



University of Cologne  
Special Research Grant SFB608  
Chairman: Prof. Dr. A. Rosch

Complex transition metal compounds with spin  
and charge degrees of freedom and disorder

Address for correspondence  
Institute of Physics II  
Zùlpicher StraÙe 77  
D-50937 Cologne, Germany

Phone (0221) 470-6386 (Trebst)  
Fax (0221) 470-6708  
E-Mail trebst@ph2.uni-koeln.de

# Strongly correlated transition metal compounds - a farewell to CRC 608

**Cologne**  
**6.3.2013 - 8.3.2013**

**Hosted by**  
**SFB 608**

## Organisation

S. Trebst, M. Braden, T. Michely,  
P. Becker-Bohatý, A. Rosch, G. Meyer

## Topics

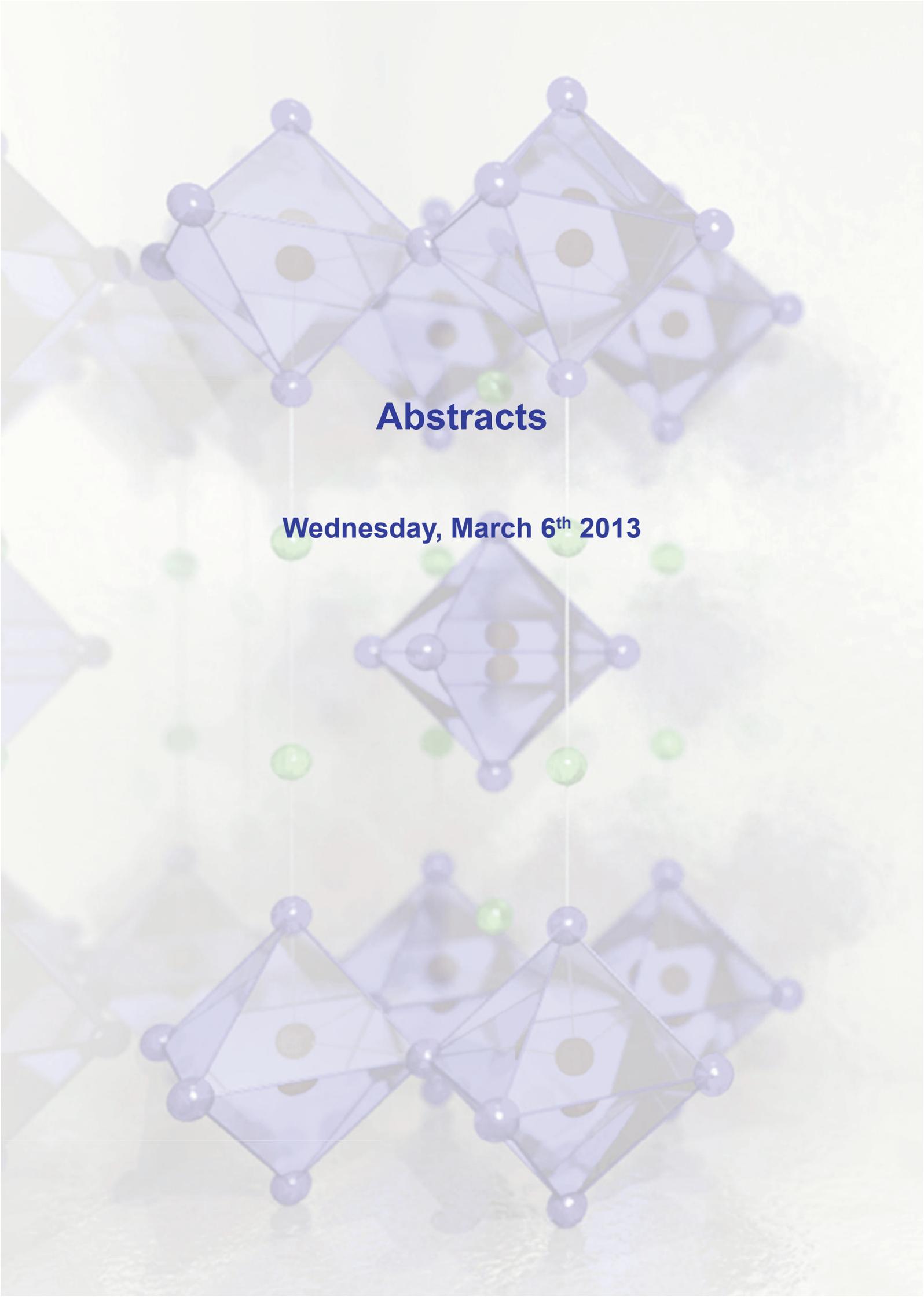
New materials  
Multiferroics  
Superconductors  
Skyrmions  
Surface physics  
Topological insulators

## Invited participants

D. Baeriswyl, E. Benckiser, S. Blùgel, B. Bùchner,  
M. Dressel, M. Fiebig, R. Gross, W. Hanke, M. Haverkort,  
M. Lang, M. Loewenhaupt, A. Mùller, C. Pfleiderer,  
K. Schmidt, C. Schùbler-Langeheine, H. Tjeng,  
G. Uhrig, M. Vojta, D. Vollhardt

**Strongly correlated transition metal compounds  
– a farewell to CRC 608**

March, 6 – 8th 2013 / Cologne



**Abstracts**

**Wednesday, March 6<sup>th</sup> 2013**

# Coupled electricity and magnetism in frustrated Mott insulators: spontaneous currents, dipoles and monopoles

D.Khomskii

Cologne University, Germany

The standard point of view is that at low energies Mott insulators exhibit only magnetic properties, while charge degrees of freedom are frozen out, because electrons are localized. I demonstrate that in general this is not true [1, 2]: for certain spin textures there exist quite nontrivial effects in the ground and lowest excited states, connected with charge degrees of freedom. In particular this may happen in frustrated systems, e.g. containing triangles or tetrahedra as building blocks. I will show that in some cases there may exist *spontaneous circular currents* in the ground state of insulators, proportional to the *scalar chirality*; this clarifies the meaning of the latter and opens the ways to directly experimentally access it. For other spin structures there may exist *spontaneous charge redistribution*, so that average charge at a site may be different from 1. This can lead to the appearance of dipole moments and possibly of the net *spontaneous polarization*. This is a novel, purely electronic mechanism of *multiferroic behaviour*. In particular I show [3] that such electric dipoles should exist in spin ice materials at every tetrahedra with three-in/one-out or one-in /three-out spin configurations, which are equivalent to magnetic monopoles. Thus there should be an *electric dipole* attached to each *magnetic monopole* in spin ice. This leads to electric activity of magnetic monopoles, and opens the possibility to control magnetic monopoles by electric field. The possibility to use chirality as qubits will be also discussed.

