MA 68: Poster 5

Time: Friday 9:30–13:00 Location: P2-OG4

MA 68.1 Fri 9:30 P2-OG4

Investigation of thermalization in giant-spin models by different Lindblad schemes — •Christian Beckmann and Jürgen Schnack — Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

The theoretical understanding of time-dependence in magnetic quantum systems is of great importance in particular for cases where a unitary time evolution is accompanied by relaxation processes. A key example is given by the dynamics of single-molecule magnets where quantum tunneling of the magnetization competes with thermal relaxation over the anisotropy barrier. In this contribution we investigate how good a Lindblad approach describes the relaxation in giant spin models and how the result depends on the employed operator that transmits the action of the thermal bath.

MA 68.2 Fri 9:30 P2-OG4

High-frequency EPR studies on lanthanide monomers in different ligand structures — •Julian Butscher[1], Changhyun Koo[1], Johannes Werner[1], Asha Roberts[2], Peter Comba[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Anorganisch-Chemisches Institut, Universität Heidelberg, Heidelberg, Germany

4f-lanthanide single molecular magnets (SMMs) find increasing interest in the SMM research field due to their high magnetic anisotropy caused by strong spin-orbit coupling in Ln ions. We report the magnetic properties of Ln monomers (Ln = Dy(III) and Tb(III)) in different ligand structures ([Dy(III)(2Li-1,2-HOPo)$_2$]pyH, [Tb(III)(2Li-1,2-HOPO)$_2$]PyH, and [Tb(III)(5Li-1,2-HOPO)$_2$]PyH) which are studied by means of high-field magnetometry and high-frequency electron paramagnetic resonance (HF-EPR). The HF-EPR spectra of all complexes, at T = 2 K, exhibit only a single resonance feature which frequency linearly increases with the external magnetic field. The associated g-factors much larger than 2 are read-off the frequency vs. magnetic field diagrams. Finite zero-field splitting (ZFS) is observed in the [Tb(III)(2Li-1,2-HOPO)$_2$]PyH-complex which indicates lifting of the degeneracy in a non-Kramers doublet. The ground states of the complexes are estimated by using high-field magnetization and HF-EPR measurements, as well as by energy level calculations.

MA 68.3 Fri 9:30 P2-OG4

Tuneable electronic structure and molecular magnetism in metal organic frameworks — •Sebastian Schwalbe[1], Kai Trepte[2], Gotthard Seifert[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Technische Universität Dresden, Theoretical Chemistry, Germany

We present an ab-initio density functional theory study and show how it is possible to tune the electronic structure and with that the local magnetism represented by single molecule magnets (SMMs) within three-dimensional metal organic frameworks (MOFs). The electronic and magnetic properties of the flexible MOF DUT-8(Ni) [1,2] were described by Trepte et al. [3]. Based on this work we performed a screening of the metal centers in a special model system [4], which is a good approximation for the electronic and magnetic properties of DUT-8(Ni). A major result of these calculations is that the electronic structure is mainly determined and influenced by the metal centers (3d metals). By changing the metal centers inside the SBU we are able to adjust magnetic properties and obtain stable ferromagnetic, antiferromagnetic or eventually even metallic secondary building units.

[1] N. Klein et al., PCCP, vol. 12, pp. 11778-11784, 2010
[2] V. Bon et al., PCCP, vol. 17, pp. 17471-17479, 2015
[3] K. Trepte et al., PCCP, vol. 17, pp. 17122-17129, 2015
[4] S. Schwalbe et al., PCCP, vol. 18, pp. 8075-8080, 2016

MA 68.4 Fri 9:30 P2-OG4

Field-induced exciton condensation in $LaCoO_3$ — •Andrii Sotnikov and Jan Kuneš — Institute of Solid State Physics, TU Wien, Austria

Motivated by recent observation of magnetic field induced transition in $LaCoO_3$ [1] we study the effect of external field in systems close to instabilities towards spin-state ordering and exciton condensation. We show that, while in both cases the transition can be induced by an external field, temperature dependencies of the critical field have opposite slopes [2]. Based on this result we argue that the experimental observations select the exciton condensation scenario. We show that such condensation is possible due to high mobility of the intermediate spin excitations. The estimated width of the corresponding dispersion is large enough to overrule the order of atomic multiplets and to make the intermediate spin excitation propagating with a specific wave vector the lowest excitation of the system.

