TT 59: Low-Dimensional Systems: Poster Session

Time: Wednesday 15:00–18:30 Location: Poster D

TT 59.1 Wed 15:00 Poster D

Finite-size effects in spin-gapped metals — •Jonas Greitemann[1,3], Stephan Hesselmann[1], Stefan Wessel[1], Fakher Assaad[2], and Martin Hohenadler[2] — [1]RWTH Aachen, Germany — [2]University of Würzburg, Germany — [3]LMU Munich, Germany

Attractive backscattering in one-dimensional models is a relevant perturbation to the Tomonaga-Luttinger fixed point, prompting the opening of a spin gap as governed by the Luther-Emery fixed point. We use complementary quantum Monte Carlo approaches to show that this crossover takes place as a function of distance, giving rise to finite-size effects below a scale set by the inverse spin gap. In particular, the finite-size scaling of the staggered charge susceptibility is argued to be unreliable for pinpointing the Peierls transition in the spinful Holstein model.

TT 59.2 Wed 15:00 Poster D

Charge and spin density in the helical Luttinger liquid — Niccolò Traverso Ziani[1], •Christoph Fleckenstein[1], Francois Crépin[2], and Björn Trauzettel[3] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Laboratoire de Physique Théorique de la Matière Condensée, UPMC, CNRS UMR 7600, Sorbonne Universités, 4 place Jussieu, 75252 Paris Cedex 05, France — [3]Department of Physics, University of California, Berkeley, California 94720, USA

Two-dimensional topological insulators represent a recently descovered phase of matter, characterized by an insulating two-dimensional bulk and metallic one dimensional edge states. These edge states are characterized by spin-momentum locking: particles with opposite spin move in opposite direction. When electron-electron interactions are taken into account, the one-dimensional edge states are conveniently described by the so called helical Luttinger liquid. Within the framework of the helical Luttinger liquid we theoretically show that, due to the absence of Friedel and Wigner parts in the density operator, density-density correlation functions do not exhibit $2k_F$ and $4k_F$ oscillations, while spin-spin correlations show anisotropic planar wave structure, which is enhanced by electron-electron interactions. Moreover, we demonstrate that the most relevant, in the renormalization group sense, impurity potentials, are not able to modify the average local electron density. Finally we show that only magnetic impurities can pin the planar spin density wave.

TT 59.3 Wed 15:00 Poster D

Criticality at the Haldane-insulator charge-density-wave quantum phase transition — Florian Lange, •Satoshi Ejima, and Holger Feshke — Institute of Physics, University of Greifswald, D-17489 Greifswald, Germany

Exploiting the entanglement concept within a matrix-product-state based infinite density-matrix renormalization group approach, we show that the spin-density-wave and bond-order-wave ground states of the one-dimensional half-filled extended Hubbard model give way to a symmetry-protected topological Haldane state in case an additional alternating ferromagnetic spin interaction is added. In the Haldane insulator, the lowest entanglement level features a characteristic twofold degeneracy. Increasing the ratio between the nearest-neighbor and local Coulomb interaction V/U, the enhancement of the entanglement entropy, the variation of the charge, spin, and neutral gaps, and the dynamical spin and density response signal a quantum phase transition to a charge-ordered state. Below a critical point, which belongs to the universality class of the tricritical Ising model with central charge 7/10, the model is critical with $c = 1/2$ along the transition line. Above this point, the transition between the Haldane insulator and charge-density-wave phases becomes first order.

TT 59.4 Wed 15:00 Poster D

Electron correlations in a one-dimensional manganite model — •Ole Schumann[1], Salvatore R. Manmana[1], Peter E. Blöchl[2], Fabian Biebl[1], and Sangeeta Rajpurohit[2] — [1]Institute for Theoretical Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institute for Theoretical Physics, TU Clausthal, Leibnizstr. 10, 38678 Clausthal-Zellerfeld

An effective 1D model for a manganite is derived for the ground state atomic structure which consists of antiferromagnetically coupled manganese dimers in the spin triplet state. The model is Hubbard like with an additional staggered magnetic field. Using the DMRG, we obtain the $T = 0$ phase diagram of the resulting many electron model. We investigate various scenarios for photo-excitation of the system and give an outlook to a more realistic modelling.