[1] L.N.Bulaevskii, C.D.Batista, M.V.Mostovoy and D.I.Khomskii, Phys.Rev.B **78**, 028402 (2008)

[2] D.I.Khomskii, JPCM **22**, 164209 (2010)

[3] D.I.Khomskii, Nature Comm. **3**, 904 (2012)

# Tunable sub-THz ESR spectroscopy of complex transition metal oxides

Bernd Büchner

Institut für Festkörperforschung, IFW Dresden

Institut für Festkörperphysik, TU Dresden

The expansion of the frequency window of ESR from the GHz- towards the THz-region opens new frontiers to explore the physics of materials with strong correlations between spin, charge and orbital degrees of freedom, such as complex transition metal oxides. In my talk I will discuss two examples of ESR studies on transition metal oxides. In lightly hole-doped  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$  ( $x \sim 0.002$ ) the ESR data provide clear-cut experimental evidence for the creation of extended spin clusters with a large spin multiplicity at low temperatures. There are multiple gapped excitations with large g factors showing a pronounced temperature dependence. The data can be modeled assuming ferromagnetic clusters with a total moment of about  $13/2 m_B$  and a substantial magnetic anisotropy. We argue that each doped hole couples ferromagnetically seven magnetic Co ions yielding a spin-state polaron with a huge local magnetic moment with a strong orbital contribution. As a second example I will discuss the 5d metal oxide  $\text{Sr}_2\text{IrO}_4$  which has been recently proposed to be a novel kind of insulator where the Mott insulating state arises due to electron correlation effects combined with strong relativistic spin-orbit coupling. Owing to a complex spin-orbital character of the effective  $J_{\text{eff}} = 1/2$  ground state of  $\text{Ir}^{4+}$  ions a rich variety of magnetically ordered phases in iridium oxides ranging from a Heisenberg to exotic quantum compass and Kitaev models have been predicted theoretically. Experimentally one observes in  $\text{Sr}_2\text{IrO}_4$  a canted antiferromagnetically (AFM) “easy-plane” ordered spin structure below  $T_N = 230$  K with an anomalously large “hidden” ferromagnetic (FM) moment. We have studied low-energy magnetic excitations at the AFM zone center in a single crystal of  $\text{Sr}_2\text{IrO}_4$  by high field ESR spectroscopy in the sub-THz frequency domain. We can identify both the “low” frequency mode due to the precession of the FM moments and the “high” frequency modes due to the precession of the AFM sublattices. We find an appreciable anisotropy of the g-factor which is expected due to the spin-orbital entanglement in the ground state. Surprisingly, despite this, the energy gap for the out-of-plane AFM excitations appears to be very small, amounting to 0.83 meV only. This suggests a rather isotropic Heisenberg character of Ir spins. We compare our ESR data with recent RIXS and INS results on iridium oxides and discuss possible reasons for the smallness of the magnon gap in  $\text{Sr}_2\text{IrO}_4$ .

# Spin-orbit assisted Mott physics in Iridates

Simon Trebst

Cologne University, Germany

While relativistic effects in electronic systems have been appreciated already in the early days of quantum mechanics – most notably in the discovery of the electron spin arising from the solution of the Dirac equation, they have long been considered well-understood, perturbative afterthoughts in solid-state physics. This perspective has dramatically changed in recent years with a plethora of novel quantum states being discovered which originate solely from (strong) spin-orbit coupling. Prominent examples include multiferroics, chiral metals exhibiting skyrmion physics, and probably most spectacularly topological insulators.

While our understanding of spin-orbit induced phenomena in these quite distinct electronic states is slowly growing, an even bigger slew of open questions arises when taking into account that for many systems the underlying electronic state is rather fragile and extremely sensitive to otherwise residual effects. One example are “heavy” 5d transition metal oxides, such as the Iridates or Osmates, where the extended nature of the 5d orbitals dampens the Coulomb interactions, thereby weakening the formation of a Mott insulating state, while also making the system exceedingly sensitive to its surrounding crystal fields. A microscopic description of these materials thus requires a delicate balance of the effects of spin-orbit coupling, strong correlations, and orbital/crystal field physics.

In this talk, I will discuss how to handle this theoretical challenge for a pair of layered Iridates,  $\text{Na}_2\text{IrO}_3$  and  $\text{Li}_2\text{IrO}_3$ . Various ordering patterns for the effective Iridium moments and their thermal stability will be considered, which allows us to connect back to thermodynamic measurements and possibly estimate microscopic coupling parameters. Finally, we discuss how applying magnetic fields might drive these systems into an exotic, topologically ordered state.

# Magnetic Monopole Heat Transport in Spin-Ice

Thomas Lorenz

Cologne University, Germany

Elementary excitations in the spin-ice compound  $\text{Dy}_2\text{Ti}_2\text{O}_7$  can be described as magnetic monopoles propagating independently within the pyrochlore lattice of magnetic Dy ions. In this talk, I will report heat-transport measurements to clarify the influence of the monopole excitations on the total thermal conductivity. From the anisotropic magnetic-field dependence and by additional measurements on reference compounds, we are able to separate the phononic and the magnetic contributions to the total heat transport, which both depend on the magnetic field. The field dependent phononic contribution arises from lattice distortions due to magnetic-field induced torques on the non-collinear magnetic moments of the Dy ions. For the magnetic contribution, we observe a highly anisotropic magnetic-field dependence, which correlates with the corresponding magnetization data reflecting the different magnetic-field induced spin-ice ground states. This anisotropic field dependence as well as various hysteresis effects suggest that the magnetic heat transport is essentially determined by the mobility of the magnetic monopole excitations in spin ice.

# Symbiosis of Intermetallic and Salt: Rare-Earth Metal Cluster Complexes with Endohedral Transition Metal Atoms

Gerd Meyer

Department für Chemistry, Universität zu Köln, 50939 Köln

Clusters of electron-poor group 3 elements (R) need an endohedral atom (Z) to stabilize the cluster  $\{ZR_x\}$  mainly through Z-R bonding interactions. There are an increasing number of rare-earth metal clusters sequestering transition metal atoms, mainly from groups 8 to 10. Isolated clusters surrounded by halide ligands (X), partly shared between the cluster complexes  $\{ZR_x\}X_2$ , are rare, as for example in  $\{IrEr_6\}I_{10}$ . In the majority of cases, clusters share common cluster atoms, mostly edges, less frequently faces. Coordination numbers of the endohedral atoms vary between 4 (tetrahedron) and 8 (cube or square antiprism) with 6 (octahedron) majoring. In  $\{Ru_5Lu_{20}\}I_{24}$ , for example, cubes and square antiprisms  $\{RuLu_8\}$  share common square faces to a one-dimensional intermetallic chain, surrounded by and connected through iodide ligands. The same polyhedra, and in addition such with nine- and ten-coordinate ruthenium atoms, are seen in the three-dimensional intermetallic compound  $\{Ru_{11}Lu_{20}\}$ .