[1] A. Ikeda *et al.*, Phys. Rev. B **93**, 220401 (2016).
[2] A. Sotnikov and J. Kuneš, Sci. Rep **6**, 30510 (2016).

MA 68.5 Fri 9:30 P2-OG4

Functional approach to electrodynamics of media — •Ronald Starke[1] and Giulio Schober[2] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg — [2]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg

By a systematic investigation of the mutual functional dependencies between induced, external and total electromagnetic field quantities we derive universal (material-independent) relations between electromagnetic response functions such as the dielectric tensor, the magnetic susceptibility and the microscopic conductivity tensor. Our formulae can be reduced to well-known identities in special cases, but more generally include the effects of inhomogeneity, anisotropy, magneto-electric cross-coupling and relativistic retardation. If combined with the Kubo formalism, they would therefore lend themselves to the ab initio calculation of all linear electromagnetic response functions, thus paving the way for a first-principles description of magneto-electric materials for spintronics applications.

MA 68.6 Fri 9:30 P2-OG4

Resonant inelastic X-ray scattering study of excitonic condensation in perovskite cobalt oxides — •Atsushi Hariki and Jan Kuneš — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Spin-state transition in perovskite cobalt oxides, such as $LaCoO_3$, is an open problem in the research of the strongly correlated electron systems. Recently, the instability towards the excitonic condensation (EC) close to the spin-state transition was theoretically studied [1,2]. However, experimental probe to detect the EC in perovskite cobalt oxides has not been realized so far.

In this study, we propose that Co $L_{2,3}$-edge resonant inelastic X-ray scattering (RIXS) is a promising experimental method to investigate the EC in perovskite cobalt oxides. We analyze the angular dependence of $L_{2,3}$ RIXS by means of an atomic model considering the effect of the EC and show that RIXS gives a distinctive spectral feature of the EC state in comparison with the contributions of the pure (atomic) spin-states (such as high-, low- and intermediate-spin states) discussed in the context of the spin-state transition so far.

[1] J. Kuneš et al., Phys. Rev. B 89, 115134 (2014).
[2] J. Kuneš et al., Phys. Rev. B 90, 235112 (2014).

MA 68.7 Fri 9:30 P2-OG4

Excitonic condensation in $LaCoO_3$ perovskite — •Juan Fernandez Afonso and Jan Kunes — Technische Universität Wien, Freihaus building, Wiedner Hauptstrasse 8 -10, 1040 Wien, AUSTRIA

We study the possibility of excitonic condensation in transition metals perovskites with d^6 electronic configuration such as $LaCoO_3$. These excitonic states arise from an intra-atomic $e_g - t_{2g}$ electron-hole coupling. It is possible to characterise them by a 3×3 complex order parameter. We present several LDA+U self-consistent solutions which correspond to distinct ordered states. We study both stability and symmetry properties of these solutions, investigate the evolution of the order parameter with the interaction strength and the effect that the spin-orbit coupling has on these states. Our results suggest that $LaCoO_3$ is close to the excitonic instability and suggest ways how the instability can be reached in the reality.

MA 68.8 Fri 9:30 P2-OG4

Domain engineering in the $4f$ uniaxial ferromagnet $CeRu_2Ga_2B$ — •Dirk Wulferding[1,2], Hoon Kim[1,3], Ilkyu

Yang[1,3], Oscar Ayala-Valenzuela[1], Roman Movshovich[4], Ryan Baumbach[5], Eric Bauer[4], Joe Thompson[4], Leonardo Civale[4], and Jeehoon Kim[1,3] — [1]CALDES, Institute for Basic Science, Pohang, Korea — [2]IPKM und LENA, TU-BS, Braunschweig, Germany — [3]Dept. of Phys., POSTECH, Korea — [4]MPA-CMMS, Los Alamos Natl. Lab., Los Alamos, USA — [5]NHML, Florida State Univ., Tallahassee, USA

The interplay of spin and electronic degrees of freedom in strongly correlated electron systems is a fruitful route towards many exotic and unexpected phenomena. In particular, rich magnetic phase diagrams can be found in systems with additional magnetic anisotropies. While the bulk magnetic properties are often well explored, the evolution of the microscopic magnetic domain structure within the phase diagram remains elusive. Using low temperature magnetic force microscopy with vector magnet capabilities [1], we explore the evolution and manipulation of magnetic domains in the centrosymmetric ferromagnet $CeRu_2Ga_2B$ [2]. This compound exhibits transitions among dendritic, stripe, and bubble domain phases. We highlight the domain evolution with a vector magnetic field in this Ising-like spin system and demonstrate the manipulation of individual bubble domains through the magnetic tip of our scanning probe microscope.