Financial support via DFG through CRC 1073 "Atomic scale control of energy conversion", project B03 is gratefully acknowledged.

TT 59.5 Wed 15:00 Poster D

Acceleration of MPS-based algorithms by using the adaptive cross approximation — •Holger Thyen, Thomas Köhler, Salvatore R. Manmana, and Stephan Kramer — Institut für Theoretische Physik, Georg-August-Universität, Göttigen

We investigate the benefits of the adaptive cross approximation (ACA) [1], used for the low-rank approximation of the matrices occurring in MPS-based DMRG algorithms. By connecting convergence criteria occurring during the ACA to the discarded weight of the approximation via the usual singular value decomposition (SVD), we obtain a stopping criterion for the iterations of the ACA and investigate possible alternative control parameters. The so obtained code based on ACA is benchmarked to codes based purely on SVD. The code development is part of the open-source SciPAL library [2].

Financial support via DFG through CRC 1073 "Atomic scale control of energy conversion", project B03 is gratefully acknowledged.

[1] M. Bebendorf and S. Rjasanow, Computing **70** 1, (2003).
[2] Stephan C. Kramer and Johannes Hagemann, ACM Trans. Parallel Comput. **1**, 2, Article 15 (2015)

TT 59.6 Wed 15:00 Poster D

Mott quantum criticality in the anisotropic 2D Hubbard model — •Benjamin Lenz[1], Salvatore R. Manmana[1], Thomas Pruschke[1], Fakher F. Assaad[2], and Marcin Raczkowski[2,3] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany — [2]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians-Universität Würzburg, Germany — [3]Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Germany

We present evidence for Mott quantum criticality in an anisotropic two-dimensional system of coupled Hubbard chains at half-filling. In this scenario emerging from variational cluster approximation and cluster dynamical mean-field theory, the interchain hopping $t_\perp$ acts as control parameter driving the second-order critical endpoint T_c of the metal-insulator transition down to zero at $t_\perp^c/t \simeq 0.2$. Below $t_\perp^c$ the volume of hole and electron Fermi pockets of a compensated metal vanishes continuously at the Mott transition. Above $t_\perp^c$ the volume reduction of the pockets is cut off by a first-order transition. We discuss the relevance of our findings to a putative quantum critical point in layered organic conductors whose location remains elusive so far.

Financial support via DFG through FOR1807 is gratefully acknowledged.

TT 59.7 Wed 15:00 Poster D

Functional renormalization group studies of spin-orbit entangled j=1/2 Mott insulators — •Finn Lasse Buessen and Simon Trebst — Institute for Theoretical Physics, University of Cologne, Germany

We apply a recently developed functional renormalization group (FRG) approach to study the collective phenomena of spin-orbit entangled j=1/2 moments in Mott insulators. The microscopic exchange of these moments can be captured by a Heisenberg-Kitaev model for various lattice geometries. We discuss technical aspects of the application of the pseudo-fermion FRG approach developed by Reuther and Wölfle and its efficient numerical implementation. Model systems to be discussed include the Heisenberg-Kitaev model on honeycomb and triangular lattice geometries, for which we discuss the formation of unconventional magnetism in the form of spin liquids or non-trivial spin textures.

TT 59.8 Wed 15:00 Poster D

Spin textures in j=1/2 Mott insulators on the triangular lattice — •Tilman Disselkamp and Simon Trebst — University of

Cologne

Spin-orbit entangled j=1/2 Mott insulators can give rise to unconventional forms of magnetism, which has sparked an interest in Heisenberg-Kitaev models thought to capture their essential microscopic interactions. Our focus is on j=1/2 Mott insulators in triangular lattice geometries relevant, e.g. to $Ba_3IrTi_2O_9$, for which we study the interplay of geometric frustration and spin-orbit coupling. While the pure Heisenberg model is known to exhibit 120 degree order, nontrivial spin textures are induced by an infinitesimal Kitaev coupling or a Dzyaloshinskii-Moriya exchange. The former stabilizes a $\mathbb{Z}_2$ vortex phase, while the latter gives rise to a skyrmion lattice. Using numerical simulation techniques, we map out the stability of these spin textures at zero and finite temperatures.