# Magnetic and orbital excitations studied by optics and RIXS

Markus Grüninger

Cologne University, Germany

In this talk we focus on the character of magnetic excitations in the cuprates and of orbital excitations in the vanadates.

In the case of magnetic excitations, we concentrate on cuprate five-leg spin 1/2 ladders. The character of magnetic excitations changes from spinons in 1D chains via triplons in two-leg ladders to magnons in 2D. The five-leg ladders form a bridge between 1D and 2D. We use optical spectroscopy to study the magnetic excitations at high energies. In particular, we look for common properties of the excitations of different compounds and for the existence of bound states.

In the case of orbital excitations, the experimental proof for the existence of low-energy orbital waves or orbitons is still lacking. Typically, superexchange is assumed to be the driving force for the propagation of orbital waves, whereas the coupling to the lattice is supposed to suppress the dispersion. Using high-resolution RIXS, we have observed orbital excitations in orbitally ordered  $\text{YVO}_3$  and  $\text{GdVO}_3$  at the V L edge and the O K edge. We find a clear momentum dependence of the excitations, which however does not follow the expectations for the dispersion within a superexchange scenario. We discuss an alternative mechanism which yields propagating orbital waves.

# Kondo correlations in real space

Ralf Bulla

Cologne University, Germany

Quantum impurity systems show a variety of renormalization group fixed points and quantum phase transitions between these fixed points, features which have been studied in detail using various theoretical and numerical techniques. Here we focus on real-space signatures of such fixed points.

An example in the context of Kondo physics is the so-called screening cloud which - in real space - signals the crossover from the Local-Moment to the Strong-Coupling fixed point. These investigations are generalized to the case of a disordered bath, and to multi-impurity models. For the latter case we study the issue of overlapping screening clouds and - on a technical level - the application of DMFT-like approaches to such systems.



**Abstracts**

**Thursday, March 7<sup>th</sup> 2013**

# Dynamic Transitions in Interaction Quenches

Götz Uhrig

Dortmund University, Germany

We show that the non-equilibrium time-evolution after interaction quenches in the one dimensional, integrable Hubbard model exhibits a dynamical transition in the half-filled case. This transition ceases to exist upon doping. Our study is based on systematically extended equations of motion. Thus it is controlled for small and moderate times; no relaxation effects are neglected. Remarkable similarities to the quench dynamics in the infinite dimensional Hubbard model are found suggesting dynamical transitions to be a general feature of quenches in such models.

# Unusual Manifestations of Ferroelectric Order in Multiferroics

Manfred Fiebig

Department of Materials, ETH Zurich, Switzerland

Materials with a coexistence of magnetic and electric order, called multiferroics, are rare because (anti)ferromagnetic and ferroelectric order tend to be mutually exclusive. Magnetic order based on transition-metal exchange interactions requires partially filled 3d orbitals while ferroelectricity of the displacive hybridisation type calls for empty 3d shells. In this sense, any occurrence of magnetoelectric multiferroicity inherently involves unusual realisations of ferroelectric order. In my talk I will highlight various examples for these „exotic ferroelectrics“ and discuss how the unconventional origin of the spontaneous polarization leads to interesting topological states or to manifestations that may be relevant for oxide-electronics devices. The experiments presented here were conducted by optical second harmonic generation and by force-microscopy techniques.

# Dynamics near the multiferroic phase transition

Joachim Hemberger

II. Physikalisches Institut, Universität zu Köln

In magnetoelectric multiferroics the onset of ferroelectricity is coupled to the onset of inversion-symmetry breaking magnetic structure. The dynamics of such complex order can be probed via the dielectric response of the system. A prominent feature is the stimulation of (electro-) magnons via electric field in the THz-range. But as well at lower frequencies diverse dispersive features can be found, especially in the region around the multiferroic phase transition. As an example we studied the dielectric response of  $\text{MnWO}_4$ , which possesses a ferroelectric phase driven by cycloidal magnetism, using linear and non-linear spectroscopy in a frequency range from mHz to THz. The results denote the critical slowing down of the dynamics above the onset of multiferroic order, while the dielectric response of the ordered phase is dominated by the dynamics of domains and domain walls respectively.

# **Magnetoelectric and multiferroic materials**

Petra Becker-Bohaty

Cologne University, Germany

The interplay between magnetism and electricity, which can manifest by the cross-coupling of electric field and magnetisation or, vice versa, by magnetic field and electric polarisation, (magnetoelectric effect), but also, particularly, by emerging ferroelectricity induced by magnetic order (magnetoelectric multiferroicity), presently is a topical issue in solid state physics and has been one of the research areas of SFB 608. Up to now, a few distinct types of microscopic origins of multiferroic behaviour are known, which constitute the basis for the development of new multiferroic materials. The present contribution will give brief insight into the search and exploration activities for new (and perhaps novel) multiferroic and magnetoelectric crystals in SFB 608 and their basic characterisation.

# **Fascinating materials and thin films: Cologne youngsters' recent results at the Max Planck in Dresden**

Hao Tjeng

MPI-CPFS Dresden, Germany

# Dynamic heat transport shining light on phonon-magnon interactions in low dimensional quantum magnets

Paul van Loosdrecht

Cologne University, Germany

Thirty-five years ago, Sanders and Walton [Phys. Rev. B 15, 1489 (1977)] proposed a method to measure the phonon-magnon interaction in antiferromagnets through thermal transport which so far has not been verified experimentally. We show that a dynamical variant of this approach allows direct extraction of the phonon-magnon equilibration time, yielding 400  $\mu\text{s}$  for the cuprate spin ladder system  $\text{Ca}_9\text{La}_5\text{Cu}_{24}\text{O}_{41}$ . The present work provides a general method to directly address the spin-phonon interaction by means of dynamical transport experiments.

# Time-resolved x-ray diffraction from complex materials

Christian Schüßler-Langeheine

Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Understanding the interplay of different degrees of freedom across phase transitions or other changes of macroscopic properties is a central goal of material science. The availability of pulsed and ultra-bright coherent x-ray sources allow for novel experimental approaches in this field that combine highly selective x-ray probes with temporal and even spatial resolution. In a pump-probe experiment the system can be driven out of equilibrium by an external stimulus and its response being tracked with femtosecond x-ray pulses. We used this method to analyze the dynamics of spin, charge and orbital order in different materials. For the case of the 4f antiferromagnet EuTe we found a complicated response of its magnetic profile to which both magnetic and lattice dynamics contribute. The fast response of the metallic 4f antiferromagnet Ho rules out predictions that large magnetic moments lead to slow magnetic dynamics.

For the case of the Verwey transition in magnetite ( $\text{Fe}_3\text{O}_4$ ) we find when the pump pulse destroys the low-temperature phase only partially that besides the ultrafast response of orbital order and lattice distortion a second time scale comes into play, on which a spatial segregation of low- and high-temperature phase regions occur. Similar effects of spatial reorganization can be found also across the insulator-to-metal transition in doped titanates, where they are quasi static and hence accessible with micro-diffraction and coherent x-ray scattering methods.