[1] Yang, et al., Rev. Sci. Instrum. 87, 023704 (2016). [2] Baumbach, et al., J. Phys.: Condens. Matter 24, 185702 (2012).

MA 68.9 Fri 9:30 P2-OG4

Resonant Elastic X-ray Scattering (REXS) from the helical phase in Cu_2OSeO_3 at VEKMAG — •Simon Pöllath[1], Chen Luo[1], Martin Schön[1], Florin Radu[2], Hanjo Ryll[2], and Christian Back[1] — [1]Universität Regensburg Institut für Experimentelle und Angewandte Physik, Regensburg, Deutschland — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Deutschland

We report successful Resonant Elastic X-ray Scattering (REXS) experiments at the BESSY II PM2 VEKMAG beamline. We investigate a single crystalline Cu_2OSeO_3 sample grown by the chemical vapor transport method. The multiferroic insulator Cu_2OSeO_3 hosts a variety of magnetically modulated states at weak externally applied fields and below its critical Temperature. In the helical phase of the chiral magnet, the structural (001) Bragg peak shows a multiple splitting at the Cu L3 edge energy, caused by the modulated magnetic texture. Reciprocal space maps of the helical phase are obtained using a pin-hole diode. Additionally, the thermodynamic phase diagram is accessible from magnetization loops of the Bragg peak intensity. The vector magnet enables precise control of the modulation directions for future studies of conical and skyrmionic phases.

MA 68.10 Fri 9:30 P2-OG4

First-principles calculations of chiral magnetic structures in multilayers: {Rh|Co|Pt} and {Pd|Co|Pt} — •Hongying Jia, Bernd Zimmermann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

The Dzyaloshinskii-Moriya interaction (DMI), which is an antisymmetric exchange interaction, plays an important role in determining the physical properties of surfaces and interfaces of low-dimensional metallic magnets, in particular for the formation of magnetic skyrmions.

Here, we determine the magnetic interaction parameters of the magnetic multilayers of {Rh|Co|Pt} and {Pd|Co|Pt} using first-principles calculations based on the full-potential linearized augmented plane-wave (FLAPW) method, which is implemented in the `FLEUR` code [1].

We find that the 4*d* (i.e. Rh and Pd) elements induce a DMI that partly cancels the large DMI produced by the heavy-metal Pt layer. Upon variation of the thickness of the Pt layer between one and five atomic layers, we investigate the interlayer exchange coupling between the magnetic Co layers. For the {Pd|Co|Pt} system, a RKKY-type oscillatory behavior between ferromagnetic and antiferromagnetic interactions is observed. The {Rh|Co|Pt} system has a qualitatively different behavior, where frustrations in between the Co layers lead to a non-collinear order along the *c* axis.

We acknowledge financial support from the MAGicSky Horizon 2020 European Research FET Open project (#665095).

[1] For the program description see http://www.flapw.de.

MA 68.11 Fri 9:30 P2-OG4

Electric coupling of magnetic monopoles in the quantum spin-ice $Pr_2Hf_2O_7$ — •Jacob Hornung[1,2], Lars Opherden[1,2], Thomas Herrmannsdörfer[1], Alexandros Samartzis[3], Bella Lake[3,4], and Jochen Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Abteilung Quantenphänomene in neuen Materialien, HZB, Berlin, Germany — [4]Institut für Festkörperphysik, TU Berlin, Germany

We report on the magnetoelectric coupling of magnetic monopole excitations in the quantum spin-ice material $Pr_2Hf_2O_7$. We have investigated $Pr_2Hf_2O_7$ single crystals by means of dynamic permittivity and susceptibility measurements down to 100 mK. The ac susceptibility, its frequency, field, and temperature dependence, and its saturation at a finite value in the low-temperature limit indicate the formation of a quantum spin-ice state. The permittivity shows a clear correlation to the monopole density and an anomaly in magnetic fields along the local [111] direction. This hints at a charge redistribution on the magnetic monopole sites, leading to the formation of electric dipole moments.