TT 59.9 Wed 15:00 Poster D

Scaling theory and universal critical behavior of topological phase transition — •Wei Chen, Markus Legner, and Manfred Sigrist — ETH Zurich, Switzerland

Topologically ordered systems are characterized by topological invariants that are often calculated from the momentum space integration of a certain curvature function, such as Berry curvature or Berry connection. Akin to stretching a messy string to reveal the number of knots it contains, a scaling procedure is proposed for the curvature function, from which one obtains the RG flow of the driving energy parameter (hopping, chemical potential, Coulomb interaction, etc) that distinguishes topological phase transitions. Several critical exponents are further identified from the critical behavior of the curvature function, and the relation between them is explored.

TT 59.10 Wed 15:00 Poster D

Inversion symmetry induced topological edge states in quantum wires — •Sudhakar Pandey[1] and Carmine Ortix[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

We demonstrate the existence of topologically non-trivial insulating phases in quantum wires as a consequence of inversion symmetry. The topologically non-trivial phases are characterized by a pair of in-gap edge states which are robust against weak disorder. We find that these topological edge states are identical to the so called Maue-Shockley surface states that can be predicted independently from the location of boundaries and the sign of the Fourier component which opens the insulating gap. We demonstrate that the insulating state can be switched between topologically non-trivial and trivial phases by suitably adjusting the controllable parameters of the Hamiltonian.

TT 59.11 Wed 15:00 Poster D

Breakdown of the bulk boundary correspondence in a strongly correlated model Hamiltonian — •Robert Triebl and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz Univerity of Technology, Petersgasse 16, 8010 Graz, Austria

We analyze the bulk boundary correspondence of a archetypal model for interacting Z_2 topological insulators, namely the Kane-Mele-Hubbard model, in particular focusing on the competition between topological and magnetic order. Both bulk and ribbon Green's functions have been calculated using the variational cluster approach, employing a two-site dynamical impurity approximation (DIA). The Z_2 invariant of the bulk can be calculated with a Wannier charge center approach by mapping the interacting system to a topological Hamiltonian, which is an effective free-particle model with the same topological properties. The resulting invariants are compared to the existence of gapless edge states of the ribbon, where we use a site-dependent antiferromagnetic Weiss field on the ribbon. It turns out that spontaneous symmetry breaking occurs locally at the edges already at much smaller interactions than in the middle of the ribbon, leading to a gap in the edge spectral function. As a consequence, the topological invariant defined in the bulk may not correspond to the existence of gapless edge states since time reversal invariance is locally broken only at the edges.

TT 59.12 Wed 15:00 Poster D

Trivial and topological phases protected by symmetries in spin-2 quantum chains — •Augustine Kshetrimayum[1], Hong-Hao Tu[2], and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Symmetry-protected trivial (SPt) phases of matter are the product-state analogue of symmetry-protected topological (SPT) phases. This means, SPt phases can be adiabatically connected to a product state by some path that preserves the protecting symmetry. Moreover, SPt and SPT phases can be adiabatically connected to each other when interaction terms that break the symmetries protecting the SPT order are added in the Hamiltonian. It is also known that spin-1 SPT phases in quantum spin chains can emerge as effective intermediate phases of spin-2 Hamiltonians. In this work, we show that a similar scenario is also valid for SPt phases. More precisely, we show that for a given spin-2 quantum chain, effective intermediate spin-1 SPt phases emerge in some regions of the phase diagram, these also being adiabatically connected to non-trivial intermediate SPT phases. We characterize the phase diagram of our model by studying quantities such as the entanglement entropy, symmetry-related order parameters, and 1-site fidelities. Moreover, we provide a field theory description of the quantum phase transitions between the SPt phases.

