TT 81: Correlated Electrons: Other Materials

Time: Thursday 15:00–17:15 Location: HSZ/0101

TT 81.1 Thu 15:00 HSZ/0101

Built-in Electric-Field-Driven Rashba Spin-Orbit Interactions in $AlO_x/Sr_{1-x}Ca_xTiO_3$ Interfaces — •Janine Gückelhorn[1], Sergi Plana-Ruiz[2,3], Gyanendra Singh[1], Saul Estandia Rodriguez[1], Roger Guzman[1], Fernando Gallego[4], Luis M. Vicente-Arche[4], Joaquim Portillo[5], Thanos Galanis[5], Manuel Bibes[4], Jaume Gázquez[1], and Gervasi Herranz[1] — [1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Bellaterra, Spain. — [2]Scientific & Technical Resources, Universitat Rovira i Virgili, Tarragona, Spain. — [3]LENS-MIND, Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Spain. — [4]Laboratoire Albert Fert, CNRS, Thales, Université Paris Saclay, France. — [5]NanoMEGAS SPRL, Brussels, Belgium.

Two-dimensional electron gases (2DEGs) at oxide interfaces exhibit strong Rashba spin-orbit coupling (SOC), arising from broken inversion symmetry and the resulting built-in electric field. However, the microscopic origin of Rashba SOC remains under debate. Density functional theory points to two key mechanisms as origin: polar lattice displacements and electric-field-driven orbital polarization. We show that the Rashba coefficient in $AlO_x/Sr_{1-x}Ca_xTiO_3$ 2DEGs increases significantly with Ca substitution, which enhances polarizability and induces ferroelectricity. Separating lattice and electrostatic effects reveals that modest structural changes accompany a near-tenfold rise in the built-in field. Our results demonstrate that nonlinear polarizability, not just structural asymmetry, dictates Rashba SOC strength, establishing polarizability as a key control of SOC in oxide 2DEGs.

TT 81.2 Thu 15:15 HSZ/0101

Non-quasiparticle states at a ferromagnetic oxide interface — Dylan Jones[1,2], Andreas Östlin[1,2], and •Liviu Chioncel[1,2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany

We propose a minimal tight-binding model for the electronic interface layer of the $LaAlO_3/SrTiO_3$ heterostructure with oxygen vacancies. In this model, the effective carriers are subject to oxygen vacancy-induced magnetic impurities. Both the effects of random on-site potentials and Zeeman-like exchange interactions between correlated carriers and magnetic impurities are taken into account. By applying the combined coherent potential approximation (CPA) and dynamical mean field theory (DMFT) for a ferromagnetic state, we analyze how magnetic impurities generate incoherent non-quasiparticle spectral weight near the Fermi level and introduce a low-energy scale that is expected to be relevant for electronic transport at the interface.

TT 81.3 Thu 15:30 HSZ/0101

Transport properties of the metal to insulator transition in Ca_2RuO_4 nanoflakes — •Roman Hartmann[1], Rosalba Fittipaldi[3], Antonio Vecchione[3], Elke Scheer[1], and Angelo Di Bernardo[1,2] — [1]FB Physik, Universität Konstanz, Konstanz, Germany — [2]Dipartimento di Fisica, Università di Salerno, Fisciano, Italy — [3]CNR-Spin, Salerno, Italy

The Mott insulator calcium ruthenate Ca_2RuO_4 (CRO) has attracted considerable attention due to its insulator to metal transition (IMT) with a transition temperature of 357 K (insulating below, metallic above) and the ability to trigger the IMT using pressure, current or an electric field of just 40 V/cm [1,2]. Unfortunately, stress from a structural transition (orthorombic to tetragonal) during the IMT combined with an increase in unit cell volume [1] generally breaks bulk crystals.

To overcome this limitation we have developed a method to fabricate sub-micron CRO flakes from bulk single crystals (despite it not being a layered material) that we can contact using standard lithographic and thin film techniques.

In these flakes we can reversibly trigger the IMT thousands of times by passing current without breaking the sample. The robustness of the devices enables us to switch at high frequencies paving the way for potential applications and enabling us to to gain further insight into the nature of the IMT [3].

[1] F. Nakamura et al., Sci. Rep. 3, 2536 (2013)
[2] R. Okazaki et al., JPSJ 82, 103702 (2013)
[3] V. K. Bhartiya et. al., arXiv:2504.17871 (2025)

TT 81.4 Thu 15:45 HSZ/0101

Many body effects in Li-ion cathode materials: how Coulomb interactions drive the redox profile — •Francesco Cassol and Silke Biermann — CPHT, Ecole Polytechnique, Palaiseau, France

In the last decades, a rising demand for energy storage has spurred consistent efforts into the design of high energy density cathode materials.

Crystallizing in layered structures, these compounds alternate lithium and transition-metal oxide planes, facilitating Li mobility during charge and discharge. Most of the battery properties are intimately related to the electronic structure, which governs the cyclic charge redistribution via oxidation and reduction of transition metal ions.

In this talk, we investigate the effects of Coulomb interactions on the corresponding redox mechanism upon delithiation, focusing on complex Li-based alloys studied within the dynamical mean-field theory (DMFT). Our results reconcile the charge profile with experiments and emphasize the importance of many-body effects for an accurate description of battery compounds.