MA 68.12 Fri 9:30 P2-OG4

NMR of the frustrated spin-ladder system Copper Sulfolane — •D. Dmytriieva[1,2], Z. T. Zhang[1,3], M. Naumann[1], J. Wosnitza[1,2], E. Wulf[4], A. Zheludev[4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [4]Neutron Scattering and Magnetism, Laboratory for Solid State Physics, ETH Zuerich, Switzerland

We present results from NMR experiments on the geometrically frustrated quantum magnet Copper Sulfolane. The ground state is a disordered spin liquid that evolves into a chiral helimagnetic phase at fields above about 4 T. NMR of ^{35}Cl nuclei on two nonequivalent sites was performed to map the local susceptibility and charge-gradient tensors close to the Cu^{2+} $S = 1/2$ moments. The field-driven transition into the helimagnetic state, probed via ^{13}C NMR, yields a drastic increase of slow spin fluctuations, manifested as a sharp maximum of the nuclear spin-lattice relaxation rate. Further, we investigated the effect of a dilute and random modification of the local frustration ratio, introduced by Br substitution on the nonmagnetic halogen site. Bulk thermodynamic measurements indicate that surprisingly small Br concentrations have a strong impact on the magnetic correlations of the helimagnetic state. In line with these findings, we observed a strong suppression of the dynamic properties with Br substitution.

MA 68.13 Fri 9:30 P2-OG4

The magnetic phase diagram of the frustrated spin-chain linarite as seen by neutron diffraction — •Leonie Heinze[1], Britta Willenberg[1,2], Jens-Uwe Hoffmann[2], Anja U. B. Wolter-Giraud[3], Kirrily C. Rule[4], Bachir Ouladdiaf[5], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Germany — [2]HZB, Berlin, Germany — [3]IFW Dresden, Dresden, Germany — [4]ANSTO, Kirrawee, Australia — [5]ILL, Grenoble, France

Linarite, $PbCuSO_4(OH)_2$, has been established as a model compound of the frustrated one-dimensional spin-1/2 chain with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor interactions [1,2]. Recently, a complex magnetic phase diagram has been reported for linarite in fields $B \| b$ axis for temperatures below 2.8 K consisting of five regions [3]. In particular, the so-called phase V has been established as an incommensurate spin density wave (SDW) phase as predicted by theory.

Here, we present an elastic neutron diffraction study on linarite of the magnetic phase diagram $B \| b$, with special emphasis on phase V. This way, the temperature and field dependence of the magnetic moment were established for temperatures down to 50 mK and fields up to 9.5 T. Further, the field and temperature dependence of the incommensurability vector **q** of the SDW in phase V was established. Finally, the nature of the phase transition IV-V being of first order was derived.

[1] A.U.B. Wolter et al., Phys. Rev. B **85**, 014407 (2012).
[2] B. Willenberg et al., Phys. Rev. Lett. **108**, 117202 (2012).
[3] B. Willenberg et al., Phys. Rev. Lett. **116**, 047202 (2016).

MA 68.14 Fri 9:30 P2-OG4

Breakdown of 3D topological order in a magnetic field — •David Reiss and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Intrinsic topological order in three dimensions represents interesting quantum phases featuring exotic elementary excitations which are spa-

tially extended and have anyonic statistics different from bosons and fermions. Such phases can exist at finite temperatures and might serve as future error-correcting quantum memories. One paradigmatic example of 3D topological order is Kitaev's toric code, which has a nonzero topological entanglement entropy at finite temperatures in contrast to the conventional 2D case. This phase can arise as effective low-energy Hamiltonian of 3D generalizations of the frustrated Kitaev honeycomb model which might describe frustrated quantum magnets like certain iridate compounds.

Here we study the robustness of the 3D toric code against quantum fluctuations by investigating the zero-temperature phase diagram of the 3D toric code in an arbitrary uniform magnetic field.

MA 68.15 Fri 9:30 P2-OG4

Monopole heat transport and residual entropy in dilute spin ice $(Dy_{1-x}Y_x)_2Ti_2O_7$ — •Daniel Brüning, Simon Scharffe, Jean-Francois Welter, Gerhard Kolland, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Deutschland

The spin ice $Dy_2Ti_2O_7$ is a geometrically frustrated spin system of corner-sharing tetrahedra with an Ising anisotropy. In the ground state configuration two spins point into and two out of each tetrahedron. The lowest excitation in spin ice systems is a single spin flip which creates a pair of 1in-3out and 3in-1out configurations on neighboring tetrahedra. Such a pair can fractionalize into two individual excitations, namely magnetic monopoles, that can propagate almost independently within the pyrochlore lattice. The entropy of $Dy_2Ti_2O_7$ reveals a plateau-like feature close to Pauling's residual entropy around 0.5 K derived originally for water ice. Ultraslow thermal equilibration prevents a distinct expansion towards lower temperature. We analyze the influence of non-magnetic yttrium dilution on the low-temperature entropy of $(Dy_{1-x}Y_x)_2Ti_2O_7$. The ultraslow thermal equilibration rapidly vanishes with increasing x, the low-temperature entropy systematically decreases, and its temperature dependence strongly increases. From our data, a non-degenerate ground state can be derived that is compared to different theoretical approaches. Additionally, we present the heat transport data of the dilution series, which give insight in the monopole transport contribution.