TT 59.13 Wed 15:00 Poster D

Raman spectroscopic signature of fractionalized excitations in β-Li_2IrO_3 — •A. Glamazda[1], S.-H. Do[1], K.-Y. Choi[1], and P. Lemmens[2] — [1]Department of Physics, Chung-Ang University, Seoul, Republic of Korea — [2]IPKM, TU-BS, Braunschweig

The Kitaev honeycomb spin model is known to host exotic fractionalized quasiparticles. Using polarization resolved Raman spectroscopy we study the hyper-honeycomb compound β-Li_2IrO_3, a promising candidate of a three-dimensional Heisenberg-Kitaev system. A dynamical Raman response exhibits a broad scattering continuum with distinct polarization, which evolves into a quasielastic response with increasing temperature. The given experimental results give a signature of two-particle Majorana spinon excitations and demonstrate that β-Li_2IrO_3 is close in realizing a three-dimensional Kitaev spin liquid.

Work supported by RTG-DFG 1952/1, Metrology for Complex Nanosystems and the Laboratory for Emerging Nanometrology, TU Braunschweig.

TT 59.14 Wed 15:00 Poster D

Stabilization of stoichiometric $LaTiO_3$ thin films grown by pulsed laser deposition — •Matthias Schmitt, Philipp Scheiderer, Alex Gössmann, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

Like in the famous oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a two dimensional electron system is found at the interface between the strongly correlated Mott insulator $LaTi^{3+}O_3$ and the band insulator STO. In contrast to LAO, the stabilization of $LaTi^{3+}O_3$ requires strong reducing growth conditions since the thermodynamically stable bulk phase is the oxygen-rich $La_2Ti_2^{4+}O_7$. Therefore, we have systematically studied the impact of oxidizing and reducing background atmospheres and the influence of the substrate on $LaTi^{3+}O_3$ thin film growth by pulsed laser deposition. *In situ* x-ray photoelectron spectroscopy of the films prepared on STO exhibit overoxidation probably due to oxygen out-diffusion from the STO substrate, which is reduced for growth on $DyScO_3$ due to the lower oxygen mobility. In addition, we found that a LAO capping layer of a few unit cells thickness acting like a diffusion barrier for oxygen prevents the LTO film from overoxidation during storage in air.

TT 59.15 Wed 15:00 Poster D

Oxygen vacancy induced two-dimensional electron system in disordered-crystalline $LaAlO_3/KTaO_3$ heterostructures — •Michael Zapf[1], Judith Gabel[1], Philipp Scheiderer[1], Lenart Dudy[1], Christoph Schlueter[2], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, United Kingdom

Two-dimensional electron systems (2DESs) in oxide heterostructures based on $SrTiO_3$ are considered to be a promising platform for future microelectronic technology. A variety of interesting properties such as ferromagnetism, resistive switching and superconductivity are linked to interfacial n-doping involving oxygen vacancies. The introduction of a high Z-cation with large spin-orbit coupling like Ta offers an exciting new parameter. We report on a new oxygen vacancy induced 2DES located at the interface of disordered $LaAlO_3$ and crystalline $KTaO_3$,

which exhibits remarkably high electron mobilities and charge carrier concentrations. The number of charge carriers can be readily manipulated by the film thickness and irradiation with intense X-rays. Our synchrotron-based hard X-ray photoemission experiments provide a direct probe of the Ta 5d charge carriers at the buried interface to obtain information on the charge carrier density, its depth distribution, and the band structure.

TT 59.16 Wed 15:00 Poster D

Profiling the interfacial electron gas of $LaAlO_3/SrTiO_3$(111) Heterointerfaces — •Judith Gabel[1], Michael Zapf[1], Philipp Scheiderer[1], Philipp Schütz[1], Ozan Kirilmaz[1], Christoph Schlueter[2], Tien-Lin Lee[2], Claudia Cancellieri[3], Victor Rogalev[1,4], Vladimir Strocov[4], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, United Kingdom — [3]EMPA, Laboratory of Joining Technologies and Corrosion, Duebendorf, Switzerland — [4]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

Akin to the the well established $LaAlO_3$(LAO)/$SrTiO_3$(STO) (001) a two-dimensional electron system (2DES) also forms at the interface between LAO and STO in (111) orientation. In contrast to the (001) samples, the (111) oriented structures are predicted to display highly non-trivial topological properties induced by symmetry breaking and the peculiar real space lattice topology. We have investigated the electronic structure of the LAO/STO (111) heterostructure by hard and resonant soft X-ray photoemission. The momentum-resolved electronic structure of the interface Ti 3d states showcases the distinctive symmetry of the (111) orientation. These measurements as well as angular resolved hard X-ray photoemission measurements of the Ti 2p core level furthermore allow conclusions to be drawn about the spatial extent of the interfacial 2DES.

