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Ulrich Eckern, Philipp Gegenwart

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From Electronic Correlations to Functionality

Ulrich Eckern and Philipp Gegenwart**

This Special Issue of *physica status solidi (b)* highlights some of the recent research achievements of the Transregional Collaborative Research Center "From Electronic Correlations to Functionality" (CRC/Transregio 80), which has been funded by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG, project no. 107745057) from January 2010 until June 2022. Our Transregio has been organized, in its last period, in 22 projects – arranged in three project areas – supervised by 31 principal investigators, from the University of Augsburg (applicant university), the TU Munich (co-applicant university), as well as from the LMU Munich (2010–2017), the Bavarian Academy of Sciences and Humanities (Walther Meissner Institute), the Max Planck Institute for Solid State Research, and the University of Duisburg-Essen (2018–2022).

The Transregio has focused on electronic properties of correlated matter with potential applications in future electronic technology. Unlike in ordinary metals or semiconductors, the mutual interactions between electrons may not be neglected in materials with partially filled *d* or *f* shells. Correlated electron materials display an exceptionally rich variety of quantum-mechanically entangled insulating, metallic, magnetic, or superconducting states. Our Transregio has combined highly advanced instrumentation and theoretical tools for the exploration of correlated quantum matter with new functionalities. The main research goals were as follows:

- Experimental identification of emergent functionalities driven by strong electronic correlations, and clarification of their origin in terms of underlying rigidity, symmetry breaking, and topological characteristics.
- Development of conceptual frameworks and quantitative theoretical accounts of strongly correlated electron systems that enable material-specific control of emergent functionalities.
- Design and tailoring of specific functionalities arising from strong electronic correlations in artificial systems by means of system size, shape, and materials combinations.

Most of the projects in the Transregio followed at least one of the routes: from correlations to topology, or from the bulk to surfaces and interfaces. Driven by the discovery of topology as one of the organizing principles of correlated matter, a major focus concerned non-trivial topological characteristics of the electronic and magnetic properties in both configuration and reciprocal space. This research included most prominently skyrmions, but also quantum spin liquids and Weyl semimetals. Another focus was placed on the influence of spatial confinement, for example, orbital, electronic and magnetic reconstructions on the way from the bulk to the surface or close to an interface. In several cases, the studies also involved topologically non-trivial states, like Chern insulators or topological superconductors. The understanding of how electronic correlations, spin–orbit coupling and interfaces conspire to form novel quantum states has also been central for the investigation of their emergent dynamics.

The current Special Issue features eight reviews and twelve research articles, highlighting selected recent achievements of the CRC/Transregio 80; twelve papers are experimentally oriented, five theoretically, while three contributions are devoted to the results of particularly close experimental–theoretical collaborations.

Correlated systems with non-trivial topology in real and reciprocal space

A preparation chain based on the optical floating-zone technique is used for the synthesis of high-quality bulk single crystals of quantum materials with topological magnetic or electronic states. The review by A. Bauer et al. (pssb.202100159) describes how precise control over the composition of the feed material enables the growth of chiral magnets with intentional compositional gradients. This way, the evolution of the magnetism under doping is studied in a single sample utilizing the spatial resolution of small-angle neutron scattering. Moreover, the growth of diborides with demanding metallurgy is reported, tuning the bulk properties by means of careful control of the synthesis parameters.

In a combined experiment–theory effort, J. Ketels et al. (pssb.202100151) have investigated the Fermi surface properties of, e.g., the hexaboride LaB_6. The 2D angular correlation of the positron annihilation radiation spectra is measured along high-symmetry directions and compared with first-principles calculations based on density functional theory. This allows the modeling of the Fermi surface in terms of ellipsoid electron pockets centered at *X*-points elongated along the Σ axis (Γ–*M* direction).

The electronic structure of the non-centrosymmetric transition metal monopnictide NbAs is studied by means of angular dependent quantum oscillation measurements in comparison with band-structure calculations by M. Naumann et al. (pssb.202100165). Previously unobserved pockets are found. The analysis suggests topological Weyl nodes that are located only 4 meV below the Fermi energy.

U. Eckern
Institute of Physics
University of Augsburg
86135 Augsburg, Germany
E-mail: ulrich.eckern@physik.uni-augsburg.de

P. Gegenwart
Center for Electronic Correlations and Magnetism
Institute of Physics
University of Augsburg
86135 Augsburg, Germany
E-mail: philipp.gegenwart@physik.uni-augsburg.de

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W. Kreuzpaintner et al. (pssb.202100153) review the development of polarized neutron reflectometry (PNR) as unique research tool for obtaining depth-resolved magnetization profiles from thin films and heterostructures. Dedicated insight is given on in-situ thin film growth capabilities for PNR, from early pioneering experiments to the sputter deposition system and Selene optics, integrated into the AMOR beamline at the Swiss spallation neutron source.

Two-dimensional s-wave superconductors in the presence of Rashba spin–orbit coupling, theoretically studied by S. R. Gorol et al. (pssb.202100156), possess distinct topologically nontrivial ground-state phases controlled by Zeeman splitting and band filling. These phases can be characterized in terms of spin textures in momentum space. Thermodynamic signatures directly related to the topological phase transitions of the ground state are identified.