# **Weakly doped cuprates: Fractionalized Fermi liquids?**

Matthias Vojta

TU Dresden, Germany

High-temperature superconductivity in the copper oxides constitutes one of the most fascinating and challenging problems in modern condensed matter physics. I will address the physics of underdoped cuprates, starting from the weakly

doped Mott insulator. In particular, I will focus on the concepts of selective Mott phases and fractionalized Fermi liquids, originally developed to describe non-Fermi liquid behavior in multi-band systems, and its possible relevance to the pseudogap regime of cuprates.

## Fermi surfaces in electron-doped cuprate superconductors

M.V. Kartsovnik,<sup>1</sup> T. Helm,<sup>1</sup> C. Putzke,<sup>2</sup> E. Kampert,<sup>2</sup> J. Wosnitza,<sup>2</sup> S. Lepault,<sup>3</sup> C. Proust,<sup>3</sup>  
A. Kiswandhi,<sup>4</sup> E.-S. Choi,<sup>4</sup> J.S. Brooks,<sup>4</sup> W. Biberacher,<sup>1</sup> A. Erb,<sup>1</sup> and R. Gross<sup>1,5</sup>

<sup>1</sup>Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

<sup>2</sup>Hochfeld-Magnetlabor Dresden, Dresden-Rossendorf, Germany

<sup>3</sup>Laboratoire National des Champs Magnétiques Intenses, CNRS, Toulouse, Grenoble, France

<sup>4</sup>National High Magnetic Field Laboratory, Tallahassee, USA

<sup>5</sup>Physik-Department, Technische Universität München, Garching, Germany

<http://www.wmi.badw.de>

We report on the current status of the Fermi surface studies in single crystals of the electron-doped cuprate superconductor  $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$  by means of magnetic quantum oscillations of magnetoresistance (Shubnikov-de Haas effect) [1-3]. The oscillations are observed for Ce concentrations  $x$  starting from 0.145 (optimal doping) up to 0.17 (strongly overdoped composition). The data provide evidence of a weak  $(\pi/a, \pi/a)$ -superlattice potential persisting over the whole overdoped range available for bulk crystals. The variation of the observed oscillation amplitude with the field orientation indicates a magnetic nature of the relevant ordering. The superlattice energy gap is very small ( $\approx 10$  meV) and is gradually suppressed on increasing the doping level, extrapolating to zero right at the edge of the superconducting dome ( $x \approx 0.175$ ). This suggests a close relation between superconductivity and the competing ordering instability.

The reduction of the doping level below optimal doping ( $x \approx 0.145$ ) results in a dramatic suppression of the oscillation amplitude as well as in a considerable increase of the effective cyclotron mass. The possibility of a quantum phase transition leading to a collapse of the classical cyclotron orbits on a closed Fermi surface just slightly below optimal doping is corroborated by dramatic changes in the non-oscillating component of magnetoresistance and Hall coefficient as well as by the behavior of the quantum oscillations in the sister compound  $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4$ .

This work is supported by the German Research Foundation via Grant No. GR 1132/15, EuroMagNET II under the EC Contract No. 228043, and the German Excellence Initiative via NIM.

- [1] T. Helm, M. V. Kartsovnik, M. Bartkowiak, N. Bittner, M. Lambacher, A. Erb, J. Wosnitza, R. Gross, Phys. Rev. Lett. 103, 157002 (2009).
- [2] T. Helm, M. V. Kartsovnik, I. Sheikin, M. Bartkowiak, F. Wolff-Fabris, N. Bittner, W. Biberacher, M. Lambacher, A. Erb, J. Wosnitza, R. Gross, Phys. Rev. Lett. 105, 247002 (2010).
- [3] M. V. Kartsovnik, T. Helm, C. Putzke, F. Wolff-Fabris, I. Sheikin, S. Lepault, C. Proust, D. Vignolles, N. Bittner, W. Biberacher, A. Erb, J. Wosnitza, and R. Gross, New J. Phys. 13, 015001 (2011).

# Strong correlations in inhomogeneous quantum systems

Hans Kroha

University of Bonn, Germany

The interplay of static inhomogeneities with the dynamics of local interactions can induce exotic ground states of matter and unconventional transport properties in electronic systems. In this talk two different systems involving inhomogeneity and strong correlations will be discussed.

(1 - Project D12) 2-channel Kondo (2CK) physics is one of the archetypes for non-Fermi liquid behavior. However, the 2CK effect has been notoriously difficult to realize in physical systems due to the necessity of fine-tuning of parameters. We propose a quantum impurity model consisting of a 3-level system with partial  $SU(3)$  symmetry which exhibits a generic 2CK fixed point without fine-tuning. The 2CK fixed point and a highly non-trivial temperature dependence of the entropy are obtained by NRG calculations, confirming earlier conjectures based on perturbative RG.

(2 - Project D13) Near the 1st-order Mott-Hubbard transition, the

thermodynamically stable state at finite temperature is characterized by a coexistence of metallic and insulating nanodomains, leading to the emergence of disorder from a homogeneous Hubbard system. We calculate the nanodomain size distribution in the coexistence region and derive from it the electrical conductivity, using random resistor network theory. A linear temperature dependence of the conductivity is found.

# Electronic Correlations and Structural Stability

Dieter Vollhardt

University of Augsburg, Germany

The total energy of correlated materials is computed as a function of the atomic positions and the unit cell parameters by employing a generalization of the LDA+DMFT scheme. Thereby it is possible to assess the influence of electronic correlations on structural transformations of the ionic lattice. Results are presented for two exemplary materials:

1) For paramagnetic  $\text{KCuF}_3$  the equilibrium Jahn-Teller distortion is calculated and a direct structural optimization is performed [1]. We obtain the correct lattice constant, equilibrium Jahn-Teller distortion, antiferro-orbital order, tetragonal compression of the unit cell, and spectral properties.

2) The equilibrium crystal structure and phase stability of paramagnetic iron at the  $\alpha$ - $\gamma$  phase transition is computed. Furthermore, by combining the GGA+DMFT scheme with the method of frozen phonons the lattice dynamics and phonon dispersion relations are determined [2].

In both cases electronic correlations are shown to be the driving force behind the structural transformation of the solid.

[1] I. Leonov, N. Binggeli, D. Korotin, V. I. Anisimov, N. Stojic, and D. Vollhardt, Phys. Rev. Lett. **101**, 096405 (2008); I. Leonov *et al.*, Phys. Rev B **81**, 075109 (2010).

[2] I. Leonov, A. I. Poteryaev, V. I. Anisimov, and D. Vollhardt, Phys. Rev. Lett. **106**, 106405 (2011) and Phys. Rev. B **85**, 020401 (2012).