TT 59.17 Wed 15:00 Poster D

Electronic reconstruction at the interface between the Mott insulator $LaVO_3$ and the band insulator $SrTiO_3$ — •Martin Stübinger, Judith Gabel, Philipp Gagel, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

Akin to the well known oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) the formation of a conducting interface is found between the strongly correlated, polar Mott insulator $LaV^{3+}O_3$ (LVO) and the non-polar band insulator STO. Since $LaV^{3+}O_3$ tends to overoxidize to the thermodynamically more favourable $LaV^{5+}O_4$ phase when exposed to air, a suitable passivation is required. Therefore, we have employed pulsed laser deposition thin film growth of LVO films with a crystalline LAO capping layer. *In situ* photoemission measurements of samples before and after being exposed to air show that the V oxidation state can indeed be stabilized by the LAO capping layer. By transport measurements, we identify an insulator-to-metal transition at a combined LAO/LVO overlayer thickness of 4 to 5 unit cells. With LVO being a Mott insulator, passivation by the LAO capping opens the opportunity to study a band-filling controlled Mott insulator to metal transition induced by a purely electrostatic mechanism without interfering overoxidation of the LVO film.

TT 59.18 Wed 15:00 Poster D

Stoichiometry control of $SrVO_3$ thin films grown by pulsed laser deposition — •Philipp Scheiderer, Matthias Schmitt, Michael Sing, and Ralph Claessen — Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany

Oxide heterostructures exhibit fascinating properties, e.g., the coexistence of superconductivity and ferromagnetism at the interface of $LaAlO_3/SrTiO_3$, but the extraordinary electronic properties of transition metal oxides caused by electron correlation yet wait to be fully harnessed. One suitable candidate for future device applications is the correlated metal $SrVO_3$, which can be prepared by pulsed laser deposition (PLD) on commonly used substrates such as $SrTiO_3$. Sample fabrication by PLD offers a wide variety of possibilities to manipulate the structural and electronic properties of the grown films in a controlled way. Here we report on the manipulation of the cation and oxygen stoichiometry of $SrVO_3$ thin films by tuning the laser flux density of the PLD-ablation process and the oxygen background pressure during growth, respectively. *In situ* photoemission, x-ray diffraction, and temperature dependent resistivity measurements enable us to monitor the structural and electronic changes: Cation off-stoichiometry causes a strong increase of the out-of-plane lattice constant as well as a lower residual resistivity ratio, while excess oxygen is found to induce a shift to higher vanadium valences. After exposure to air a similar shift is detected, indicating an overoxidation of the $SrVO_3$ film.

TT 59.19 Wed 15:00 Poster D

Oxygen vacancies at the spinel/perovskite γ-$Al_2O_3/SrTiO_3$ heterointerface probed by resonant photoelectron spectroscopy — •Philipp Schütz[1], Florian Pfaff[1], Michael Zapf[1], Judith Gabel[1], Lenart Dudy[1], Götz Berner[1], Yunzhong Chen[2], Nini Pryds[2], Christoph Schlüter[3], Tien-Lin Lee[3], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Würzburg, Germany — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Risø Campus, Denmark — [3]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, United Kingdom

The spinel/perovskite heterointerface between the band insulators γ-Al_2O_3 and $SrTiO_3$ hosts a two-dimensional electron system (2DES) with exceptionally high electron mobility. Soft x-ray resonant photoelectron spectroscopy at the Ti L absorption edge is used to probe the Ti 3d derived interface states. Marked differences in the resonance behavior are found for the $SrTiO_3$ valence band and the different interface states, which are observed in the band gap of $SrTiO_3$. A comparison to x-ray absorption spectra of Ti $3d^0$ and Ti $3d^1$ systems reveals the presence of different types of electronic states with Ti 3d character, i.e., oxygen vacancy induced, trapped in-gap states and itinerant states contributing to the 2DES. Exposure to low doses of oxygen during irradiation allows for the reversible manipulation of the oxygen stoichiometry, thus revealing the presence of an oxygen vacancy-induced state, which is characteristic for this spinel/perovskite interface.