15 min. break

TT 81.5 Thu 16:15 HSZ/0101

Separating magnetic bulk and surface properties of Czochralski-grown FeSi — •Gilles Gödecke[1], Philipp Herre[1], Markus Etzkorn[2,3], Musfira Aqeel[2,3], Alexander Frantz[4], Dirk Baabe[4], Stefan Süllow[1], and Dirk Menzel[1,2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, TU Braunschweig, Germany — [3]Institut für Angewandte Physik, TU Braunschweig, Germany — [4]Institut für Anorganische und Analytische Chemie, TU Braunschweig, Germany

The narrow-gap semiconductor FeSi has been extensively discussed regarding its low-temperature electronic transport and magnetic properties, ranging from Kondo-insulating behavior to the emergence of conducting and magnetic surface states. We present resistivity measurements on FeSi single crystals grown by the Czochralski method. To separate bulk and surface contributions, the sample thickness is continuously decreased by polishing. In addition, we conduct magnetization measurements of FeSi powder samples with decreasing grain sizes prepared by ball milling. The increase of the surface-to-volume ratio leads to enhanced surface contributions in the conductivity and magnetization. The results enable us to distinguish between the electrical and magnetic bulk and surface contributions and further estimate the dimensions of the surface states.

TT 81.6 Thu 16:30 HSZ/0101

Flat phonons in Eu_2AuGe_3 — •Aleksandr Sukhanov[1], Oleg Utesov[2], Artem Korshunov[3], Vinicius Frehse[1], and Marein Rahn[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), Daejeon, Korea, 34126 — [3]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 20018 San Sebastian, Spain

We employed inelastic x-ray scattering (IXS) to study the lattice dynamics in a single crystal of Eu_2AuGe_3 (orthorhombic, space group $Fmmm$). Within its crystal structure, a structural motif consisting of one Au atom and three Ge atoms plays a special role. Its atomic displacements can be effectively mapped out to the well known electronic cross-stitch model, which is a toy model for the electronic flat bands. We show that the same simple model can be applied to predict a flat phonon mode in Eu_2AuGe_3. In our experimental IXS spectra, we resolve the flat mode and show that it softens on cooling and leads to a charge density wave transition. Our first-principle calculations of the lattice dynamics further support the experimental findings.

TT 81.7 Thu 16:45 HSZ/0101

Tuning through a tetragonal collapse in $Ca_{1-x}Sr_xCo_2As_2$ single crystals investigated by thermal expansion — •Sven Graus[1], Adrian Valadkhani[2], N. S. Sangeetha[1], Markus Garst[3], Roser Valentí[2], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr University Bochum,

Bochum, Germany — [2]Institute for Theoretical Physics, Goethe University Frankfurt, Frankfurt am Main, Germany — [3]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

$Ca_{1-x}Sr_xCo_2As_2$ crystallizes in the tetragonal $ThCr_2Si_2$-type structure and undergoes a rare substitution-driven crossover from a collapsed tetragonal to an uncollapsed tetragonal structure. The resulting rich magnetic and electronic phase diagram provides an interesting platform to investigate the complex interplay between lattice, magnetic and electronic degrees of freedom.

High-resolution thermal-expansion measurements reveal strong anisotropy between in-plane and out-of-plane directions and identify a critical region near $x \approx 0.48$, where the thermal expansion coefficients $\alpha_{\mathbf{a}}/T$ and $\alpha_{\mathbf{c}}/T$ diverge at low temperatures. Analysis of the temperature dependence of the c/a ratio shows an accumulation of entropy in this region. The thermal-expansion behavior is well captured by a simple model of a pressure-tuned Van Hove singularity which is supported by density-functional theory calculations.

We acknowledge support from the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

TT 81.8 Thu 17:00 HSZ/0101

Synthesis of $CsMn_2P_2$ single crystals and study of their low temperature properties — •Martin Kostka, Ashiwini Balodhi, Matthias Kroll, N. S. Sangeetha, Sven Graus, Maik Golombiewski, Andreas Kreyssig, and Anna E. Böhmer — Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany

$CsMn_2P_2$ is an intriguing material because it exhibits unusual dynamic magnetic behavior not present in other AMn_2P_2 compounds, likely related to a mixed Mn^{2+}/Mn^{3+} valence state and enhanced magnetic fluctuations [1]. However, the synthesis of $CsMn_2P_2$ single crystals is a challenge due to the high reactivity of Cs, the high vapor pressure of Cs and P, and the high melting point of Mn. We succeeded in optimizing the growth conditions for reproducible synthesis of ~1 mm sized $CsMn_2P_2$ single crystals by systematically studying various growth techniques. The resulting samples were characterized by x-ray diffraction, electron microscopy, energy-dispersive x-ray spectroscopy, and electrical-transport measurements. The electrical resistance shows multiple intriguing phase transitions. However, it is sample dependent and varies with synthesis parameters. A relation with the lattice parameter c is observed.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] F. Hummel, Magnetism and superconductivity in layered manganese and iron pnictides, Diss. LMU (2015)