# Stripe-like ordering of charges, orbitals and spins in layered manganites

Markus Braden

Cologne University, Germany

Layered manganites of the type  $R_{1-x}A_x\text{MnO}_4$  allow for detailed microscopic investigations of the coupling of charge, orbital, and magnetic ordering. The magnetic excitations in half-doped  $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$  can be perfectly described by only four parameters. This gives very strong support for the Goodenough model with charge and orbital ordering occurring at the Mn sites. A higher amount of doping results in complex stripe-like order patterns with three incommensurate and one commensurate order parameters that are closely coupled. Orbital stripes form the dominant ordering feature in these overdoped phases. The magnetic excitations in overdoped manganites exhibit an hourglass-like dispersion which closely resembles those observed in cuprates high-temperature superconductors in spite of the insulating nature of the former. In addition to a large ratio between intra- and inter-stripe magnetic interaction parameters, the correlation length seems to be decisive for the formation of the characteristic hourglass dispersion in stripe phases. Reduction of the doping below half-doping also induces incommensurate ordering but over- and under-doping are highly asymmetric. For doping levels of  $x=0.25$  and  $0.33$  we still find evidence for magnetic correlations closely related with those at half-doping but these coexist with short-range correlations of the nearest-neighbour antiferromagnetic order in undoped  $\text{LaSrMnO}_4$ .

# Magnetic Properties and Lattice Dynamics of Triangular and Honeycomb Lattices

Angela Möller

## Angela Möller

Texas Center for Superconductivity and Department of Chemistry, University of Houston, 136 Fleming Building, Houston, Texas 77204-5003, United States; email: [amoeller@uh.edu](mailto:amoeller@uh.edu)

The  $A\text{Ag}_2M[\text{VO}_4]_2$  type of compounds can be chemically modified to address magnetic super-exchange ( $M$ -site,  $3d^n$  transition metals) via non-magnetic vanadate groups on the triangular and honeycomb lattices. We will present recent experimental work targeting (i) structural aspects, (ii) chemical modifications including alteration of charges at the  $A$ - and  $M$ -sites, and (iii) anti- and ferromagnetic ground states. Previously, we have reported the ferromagnetic insulators of the  $A\text{Ag}_2M[\text{VO}_4]_2$  series.<sup>1-3</sup> Here, we will discuss two new examples for geometrically frustrated systems on a triangular lattice and give first insights into the honeycomb members of this class of materials. Furthermore, we will comment on the lattice dynamic studies by Raman spectroscopy and DFT methods.

*Acknowledgement:* This work has been supported by the NSF (Grant DMR-1149899) and by the State of Texas through the Texas Center for Superconductivity at the University of Houston.

## References:

- [1] A. Möller, N.E. Amuneke, P. Daniel, B. Lorenz, C. R. de la Cruz, M. Gooch, and P. C. W. Chu, *Phys. Rev. B.*, **85**, 214422 (2012).
- [2] A.A. Tsirlin, A. Möller, B. Lorenz, Y. Skourski, and H. Rosner, *Phys. Rev. B* **85**, 014401 (2012).
- [3] N.E. Amuneke, D.E. Gheorghe, B. Lorenz, and A. Möller, *Inorg. Chem.* **50**, 2207 (2011).



**Abstracts**

**Friday, March 8<sup>th</sup> 2013**

# Spin orbit entanglement in metals

## Sr<sub>2</sub>RuO<sub>4</sub> and Bi<sub>2</sub>Se<sub>3</sub>

Maurits Haverkort

UBC Vancouver, Canada

The spin and charge degrees of freedom of electrons can be entangled due to relativistic spin-orbit coupling. For heavy elements spin-orbit coupling is substantial compared to the band-width, leading to exciting effects as topological protected surface states with a well defined relation between orbital and spin character. This is the case for Bi<sub>2</sub>Se<sub>3</sub>. For most solids containing light elements the spin-orbit coupling is small compared to the band width and orbital momentum is quenched. In those cases spin-orbit coupling only plays a major role if there is an accidental degeneracy between orbitals at the Fermi energy. Reducing the dimensionality of a system, either by crystal structure or by artificial multilayers can reduce the band width and more importantly can lead to degenerate orbitals in a large part of the Brillouin zone. This is the case for Sr<sub>2</sub>RuO<sub>4</sub>, a layered perovskite with a two dimensional electronic structure. Although the band-width is larger than the size of the spin-orbit coupling, due to dimensionality constraints there are degenerate bands at the Fermi energy.

In this talk I will show how, with the use of polarization dependent, spin and angle resolved photoemission, one can measure this entanglement and discuss their consequences.

# Interaction effects on almost flat surface bands in topological insulators

Lars Fritz

Cologne University, Germany

We consider ferromagnetic instabilities of two-dimensional helical Dirac fermions hosted on the surface of three-dimensional topological insulators. We investigate ways to increase the role of interactions by means of modifying the bulk properties, which in turn changes the surface Dirac theory characteristics. We discuss both long-range Coulomb interactions controlled by the dimensionless coupling constant  $\alpha = e^2/(\hbar \epsilon v_F^{\text{surf}})$  as well as short-ranged Hubbard-like interactions of strength  $U$  which can induce spontaneous surface ferromagnetism, thereby gapping the surface Dirac metal. In both cases, we find that a prerequisite for observing this effect is to reduce the Fermi velocity  $v_F^{\text{surf}}$ , and we consider different mechanisms to achieve this. While for long-range Coulomb interactions we find that screening hinders ferromagnetism, for short-range interactions screening is not that vital and the instability can prevail.

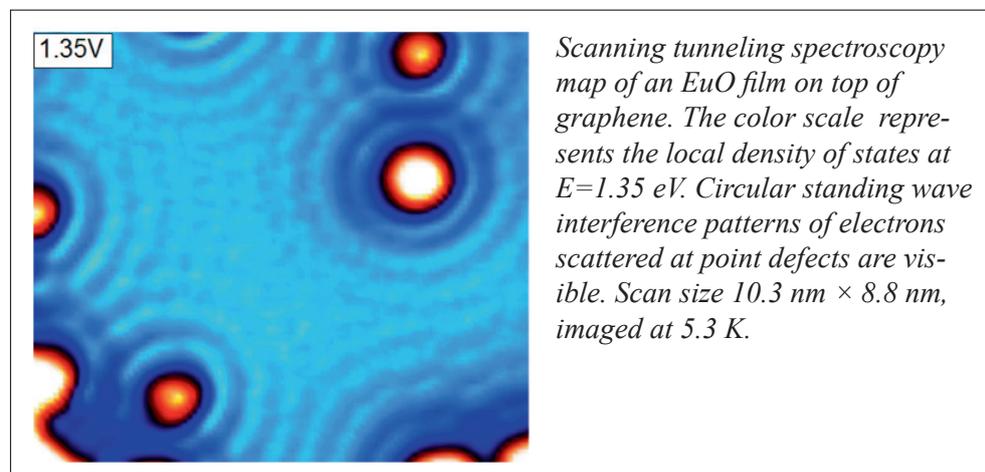
# EuO on graphene: Growth, magnetic properties, and the surface state

Carsten Busse

II. Physikalisches Institut, Universität zu Köln

The ferromagnetic semiconductor EuO has a large exchange splitting of its conduction band below the Curie temperature  $T_C$ . Therefore, it can be employed as a spin injector when used as a tunnel barrier between two electrodes, leading to almost 100% spin polarized conduction electrons, essential for the operation of spintronic devices. Ideally, a spin injector has to be coupled with a good spin conductor, i.e. a material with a high spin coherence length, a property found in the new material graphene. Consequently, we have developed a process to grow thin films of stoichiometric EuO in (100) orientation on top of in situ prepared graphene. We investigate the structural, magnetic, and electronic properties of this system using scanning tunneling microscopy / spectroscopy (STM/STS) and the magneto-optical Kerr effect (MOKE).