Supported by the DFG via CRC 1238 and project LO 818/2-1.

MA 68.16 Fri 9:30 P2-OG4

Quantum phase diagram of a bilayer Kitaev model with interlayer Heisenberg interaction — •Julian Gritsch[1], Matthias Vojta[2], and Kai Phillip Schmidt[1] — [1]FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The Kitaev honeycomb model is an extensively studied two-dimensional quantum spin model exhibiting exotic spin-liquid phases. In this project, we study two layers of the Kitaev honeycomb model coupled by a Heisenberg interaction and we focus on the regime where the isolated Kitaev models would be in the topologically ordered Abelian phase. Consequently, as a function of the interlayer coupling, there must be at least one quantum phase transition separating the topologically ordered phase from the valence bond solid present at large interlayer Heisenberg coupling where the ground state is adiabatically connected to the limit of isolated singlets. In this work we study this quantum phase transition by investigating the elementary excitations of both quantum phases.

MA 68.17 Fri 9:30 P2-OG4

Dielectric spectroscopy of doped spin ice — •Lena Klaas, C. P. Grams, J. Engelmayer, T. Lorenz, and J. Hemberger — II. Physikalisches Institut, Universität zu Köln, Cologne, Germany

Spin-ice systems have raised strong interest due to the emergence of magnetic monopoles. In $Dy_2Ti_2O_7$ the condensation of these excitations was demonstrated to undergo a first-order phase transition with a critical endpoint at T=0.36 K and $\mu_0 H$=1 T in crystallographic [111]-direction. Furthermore, magnetic monopoles also carry electric dipoles[1], making their dynamics accessible by dielectric spectroscopy. Measurements on $Dy_2Ti_2O_7$ have demonstrated unusual fluctuation dynamics above the critical temperature, a *critical speeding-up*[2]. To investigate the influence of defects on this relaxation dynamics we studied the system $(Dy_{1-x}Y_x)_2(Ti_{1-y}Zr_y)_2O_7$ with different doping levels of non-magnetic Y^{3+}- or Zr^{4+}-ions. Here, we show dielectric measurements up to frequencies of 1 MHz and down to temperatures of 0.2 K and demonstrate that critical speeding-up is observed for Y doping with x up to 10% above which the spin-ice behaviour is suppressed[3].

Supported by the Deutsche Forschungsgemeinschaft through Projects HE-3219/2-1, LO-818/2-1, and CRC 1238.

[1] D. I. Khomskii, Nat. Commun. **3**, 1-13. (2012)
[2] C. P. Grams, M. Valldor, M. Garst, and J. Hemberger, Nat. Commun. **5**, 4853. (2014)
[3] S. Scharffe, O. Breunig, V. Cho, P. Laschitzky, M. Valldor, J. F.Welter, and T. Lorenz, Phys. Rev. B **92**, 180405 (2015)

MA 68.18 Fri 9:30 P2-OG4

Nonlinear dynamics of topological spin systems — •Alexander F. Schäffer and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Germany

Topological spin systems are one of the most interesting topics both from a fundamental and application point of view.

In this contribution we present research on the nonlinear dynamics in such systems with particular emphasis on the creation and annihilation of these topologically protected objects. We investigate possible ways to drive and control skyrmionic materials via external fields such as those imparted electron beams or by material composition such as composite engineered multiferroic systems.

