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

$LaInO_3/BaSnO_3$ heterostructures have lately attracted a lot of interest due to the high electron mobility of $\sim 300 cm^2/Vs$ in $BaSnO_3$ and the formation of a 2DEG at the interface. In $LaAlO_3/SrTiO_3$ system, the origin of the 2DEG is attributed to the polar discontinuity and an electronic reconstruction at the n-type LaO-TiO_2 interface. Controlling the interface termination is therefore crucial to accomplish heterostructures with desired properties. Here, we combine density-functional theory, atomic resolution transmission electron microscopy, energy dispersive X-ray spectroscopy, and electron energy loss spectroscopy (EELS) to study the $LaInO_3/BaSnO_3$ interface. Experiment and theory are in excellent agreement and show that free $BaSnO_3$ (100) surfaces are BaO terminated, while the interface between $BaSnO_3$ and $LaInO_3$ is SnO_2 terminated. This finding indicates that during the growth of $LaInO_3$ layer on $BaSnO_3$ Ba atoms exchange from the subsurface to the surface. Preliminary EELS analysis of a few monolayer thick $LaInO_3$ grown on $BaSnO_3$ shows indications of Ba atoms on the $LaInO_3$ surface, confirming that atomic exchange in this system promotes the energetically favorable SnO_2-LaO interface.

Invited Talk HL 16.3 Wed 10:15 H17

Designing novel electronic phases at oxide interfaces from first principles — •Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany

Transition metal oxide interfaces exhibit a rich plethora of functional properties that are not available in the respective bulk compounds and open possibilities for electronics, spintronics and energy conversion applications. Over the past years several control parameters of novel behavior have been identified and systematically explored such as the symmetry breaking at the interface, the effect of strain, confinement and crystallographic orientation, the electrostatic doping at polar interfaces [1]. Based on the insight from density functional theory calculations including an on-site Hubbard term, I will address the formation of unanticipated charge, spin and orbital reconstructions in perovskite-derived superlattices and thin films with (001) and (111) orientation that can lead to e.g. metal-to-insulator transitions and/or topologically nontrivial states which are fascinating not only from a fundamental point of view but also potentially interesting for thermoelectric applications [2].

Research supported by the German Research Foundation DFG within CRC/TRR80. [1] M. Lorenz et al., J. Phys. D: Appl. Phys. 49, 433001 (2016). [2] B. Geisler, P. Yordanov, M. E. Gruner, B. Keimer, R. Pentcheva, Phys. Status Solidi B 259, 2100270 (2022)

HL 16.4 Wed 10:45 H17

Orbital engineering in vanadate heterostructures — •Padma Radhakrishnan[1], Benjamin Geisler[2], Katrin Fürsich[1], Daniel Putzky[1], Yi Wang[1], Sven Ilse[3], Georg Christiani[1], Gennady Logvenov[1], Peter Wochner[1], Peter van Aken[1], Eberhard Goering[3], Rossitza Pentcheva[2], and Eva Benckiser[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Lothastrasse 1, 47057 Duisburg, Germany — [3]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

A promising approach for the manipulation of quantum states involves the epitaxial stabilization of certain orbital occupations, i.e. orbital engineering. Here we use resonant x-ray reflectometry to extract quantitative depth-dependent x-ray linear dichroism profiles of thin slabs of YVO_3 embedded in a superlattice with $LaAlO_3$. Our data reveal an artificial, layered orbital polarization, where the average occupation of xz and yz orbitals at the interface is inverted compared to the central layers of YVO_3. We attribute this effect to a combination of epitaxial strain and spatial confinement by $LaAlO_3$. Further, insights from *ab initio* calculations and scanning transmission electron microscopy indicate that the selection of a suitable spacer layer material, layer thickness of the transition metal oxide, facet of substrate, and sign of strain can together implement a desired orbital polarization pattern. Our study demonstrates the use of orbital engineering as a promising approach for the theory-guided rational design of quantum materials.