Our films have a ferromagnetic behavior with a Curie temperature significantly higher than the value expected for such thin films, which hints at a magnetic exchange coupling mediated by graphene. Low-temperature STS reveals standing electron wave patterns arising from scattering at defects. This proves experimentally the existence of a surface state in EuO as predicted by theory more than ten years ago. We observe a pronounced shift of the energy of the surface state above the Curie temperature which indicates a spin-polarization of this state.

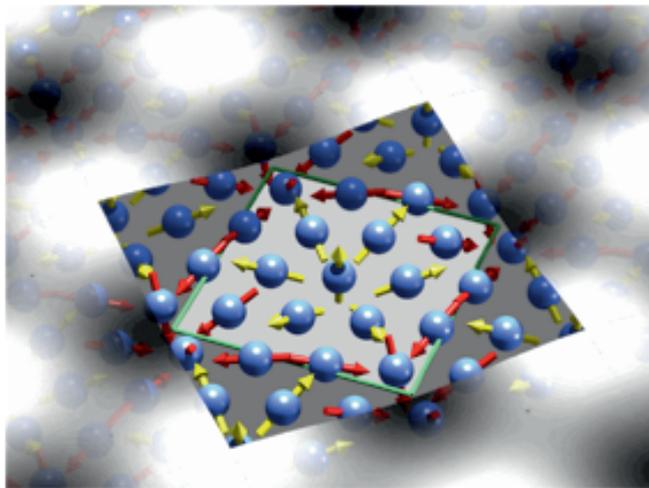


# Topologically protected Spin Textures at Metal Surfaces

Stefan Blügel

*Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany*

Applying first-principles calculations based on the density functional theory we explored the Dzyaloshinskii-Moriya interaction caused by spin-polarized electrons in the structure inversion asymmetric environment of 3d metal films on W substrates. We found that due to the large spin-orbit interaction of the W substrate the Dzyaloshinskii interaction exceeds a critical strength and competes with the exchange interaction and causes the formation of one-dimensional short-period cycloidal magnetic spirals of unique winding sense in the Fe film [1, 2]. The phenomenon is more general than expected and was also found for finite magnetic wires of Fe-double chains grown in troughs of the reconstructed Ir(100)5x1 substates [3]. Also the effect of the Dzyaloshinskii-Moriya interaction on the domain-walls will be discussed [4]. Recently we could go one step further and theoretically design a magnetic film, a monolayer of Fe on Ir(111) that exhibits a lattice of non-trivial two-dimensional magnetic structures, a nano-Skyrmion lattice [5]. We explore the phase diagram of the magnetic system based on parameters obtained from first-principles and finite size effects e.g. finite Fe clusters on Ir(111).



Nano-skyrmion of 15 atoms of iron on a Ir(111) surface are the building blocks forming a two dimensional magnetic lattice incommensurate to the atomic lattice of the substrate. The local magnetic moments at Fe atoms shown as yellow and red arrows have quantization axis that rotate from atom to atom. The magnetic structure has unique winding sense.

## Acknowledgement:

This work was carried out in collaboration with Marcus Heide, Samir Lounis, Gustav Bihlmayer, Stefan Heinze from the theory side and Matthias Bode, Andre Kubetzka, Kirsten von Bergmann of the Wiesendanger group from the experimental side.

- [1] M. Bode, M. Heide, K. von Bergmann, S. Heinze, G. Bihlmayer, A. Kubetzka, O. Pietzsch, S. Blügel, R. Wiesendanger, *Nature* **447**, 190 (2007).
- [2] P. Ferriani, K. von Bergmann, E.Y. Vedmedenko, S. Heinze, M. Bode, M. Heide, G. Bihlmayer, A. Kubetzka, S. Blügel, R. Wiesendanger, *Phys. Rev. Lett.* **101**, 027201 (2008).
- [3] M. Menzel, Y. Mokrousov, R. Wieser, J. E. Bickel, E. Vedmedenko, S. Blügel, S. Heinze, K. von Bergmann, A. Kubetzka, and R. Wiesendanger, *Phys. Rev. Lett.* **108**, 197204 (2012).
- [4] M. Heide, G. Bihlmayer, and S. Blügel, *Phys. Rev. B* **78**, 140403 (R) (2008); and *Physica B* **404**, 2678 (2009).
- [5] S. Heinze, K. von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer, and S. Blügel, *Nature Phys.* **7**, 713 (2011).

# **A model for elasticity and pinning of domain walls in helical magnets**

Thomas Nattermann

Cologne University, Germany

The theory of elasticity and coercivity of domain walls in both, centrosymmetric and noncentrosymmetric helical magnets, is developed. Generically these walls consist of regular arrays of magnetic vortex lines. Exceptions are walls oriented along high symmetry directions. The elasticity of the latter turns out to be non-local below their roughening transition, pinning of these walls by disorder is negligible. In contrast, weak anisotropy, breaking the  $U(1)$  symmetry of the helix, results in domain wall pinning by the bulk. Walls of other orientations consist of pairs of vortex lines separated by vortex free parts. These are strongly pinned by disorder. The application to chiral liquid crystals is briefly discussed.

# Universal Aspects of Non-Centrosymmetric Cubic Helimagnets

Christian Pfleiderer

TU Munich, Germany

The magnetic properties of non-centrosymmetric cubic materials with  $P2_13$  space group are characterised by a hierarchy of energy scales comprising exchange interactions on the strongest scale, Dzyaloshinsky-Moriya spin-orbit interactions on an intermediate scale and higher order spin-orbit interactions on the weakest scale. This hierarchy of energy scales is at the heart of a remarkably universal appearance of the spectrum of spin excitations as well as the magnetic phase diagram, which supports the formation of a skyrmion lattice as a new form of magnetic order.

# Dynamics of magnetic whirls in chiral magnets

Achim Rosch

Cologne University, Germany

Spin orbit interactions and tiny magnetic fields induce magnetic whirls in chiral magnets. These whirls have the topology of skyrmions. They are efficiently coupled to electric currents by Berry phases which can be described by emergent magnetic and electric field. We discuss how currents, electric and magnetic fields can be used to control, excite and measure the skyrmions.