MA 68.19 Fri 9:30 P2-OG4

Investigation of pyrochlore spin-ice compounds with reduced lattice parameters — •T. Stöter[1,2], M. Antlauf[3], L. Opherden[2], M. Doerr[1], E. Kroke[3], T. Herrmannsdörfer[2], and J. Wosnitza[1,2] — [1]Institut für Festkörperphysik/TU Dresden — [2]Hochfeld-Magnetlabor Dresden/Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Anorganische Chemie/TU Bergakademie Freiberg

The pyrochlores $R_2X_2O_7$ (R = rare earth, X = Ti, Ge, Sn, Hf, ...) have attracted interest for their geometrical frustration from which unusual magnetic states such as spin-ice emerge. Possibly, the effective interaction comes from the competition of dipolar and exchange interaction. The strength of these competing interactions strongly depends on the distance between magnetic moments, i.e., the lattice parameters. Materials with small lattice parameters are most promising to have new interesting properties. The germanate pyrochlore $Dy_2Ge_2O_7$ possesses one of the smallest known lattice constants (a = 9.929 Å), requiring high pressures over 5 GPa for its synthesis. Additionally, we applied high-pressure synthesis of more than 10 GPa to produce pyrochlores with even smaller lattice parameters by partially substituting silicon for germanium using the multianvil technique. First results on the evolution of magnetization and susceptibility down to cryogenic temperatures will be reported.

The work is supported by DFG (SFB 1143).

MA 68.20 Fri 9:30 P2-OG4

XMCD and RXR study of the magnetic and electronic properties of Vanadium-doped TIs — •Abdul-Vakhab Tcakaev[1], Volodymyr Zabolotnyy[1], Michael Dettbarn[1], Benjamin Katter[1], Enrico Schierle[2], and Vladimir Hinkov[1] — [1]University Würzburg, Am Hubland, 97074 Würzburg — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert Einstein-Str. 15, 12489 Berlin.

Bismuth and antimony tellurides, Bi_2Te_3 and Sb_2Te_3, and the alloys based on these materials play a significant role in thermoelectric technology. Recently these materials became most famous as topological insulators (TIs) with potential applications in spintronics.

Here we report on electronic and magnetic properties of vanadium-doped thin films (10 nm) of $(Bi_{1-x}Sb_x)_2Te_3$ that were grown by molecular beam epitaxy on Si(111) substrates [1]. First-principle calculations predict that vanadium orders ferromagneticaly in Bi_2Te_3 at sufficiently high concentrations. Due to its non-destructive nature and element-specificity, Resonant X-Ray Reflectivity (RXR) in combination with x-ray magnetic circular dichroism (XMCD) is an optimal experimental tool to study magnetic and electronic properties of vanadium-doped TIs. XMCD sum rules allow to extract spin and orbital moments separately. The sum rules can be readily applied for the late 3d transition metals, but for the V complex structure of absorption edge complicates deconvolution of the individual $L_{2,3}$ contributions. To resolve this difficulty we supplement our experimental data with crystal field calculations. [1] S. Grauer *et al.*, Phys. Rev. B 92, 201304(R), 2015.

MA 68.21 Fri 9:30 P2-OG4

Absence of strong skew scattering in crystals with multisheeted Fermi surfaces — •Albert Hönemann[1], Christian

Herschbach[1], Dmitry Fedorov[2,1], Martin Gradhand[3], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]University of Bristol, Bristol, United Kingdom

Transport phenomena caused by spin-orbit coupling like spin Hall effect (SHE) [1] and anomalous Hall effect (AHE) [2] are highly interesting topics of current research. In magnetic materials both effects can be observed simultaneously to explore underlying microscopic processes.

Using an *ab initio* relativistic Kohn-Korringa-Rostoker method [3] to solve the linearized Boltzmann equation [4,5], we investigated SHE and AHE for Fe, Co and Ni crystals alloyed with transition metals or Bi. In the considered dilute alloys the dominant extrinsic contribution to both effects is caused by skew scattering [6]. Nevertheless, the strength of skew scattering in these systems is greatly reduced compared to others [7-9]. Our study attributes this to the number of sheets in the host system's Fermi surface. We also discuss different relations between SHE and AHE present in the considered alloys.

[1] Sinova *et al.*, Rev. Mod. Phys. **87**, 1213 (2015); [2] Nagaosa *et al.*, Rev. Mod. Phys. **82**, 1539 (2010); [3] Gradhand *et al.*, PRB **80**, 224413 (2009); [4] Gradhand *et al.*, PRL **104**, 186403 (2010); [5] Zimmermann *et al.*, PRB **90**, 220403(R) (2014); [6] Lowitzer *et al.*, PRL **106**, 056601 (2011); [7] Gradhand *et al.*, PRB **81**, 245109 (2010); [8] Niimi *et al.*, PRL **109**, 156602 (2012); [9] Fedorov *et al.*, PRB **88**, 085116 (2013).