Kitaev's honeycomb model stands out as rigorously solvable spin model that harbors gapped and gapless quantum spin liquids with emergent fractional excitations obeying non-Abelian statistics. A. A. Tsirlin and P. Gegenwart review the experimental progress towards solid-state realization of the Kitaev interaction on spin lattices of different dimensionality and topology in three different polytypes of Li_2IrO_3 (pssb.202100146).

S.-H. Lin et al. (pssb.202100172) employ artificial neural networks as a new tool for approximating quantum many-body states. The variational power of the restricted Boltzmann machine quantum states and different shallow and deep neural autoregressive quantum states to simulate the global quench dynamics of a nonintegrable quantum Ising chain is benchmarked.

Dynamics and generic excitations of complex phases of correlated matter

Magnets with exotic ground states continue to attract attention because their properties may be tailored via the lattice and/or the electronic band structure. The layered Kagome ferromagnet Fe_3Sn_2 is paradigmatic for the interplay between lattice structure and spin order. For this system, G. He et al. (pssb.202100169) present polarization- and temperature-dependent Raman data along with theoretical simulations. Eight out of the nine predicted phonon modes are identified. The temperature-dependent frequency and linewidth anomalies of the mode at the lowest energy are indicative of the spin re-orientation occurring close to 100 K, and related to eigenvector-specific spin–phonon coupling.

Tuning the electronic properties of transition-metal and rare-earth compounds by virtue of changes of the crystallographic lattice constants offers controlled access to new forms of order. The article by P. Jorba et al. (pssb.202100623) reviews the development of tungsten carbide and moissanite Bridgman cells conceived for studies of the electrical resistivity up to 10 GPa, as well as diamond anvil cells for neutron depolarization studies up to 20 GPa. Three examples are presented: (i) evidence of ferromagnetic order in $SrRuO_3$ close to a putative quantum phase transition, (ii) the emergence of incipient superconductivity in CrB_2 studied under hydrostatic, uniaxial, and quasi-hydrostatic pressure, and (iii) the evolution of the magneto-elastic coupling in $CeCuAl_3$.

The review by T. Keller et al. (pssb.202100164) discusses the application of neutron spin-echo (NSE) spectroscopy to study magnon lifetimes and magnetic critical dynamics, the unique property of NSE being the energy resolution in the μeV range. While the first NSE spectrometers were optimized for quasielastic scattering at small momentum transfers, the subsequent resonant NSE technique extends the parameter range toward large momentum and energy transfers and permits the measurement of magnon lifetimes across the Brillouin zone. Resonant NSE also comprises the Larmor diffraction (LD) mode with a resolution for lattice spacings and their variance of about 10^{-6}, proving useful for determining magnetostriction effects, small lattice distortions related to magnetic ordering, mosaic spread in crystals, and the size distribution of antiferromagnetic domains.

Nuclear and electron spin resonance techniques are applied by M. Prinz-Zwick et al. (pssb.202100170) in order to characterize the electronic structure and collective magnetic excitations of the lacunar spinels GaV_4S_8 and GaV_4Se_8. Cycloidal, Néel-type skyrmion lattice and ferromagnetically polarized phases are apparent. ^{71}Ga NMR provides a local probe of the rhombohedral distortion and the resulting uniaxial magnetic anisotropy via the detection of electric field gradients and hyperfine coupling. Broadband ESR allows the identification of clockwise, counterclockwise, and breathing modes of the skyrmion-lattice phase supported by theoretical simulations.

The review by K. Geirhos et al. (pssb.202100160) focuses on recent progress in the field of optical, dielectric, and magnetoelectric properties of ferro- and antiferroelectric lacunar spinels (AM_4X_8). This class of narrow-gap semiconductors offers a fertile ground to explore correlation and quantum phenomena. The lattice dynamics and electronic structure of these compounds are discussed on the basis of optical spectroscopy measurements. Dielectric and polarization studies reveal the main characteristics of their low-temperature ferro- or antiferroelectric phases. Strong couplings between spin, lattice, and orbital degrees of freedom entail, e.g., the emergence of various multiferroic phases and exotic domain-wall functionalities.

The article by M. Alexander and M. Kollar (pssb.202100280) describes prethermalization phenomena in weakly interacting Hubbard systems after applying electric-field pump pulses. A scaling behavior with pulse duration is observed for the absorbed energy as well as individual prethermalized momentum occupation numbers. A pronounced non-thermal momentum distribution can be created employing suitable resonance frequencies.

The dynamics of entanglement in a Wannier–Stark many-body localized system coupled to a dephasing environment is investigated by E. Wybo et al. (pssb.202100161). The third Rényi negativity is used as entanglement proxy, as it captures the characteristic logarithmic growth of interacting localized phases in the intermediate-time regime, where the effects of the coupling to the bath are not yet dominating the dynamics.