An interesting question is also how one can change the topology of a magnetic structure. We thereby investigate the destruction of the skyrmion lattice when the external field is reduced. We argue that the transition is driven by singular hedgehog defects which act as emergent magnetic monopoles.

# Poster

## P1

### **Inhomogeneous, strongly correlated systems**

K. Ballmann, L. Borda, E. Fuh Chuo, T. Stollenwerk, and J. Kroha

## P2

### **Charge, orbital and spin ordering in layered transition-metal oxides**

T. Bardenheuer, H. Ulbrich, N. Qureshi, L. Hamdan, S. Kunkemöller, J. Engelmayer, N. Hollmann, P. Steffens, Y. Sidis, D. Lamago, A. Cousson, A. Nugroho, T. Lorenz, and M. Braden

## P3

### **Controlling domains in multiferroic and magnetoelectric materials**

M. Baum, J. Stein, T. Finger, S. Holbein, N. Qureshi, P. Becker, L. Bohaty, G. Eckold, J. Leist, Y. Sidis, M.T. Fernandez-Diaz, K. Schmalzl, L.P. Regnault, and M. Braden

## P4

### **Neutron scattering studies on magnetic correlation in FeAs-based superconductors**

N. Qureshi, J. Brand, F. Waßer, P. Steffens, A. Stunnault, Y. Sidis, D. Lamago, M. Meven, R. Ewings, L. Harnagea, I. Morozov, S. Aswartham, S. Wurmehl and B. Büchner, K. Kihou, C.-H. Lee, and M. Braden

## P5

### **Real space Correlations of Impurities in a Dissipative Environment**

Etienne Gärtner and Ralf Bulla

## P6

### **The prolific $\{TnR3\}X3$ type - structure, bonding, magnetism**

E. Meyer, S. Steinberg, M. Wolberg, and G. Meyer

## P7

### **{Ru<sub>5</sub>La<sub>14</sub>}<sub>2</sub>Br<sub>39</sub> - an anti-Werner type compound with a pentameric {Ru<sub>5</sub>La<sub>14</sub>} supercluster**

S. Steinberg and G. Meyer

## P8

### **Nanometer Scale Electronic Structure and Magnetism of EuO(100) on Graphene**

Jürgen Klinkhammer<sup>1</sup>, Daniel F. Förster<sup>1</sup>, Stefan Schumacher<sup>1</sup>, Fabian Craes<sup>1</sup>, Sven Runte<sup>1</sup>, Hans P. Oepen<sup>2</sup>, Thomas Michely<sup>1</sup>, and Carsten Busse<sup>1</sup>

1. II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

2. Institut für Angewandte Physik, Jungiusstraße 11, 20355 Hamburg, Germany

## P9

### **Orbital reflectometry of nickelate superlattices**

M. Wu, E. Benckiser, M.W. Haverkort, S. Brück, P. Audehm, E. Goering, S. Macke, A. Frañó, Y. Lu, X. Yang, O.K. Andersen, G. Cristiani, S. Heinze, H.-U. Habermeier, A.V. Boris, I. Zegkinoglou, P. Wochner, V. Hinkov, and B. Keimer

## P10

### **Theory of de Haas-van Alphen oscillations in graphene**

C. Kueppersbusch and Lars Fritz

## P11

### **Kinetic theory of Coulomb Drag in graphene**

J. Lux and Lars Fritz

## P12

### **Spin dynamics in Swedenborghites**

S. Buhrandt, J. Reim, W. Schweika, and Lars Fritz

## P13

### **Robustness and spectroscopy of topologically-ordered systems**

Kai Schmidt

## P14

### Entanglement Entropies and Quantum Monte Carlo

P. Bröcker and S. Trebst

## P15

### Thermodynamics of the XXZ- and Ising-type spin chain systems $\text{Cs}_2\text{CoCl}_4$ and $\text{CoNb}_2\text{O}_6$ in transverse magnetic field

O. Breunig<sup>1</sup>, S. Scharffe<sup>1</sup>, C. Grams<sup>1</sup>, A. Rosch<sup>2</sup>, M. Garst<sup>2</sup>, E. Sela<sup>2,4</sup>,  
B. Buldmann<sup>2</sup>, P. Becker<sup>3</sup>, L. Bohatý<sup>3</sup>, J. Frielingsdorf<sup>1</sup>, R. Müller<sup>1</sup>, M. Valldor<sup>1</sup>,  
J. Hemberger<sup>1</sup>, T. Lorenz<sup>1</sup>

<sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Germany

<sup>2</sup>Institut für Theoretische Physik, Universität zu Köln, Germany

<sup>3</sup>Institut für Kristallographie, Universität zu Köln, Germany

<sup>4</sup>Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University,  
Tel Aviv 69978, Israel

## P16

### Monopole dynamics in the Spin-Ice $\text{Dy}_2\text{Mn}_2\text{O}_7$

P. Laschitzky, C. Grams, G. Kolland, O. Breunig, S. Scharffe, M. Hiertz,  
J. Frielingsdorf, M. Valldor, J. Hemberger and T. Lorenz

## P17

### Skymionic excitations in magnetoelectric $\text{Cu}_2\text{OSeO}_3$

Steffen Harms<sup>1</sup>, Maria Belesi<sup>2</sup>, Helmuth Berger<sup>3</sup>, Jean-Philippe Ansermet<sup>3</sup>,  
Christoph Grams<sup>1</sup>, Daniel Niermann<sup>1</sup>, and Joachim Hemberger<sup>1</sup>

<sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Germany

<sup>2</sup>Leibniz Institute for Solid State and Material Research, Dresden, Germany

<sup>3</sup>Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne

## P18

### Critical dynamics in $\text{LiCuVO}_4$

C. Grams, M. Schalenbach, P. Becker, and J. Hemberger

## P19

### Low dimensional spin chain AM<sub>2</sub>V<sub>2</sub>O<sub>8</sub> compounds

S. Niesen, M. Seher, O. Breunig, G. Kolland, O. Heyer, M. Valldor, and T. Lorenz

## P20

### Magnetoelectric multiferroics and linear magnetoelectrics

M. Ackermann, M. Baum, S. Albiez, A.C. Komarek, A. Schneidewind, M. Meven, A. Hieß, M.T. Fernandez-Diaz, G. André, Y. Sidis, K. Schmalzl, P. Steffens, L.P. Regnault, M. Braden, T. Lorenz, P. Becker, and L. Bohatý