MA 68.22 Fri 9:30 P2-OG4

Multi-orbital quantum antiferromagnetism in iron pnictides — effective spin couplings and quantum corrections to sublattice magnetization — •Sayandip Ghosh[1,2], Nimisha Raghuvanshi[1], Shubhajyoti Mohapatra[1], Ashish Kumar[1], and Avinash Singh[1] — [1]Department of Physics, Indian Institute of Technology, Kanpur, India 208016 — [2]Institute for Theoretical Physics, TU Dresden, D-01062 Dresden, Germany

Effective spin couplings and spin fluctuation induced quantum corrections to sublattice magnetization are obtained in the stripe AFM state of a realistic three-orbital interacting electron model involving xz, yz, and xy Fe 3d orbitals, providing insight into the multi-orbital quantum antiferromagnetism in iron pnictides. The xy orbital is found to be mainly responsible for the generation of strong ferromagnetic spin coupling in the b direction, which is critically important to fully account for the spin wave dispersion as measured in inelastic neutron scattering experiments. The ferromagnetic spin coupling is strongly suppressed as the xy band approaches half filling, and is ascribed to particle-hole exchange in the partially filled xy band. The strongest AF spin coupling in the a direction is found to be in the orbital off-diagonal sector involving the xz and xy orbitals. First order quantum corrections to sublattice magnetization are evaluated for the three orbitals, and yield a significant 37% average reduction from the Hartree-Fock value.

MA 68.23 Fri 9:30 P2-OG4

Discrete magnetic layer-by-layer switching in antiferromagnetically coupled Fe/MgO(001) superlattices — •Tobias Warnatz[1], Fridrik Magnus[2], Gunnar K. Palsson[1], Vassilios Kapaklis[1], Victor Ukleev[1,3], Reda Moubah[4], Anton Devishvili[1], Justinas Palisaitis[5], Per O. Å. Persson[5], and Björgvin Hjörvarsson[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Science Institute, University of Iceland, Reykjavik, Iceland — [3]RIKEN Center for Emergent Matter Science, Wako-shi, Japan — [4]Faculté des Sciences, Université Hassan II-Casablanca, Casablanca, Morocco — [5]Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden

Multilayer structures with an insulating spacer layer are widely studied due to their huge tunnel-magnetoresistance. However, it is less well known (and studied) that such structures can also exhibit an interlayer exchange coupling (IEC), when prepared with a high crystalline quality. Here, we present a discrete layer-by-layer magnetic switching in Fe/MgO(001) superlattices of 10 repetitions with an antiferromagnetic IEC [1]. The structures were prepared via sputtering and the crystalline quality and layering was investigated via x-ray diffraction and reflectivity, respectively as well as via transmission electron microscopy. The magnetic properties were studied via the longitudinal magneto-optical Kerr effect as well as with polarized neutron reflectivity.

[1] R. Moubah, F. Magnus, T. Warnatz, et al. Phys. Rev. Applied 5, 044011 (2016).

MA 68.24 Fri 9:30 P2-OG4

Magnetic anisotropy in Ni-PtMnGa — •Luana Caron[1], Sanjay Singh[1], Biswanath Dutta[3], Jayita Nayak[1], Sunil W. D'Souza[1], Riccardo Cabassi[2], Fulvio Bolzoni[2], Simone Fabbrici[2], Franca Albertini[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]IMEM-CNR, Parma, Italy — [3]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Magnetic shape memory in Heusler alloys attracts a great deal of interest due to their possible applications as actuators. In materials such as Ni_2MnGa[1] strong magneto crystalline anisotropy(MCA) gives rise to large magnetic field induced strain (MFIS) at low applied fields which greatly exceed those induced by temperature in non-magnetic shape memory alloys. Practical application of the large MFIS in Ni_2MnGa is hindered by a low martensitic transition temperature (T_M) and poor mechanical stability, which still remain a challenge. Within this scope, Pt substituted Ni_2MnGa alloys have been put forward as promising MFIS materials for applications. Pt substitution elevates T_M[2,3], making it possible to use these materials in room temperature applications. However, practical MFIS applications depend on T_M as well as on the large MCA. In this work we present a detailed study of the MCA in $Ni_{2-x}Pt_xMnGa$ with $x \leq 0.25$ using ab initio calculations and the singular point detection technique.[4]

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MA 68.25 Fri 9:30 P2-OG4

Probing multi-caloric effects (magneto-, baro-, and elasto-) in all-d-metal magnetic Heusler shape memory alloys — •Enke Liu[1,2], Zhiyang Wei[2], Catalina Salazar Mejia[3], Mahdiyeh Ghorbani-Zavareh[1], Zhaosheng Wang[3], Jian Liu[4], Xuekui Xi[2], Wenhong Wang[2], Guangheng Wu[2], Xixiang Zhang[5], and Claudia Felser[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Insititute of Physics, Chinese Academy of Sciences, Beijing, China. — [3]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. — [4]Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, China. — [5]King Abdullah University of Science and Technology, Thuwal, Saudi Arabia.