TT 59.20 Wed 15:00 Poster D

2DESs at the surface of locally doped insulating titanates studied by ARPES — •Tobias C. Rödel[1,2], Franck Fortuna[1], François Bertran[2], Thomas Maroutian[3], Philippe Lecoeur[3], Patrick Le Fèvre[2], and Andrés Felipe Santander-Syro[1] — [1]CSNSM, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, 91405 Orsay, France — [2]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin-BP48, 91192 Gif-sur-Yvette, France — [3]Institut d'Electronique Fondamentale, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France

Two-dimensional electron systems (2DESs) in transition metal oxides are currently a field of intense research in the quest of novel functionalities in materials showing competing ground states. The 2DESs in $SrTiO_3$-based interfaces have been the cornerstone of such research. The building block of $SrTiO_3$ and other titanates is the oxygen octahedron. Here we show, using (angle-resolved) photoemission spectroscopy in UHV that the stacking order and the rotation of those octahedra determines the order and hybridization of the t_{2g} orbitals as well as the (de)localized character of the excess electrons in 2DESs. To study different lattice configurations, we characterized the 2DESs at the surface of $SrTiO_3$, $CaTiO_3$ and TiO_2.

TT 59.21 Wed 15:00 Poster D

Thermoelectric and spincaloric properties of epitaxial $LaNiO_3/SrTiO_3$ superlattices from first principles — •Benjamin Geisler[1,2], Ariadna Blanca-Romero[3], and Rossitza Pentcheva[2] — [1]FRM II, Technische Universität München, 85748 Garching, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany — [3]Imperial College, London, United Kingdom

Modern layer-by-layer fabrication techniques make it possible to grow epitaxial oxide superlattices with atomic precision. By combining accurate DFT+U calculations to determine the atomic and electronic structure and Boltzmann transport theory we show how a targeted design of the interface composition can be used to optimize the thermoelectric and/or spincaloric properties of $LaNiO_3/SrTiO_3$(001) superlattices. A TiO_2/LaO interface induces n-type doping, and a (potentially highly spin-polarized) charge current arises solely in-plane in the NiO_2 layers. The out-of-plane resistance is high, since the $SrTiO_3$ layers act as tunneling barriers. In contrast, a NiO_2/SrO interface leads to p-type doping. In this case, also the valence band of $SrTiO_3$ contributes to the transmission, thereby reducing the out-of-plane resistance significantly. Besides this doping effect we find that the inter-

face composition influences the electronic band structure, which leads to a nontrivial behavior of the Seebeck coefficient.

Funding by the DFG within TRR 80 (G3 and G8) is acknowledged.

TT 59.22 Wed 15:00 Poster D

Correlated Electronic Properties of Different $SrIrO_3$/$SrTiO_3$ Heterostructures — •Gernot J. Kraberger and Markus Aichhorn — Institute of Theoretical and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Strontium iridates are materials that combine strong electronic correlations with pronounced spin-orbit coupling, giving rise to fascinating physical properties. Strategies to purposefully influence and design these materials are a crucial step to further advance this field. A highly promising candidate for achieving this goal is the formation of heterostructures with other materials. Motivated by this quest, we perform calculations within the DFT+DMFT framework to investigate how the geometry of heterostructures of perovskite $SrIrO_3$ with $SrTiO_3$ influences their correlated electronic structure. We explore the differences between (001)- and (111)-stacked heterostructures, where the latter are particularly interesting because they form buckled honeycomb lattices that have non-trivial topological properties. For the (001)-heterostructures the effect of varying the thickness of the $SrIrO_3$ layers, and thus their effective dimensionality, are studied. As an important ingredient we have to consider the effect of lattice distortions – in the form of a rotation of the oxygen cages – on the electronic correlations. We argue how the interplay of all these factors together allows a targeted modification of the electronic properties of the material.