## P21

### Phonon-magnon interaction in low dimensional quantum magnets observed by dynamic heat transport measurements

Matteo Montagnese<sup>1</sup>, Marian Otter<sup>1</sup>, Xenophon Zotos<sup>2</sup>, Dmitry A. Fishman<sup>\*1</sup>, Nikolai Hlubek<sup>3</sup>, Oleg Mytiashkin<sup>3</sup>, Christian Hess<sup>3</sup>, Romuald Saint-Martin<sup>4</sup>, Surjeet Singh<sup>†4</sup>, Alexandre Revcolevschi<sup>4</sup>, and Paul H.M. van Loosdrecht<sup>1</sup>

<sup>1</sup> Zernike Institute for Advanced Materials, Rijksuniversiteit Groningen, Nijenborgh 4, 9747 AG, The Netherlands

<sup>2</sup> Department of Physics, University of Crete and Foundation for Research and Technology-Hellas, 71003 Heraklion, Greece

<sup>3</sup> IFW-Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany

<sup>4</sup> Laboratoire de Physico-Chimie de L'Etat Solide, ICMMO, UMR8182, Université Paris-Sud, 91405 Orsay CEDEX, France

\* Present address: Department of Chemistry, University of California at Irvine, Irvine, California 92697, USA

† Present address: Indian Institute of Science Education and Research 900, NCL Innovation Park, Pune 411008, India

## P22

### Magnetic and electric excitations of helices and skyrmions in chiral magnets

J. Waizner, M. Garst, A. Rosch, I. Stasinopoulos, T. Schwarze, A. Bauer, H. Berger, C. Pfleiderer and D. Grundler

## P23

### Skyrmions: Berry phase physics and spin torques

K. Everschor-Sitte, R. Bamler, M. Garst and A. Rosch

## **P24**

### **Mott metal-insulator transition on compressible lattices**

M. Zacharias, L. Bartosch, and M. Garst

## **P25**

### **Interaction effects on almost flat surface bands in topological insulators**

M. Sitte, L. Fritz, and A. Rosch

## **P26**

### **Spin liquids and conventional magnetic order in layered Iridates**

E. Sela, H.-C. Jiang, M. Gerlach, O. Wohak, and S. Trebst

## **P27**

### **Orbitons and bi-orbitons in GdVO<sub>3</sub> and YVO<sub>3</sub>**

L. Fels, M. Voigt, K. Thirunavukkuarasu, E. Benckiser, M. Haverkort, G. Ghiringhelli, M. Moretti Sala, T. Schmitt, G.R. Blake, N. Mufti, A.A. Nugroho, P. Marra, K. Wohlfeld, J. van den Brink, T.T.M. Palstra, and M. Grüninger

## **P28**

### **Broadband cw THz spectroscopy at low temperatures and high magnetic fields**

M. Langenbach, K. Thirunavukkuarasu, T. Hissen, P. Schumacher, H. Schmitz, A. Roggenbuck, I. Cámara Mayorga, R. Güsten, J. Hemberger, and M. Grüninger

## **P29**

### **Temperature-dependent optical conductivity of RVO<sub>3</sub> and of doped RTiO<sub>3</sub> studied by ellipsometry**

J. Reul, I. Vergara Kausel, A.A. Nugroho, T.T.M. Palstra, A. Komarek, M. Braden, and M. Grüninger

# Participants

## Invited Participants

Dionys **Baeriswyl**, Universite de Fribourg

Eva **Benckiser**, Max Planck Institute for Solid State Research

Stefan **Blügel**, Forschungszentrum Jülich

Bernd **Büchner**, IFW Dresden

Martin **Dressel**, University of Stuttgart

Manfred **Fiebig**, ETH Zurich

Rudolf **Gross**, TU Munich

Maurits **Haverkort**, University of British Columbia

Michael **Lang**, Goethe-University Frankfurt

Michael **Loewenhaupt**, TU Dresden

Angela **Möller**, University of Houston

Christian **Pfleiderer**, TU Munich

Christian **Schüssler-Langeheine**, Helmholtz-Zentrum Berlin

Kai **Schmidt**, TU Dortmund

Hao **Tjeng**, Max Planck Institute for Chemical Physics of Solids Dresden

Götz **Uhrig**, TU Dortmund

Dieter **Vollhardt**, University of Augsburg

Matthias **Vojta**, TU Dresden

## University of Cologne, Institute of Physics II

Mohsen **Abd-Elmequid**

Thomas **Bardenheuer**

Max **Baum**

Markus **Braden**

Johanna **Brand**

Oliver **Breunig**

Marcel **Buchholz**

Carsten **Busse**

Tobias **Cronert**

Johannes **Engelmeyer**

Luis **Fels**

Thomas **Finger**

Axel **Freimuth**

Christoph **Grams**

Markus **Grüninger**

Lucie **Hamdan**

Carmen **Handels**

Joachim **Hemberger**

Norbert **Henn**

Tobias **Hissen**

Felix **Huttmann**

Wouter **Jolie**

Daniël **Khomskii**

Harald **Kierspel**

Jürgen **Klinkhammer**

Thomas **Koethe**

Gerhard **Kolland**

Stefan **Kunkenmüller**

Malte **Langenbach**

Peter **Laschitzky**

Thomas **Lorenz**

Ralf **Müller**

Gerd **Meyer**

Thomas **Michely**

Matteo **Montagnese**

Beate **Neugebauer**

Daniel **Niermann**

Sandra **Niesen**

Navid **Qureshi**

Elia **Rampi**

Julia **Reul**

Reinhard **Rückamp**

Sven **Runte**

Simon **Scharffe**

Ulrike **Schröder**

Andrea **Severing**

Inge **Simons**

Jonas **Stein**

Fabio **Strigari**

Martin **Sundermann**

Paul **van Loosdrecht**

Ignacio Vergara **Kausel**

Rolf **Versteeg**

Jonas **Weinen**

## University of Cologne, Institute for Theoretical Physics

Robert **Bamler**

Johannes **Helmes**

Michael **Becker**

Maria **Hermanns**

Stefan **Buhrandt**

Carolin **Küppersbusch**

Benjamin **Buldmann**

Jonathan **Lux**

Ralf **Bulla**

Thomas **Nattermann**

Olga **Dimitrova**

Achim **Rosch**

Karin **Everschor-Sitte**

Hannes **Schenk**

Lars **Fritz**

Matthias **Sitte**

Markus **Garst**

Simon **Trebst**

Etienne **Gärtner**

Johannes **Waizner**

Max **Gerlach**

Mario **Zacharias**

## University of Cologne, Institute of Inorganic Chemistry

Gerd **Meyer**

Simon **Steinberg**

Eva **Meyer**

Marike **Wolberg**

## University of Cologne, Institute of Crystallography

Petra **Becker-Bohaty**

Matthias **Ackermann**

Ladislav **Bohaty**

## University of Bonn, Department of Physics

Katinka **Ballmann**

Zhong **Lai**

Evaristus Fuh **Chuo**

Ammar **Nejati**

Roman **Katzner**

Tobias **Stollenwerk**

Hans **Kroha**

Maricio **Trujillo-Martinez**