Caloric effects, driven by different external fields in phase transitions, are drawing increasing attention from solid-state cooling in very recent years. In this work, I will show the multi-caloric effects in a new family of magnetic shape memory alloys of all-d-metal Heusler Ni(Co)-Mn-Ti under different external fields of hydrostatic pressure, axial stress, and pulsed high magnetic field. A pressure driving efficiency of $dTt/dp = 56$ K/GPa was obtained based on the large volume change of $\Delta\omega = 2$ percent during the hydrostatic pressure, leading to a large $\Delta\omega|dTt/dp|$-1 of 0.036 percent K GPa-1. Large adiabatic temperatures of 10 K and 9 K were, respectively, observed during the axial loading and the pulsed magnetic fields. Large multi-caloric effects can be gained in the all-d-metal Heusler Ni(Co)-Mn-Ti based on the strong magnetostructural coupling.

MA 68.26 Fri 9:30 P2-OG4

Magnetic vortex core pinning and its influence on core gyration detection by STM — •Marvin Knol — II. Physikalisches Institut B, RWTH Aachen University

A magnetic vortex is the simplest non-trivial magnetic order of thin magnetic platelets with low magnetic anisotropy. The center of this chiral magnetic structure features an out of plane magnetic moment called the vortex core. We use external magnetic fields to manipulate the core within Fe islands prepared in UHV on W(110) probing it via spin polarized STM [1]. As expected, the vortex core is squeezed by an oppositely oriented out-of-plane field up to 1.6 T and shifted by an in-plane field. Moreover, we find Barkhausen like jumps [2] in the magnetization during in-plane field sweeps when the vortex core is additionally squeezed by an out-of-plane field. We attribute the jumps to pinning most likely at remaining surface adsorbates.

Micromagnetic simulations [3] reveal that the vortex core gyration is only excitable by spin polarized STM, if a resonant high frequency current is applied to a tip of canted magnetization with respect to the vortex core and the core is additionally squeezed. Thus, overcoming the pinning of the squeezed core is mandatory for dynamic experiments.

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MA 68.27 Fri 9:30 P2-OG4

Magnetic band gap opening at the Dirac point in Mn-doped bismuth telluride — •Partha S. Mandal[1], Emile Rienks[1,2,3], Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Gunther Springholz[3], Valentine Volobuiev[4,5], and Günther Bauer[3] — [1]Helmholtz-Zentrum Berlin, Albert-Einsteins-Str. 15, 12489 Berlin — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, 01069 Dresden — [3]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden — [4]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität, 4040 Linz, Austria — [5]Kharkiv Polytechnic Institute, 61002 Kharkiv, Ukraine

We have recently shown that the large (approx. 100 meV) band gap at the Dirac point of Mn-doped bismuth selenide is not of magnetic origin [1]. Here we demonstrate by angle-resolved photoemission a magnetic band gap of about 25 meV in Mn-doped bismuth telluride at 1 K. In contrast, Mn-doped bismuth selenide does not show any magnetic band gap when cooled below its Curie temperature of about 6 K. The different behavior of the two systems will be explained in the presentation.

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MA 68.28 Fri 9:30 P2-OG4

Dry-coating of magnetocaloric La(Fe,Si)13 — •Madhuri Wuppulluri, Snehajyoti Saha, Juliane Thielsch, Samuel Grasemann, and Anja Waske — IFW Dresden

La(Fe,Si)13 is a promising magnetocaloric material class with Curie transition near room temperature. However, forming regenerator beds for magnetocaloric cooling applications is challenging due to its poor mechanical strength. Pure elemental metal coating on La-Fe-Si results in higher mechanical strength, thermal conduction and reduces corrosion. Here dry coating of LaFeSi-based particles is presented and compared to that of ball milling. Magnetic and structural characterization of the coated powders is discussed.

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