Novel electronic and transport properties of correlated matter in thin films, at interfaces, and in nano- and heterostructures

The nondestructive investigation of electronic and magnetic modifications at buried interfaces contributes significantly to the understanding of the underlying interactions, which is essential for the design of electronic devices based on complex quantum materials. In the article by E. Benckiser et al. (pssb.202100253) the

application of resonant X-ray and neutron reflectometry for the study of perovskite transition metal oxide heterostructures is reviewed. Both methods are well suited for the nondestructive study of interfacial reconstructions and interactions of spin, charge, and orbitals at the nanoscale. Cases are highlighted in which both methods are complementary and thus provide unique insights into the physics of oxide heterostructures.

Structural voids are a defining feature of the half-Heusler structure. Using temperature-dependent neutron diffraction, complemented by room-temperature X-ray diffraction and high-resolution neutron diffraction as well as calorimetry and macroscopic magnetization measurements, the thermal disordering of these vacancies is followed by G. Neibecker et al. (pssb.202100174) across the half- to full-Heusler transition in samples of $Ni_{1+x}MnSb$ with increasing x. Strongly differing relaxation rates of order and vacancy concentrations are found, which implies that in these and related systems the thermal history potentially determines material properties such as ordering temperatures much more strongly than usual.

In close cooperation between experiment and theory (R. Bartel et al., pssb.202100154) different facets of magnetotransport in selected 2D spin–orbit-coupled systems are analyzed and characterized by their single- or multiband behavior. A remarkable interplay of weak antilocalization and electron-electron interaction is revealed near the ground state of the single-band system $BaPbO_3$/$SrTiO_3$. Further investigations of multiband effects, as in $LaAlO_3$/$SrTiO_3$, predict a huge impact of filling on the Hall effect due to intermingled Hofstadter bands with striking deviations from single-band behavior, already at weak coupling strength.

The transport properties of a magnetic layer of correlated electrons sandwiched between noninteracting normal-metal leads are studied within model calculations by A. Weh et al. (pssb.202100157). The role of band structure effects for the transmission is clarified. For a strong coupling between the leads and the central layer, high-intensity localized states are formed outside the overlapping bands, while for weaker coupling this high-intensity spectral weight is formed within the leads' continuum band around the Fermi energy.

In the review article by B. Geisler et al. (pssb.202100270), advanced growth and characterization techniques are combined with state-of-the-art first-principles simulations in the frameworks of density functional and Boltzmann transport theory, in order to elucidate the performance of transition metal oxide thin films and superlattices for thermoelectric applications. Specifically, the impact of oxygen diffusion, interface polarity, epitaxial strain, quantum confinement, and topology on the thermoelectric response is explored for delafossite, perovskite, and rock-salt-derived thin films and heterostructures. Challenges and future topics of research in oxide thermoelectrics are discussed.

An optimized chemical vapor transport technique using $SeCl_4$ as a transport agent (TA) has been developed in the work by A. Aqeel et al. (pssb.202100152) to selectively produce large high-quality Cu_2OSeO_3 single crystals. This method is more efficient and at the same time simpler than the common technique (with HCl gas as TA). The crystals are of very high quality; their absolute structures are fully determined by simple single-crystal X-ray diffraction. Enantiomeric crystals with either left- or right-handed chiralities are observed.

All in all, the research efforts of the CRC/Transregio 80, which were devoted to the design, characterization and modeling of materials from the bulk to surfaces and near interfaces, as well as to the tailoring of their emergent topological, dynamic, and functional properties, have led us to numerous fascinating discoveries, some of which are described in this Special Issue. In particular, despite considerable achievements, we are confident that this line of research is by no means closed: rather, our results indicate various aspects which invite follow-up studies, in particular, with respect to the adaption of different functionalities to concrete technological applications.

Augsburg, March 2022

Ulrich Eckern studied physics at the University of Dortmund, where he received his diploma in 1975, then moved on with his supervisor, Prof. Albert Schmid, to the University of Karlsruhe where he earned his Ph.D. in 1979. Following two years as postdoctoral associate at Cornell University (1980–1982), he returned to Karlsruhe to complete his habilitation in 1984. In 1989 he was awarded a Heisenberg fellowship, but decided a year later to join the Research Center Karlsruhe, Institute for Solid State Physics, as senior scientist. From 1993 until 2020 he headed the chair for Theoretical Physics II (Theoretical Solid State Physics) at the University of Augsburg. Eckern has been a principal investigator in the CRC/Transregio 80 from its establishment in 2010.

Philipp Gegenwart studied physics at TU Darmstadt, Germany, and received his Ph.D. in 1998, under the supervision of Prof. Frank Steglich. He continued as a group leader at the Max Planck Institute for Chemical Physics of Solids in Dresden and as a visiting researcher at St. Andrews University in Scotland. From 2006 to 2013, he has been professor of Experimental Physics (Low-Temperature Physics) in Göttingen. Since 2014, he is the head of Experimental Physics VI chair at the Center for Electronic Correlations and Magnetism, University of Augsburg, and since 2017 he is spokesperson of the Collaborative Research Center "From Electronic Correlations to Functionality" (CRC/Transregio 80), funded by the German Research Foundation.