MA 35: Spin dependent Transport Phenomena

Time: Wednesday 15:00–18:15 Location: H33

MA 35.1 Wed 15:00 H33

Ab initio theory of spin-orbitronics transport effects in disordered Heusler and antiferromagnetic alloys — •Libor Šmejkal[1,2], Karel Carva[2], Ilja Turek[2], and Tomáš Jungwirth[1] — [1]IoP, ASCR, Cukrovarnicka 10/112, CZ-16253 Prague, Czech Republic — [2]DCMP, Charles University, Ke Karlovu 5, CZ-12116 Prague, Czech Republic

We present unified fully relativistic tight-binding linear-muffin-tin-orbital framework for ab initio calculation of spin-orbit torque, anomalous Hall effect, and anisotropic magnetoresistance (AMR) in disordered systems based on coherent potential approximation and Bastin formula.[1-2] We compare our implementation with non-equilibrium Green functions technique, and FLEUR ab initio package.[2-3] Within the developed formalism are calculated aforementioned effects in materials promising for room temperature spin-orbitronics applications (Heusler alloys XMnSb, non-collinear antiferromagnets (AFM) XMn3, and AFM CuMnAs). Finally, the physics gathered from the first-principles calculations is discussed. For instance, the results provide a microscopic theory confirmation of the experimentally measured AMR signals in Ni-rich NiMnSb thin films.[3] AMR has a negative sign and a magnitude reaching 1% for current along the [110] direction, while a strong crystalline term yield an almost perfect cancellation of the AMR for current along the [100] direction.

[1]I. Turek et al., Phys. Rev. B 89 (2014)
[2] F. Freimuth et al., Phys. Rev. B 92 (2015)
[3] C. Ciccarelli et al., eprint arXiv:1510.03356 (2015)

MA 35.2 Wed 15:15 H33

Anomalous magnetothermopower in a metallic frustrated antiferromagnet — •Stevan Arsenijević[1,2,3], Jong Mok Ok[4], Peter Robinson[1,2], Saman Ghannadzadeh[1,2], Mikhail I. Katsnelson[2], Jun Sung Kim[4], and Nigel E. Hussey[1,2] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Toernooiveld 7, 6525ED Nijmegen, Netherlands — [2]Radboud University, Institute of Molecules and Materials, Heyendaalseweg 135, 6525, AJ Nijmegen, Netherlands — [3]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [4]Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea

We report the temperature T and magnetic field H dependence of the thermopower S of an itinerant triangular antiferromagnet $PdCrO_2$ in high magnetic fields up to 32 T. In the paramagnetic phase, the zero-field thermopower is positive with a value typical of good metals with a high carrier density. In marked contrast with typical metals, however, S decreases rapidly with increasing magnetic field, approaching zero at the maximum field scale for $T > 70$ K. We argue here that this profound change in the thermoelectric response is due to the strong interaction of the $4d$ correlated electrons of the Pd ions with the short-range spin correlations of the Cr^{3+} spins that persist beyond the Néel ordering temperature. Such (chiral) spin correlations are also believed to be responsible for the unconventional anomalous Hall effect that emerges in $PdCrO_2$ at elevated temperatures.

MA 35.3 Wed 15:30 H33

Spin currents injected electrically and thermally from highly spin polarized Co_2MnSi — •Alexander Pfeiffer[1,2], Shaojie Hu[3], Robert M. Reeve[1], Alexander Kronenberg[1], Martin Jourdan[1], Takashi Kimura[3,4], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Mainz, Germany — [3]Research Center for Quantum Nano-Spin Sciences, Kyushu University, Fukuoka, Japan — [4]Department of Physics, Kyushu University, 6-10-1 Hakozaki, Fukuoka 812-8581, Japan

We demonstrate the injection and detection of electrically and thermally generated spin currents in Co_2MnSi/Cu lateral spin valves. Devices with different electrode separations are patterned to measure the non-local signal as a function of the spacing and we determine a high spin polarization of the injected spins of 0.63 and the spin diffusion length in Cu is 500 nm. The electrically generated non-local signal is measured as a function of temperature with a maximum observed for a temperature of 80 K. The thermally generated non-local signal is measured as a function of current density and temperature in a second harmonic measurement detection scheme. We find different temperature dependences for the electrically and thermally generated non-local signals, which allows us to conclude that the temperature dependence of the signals is not just dominated by the transport in the Cu wire, but there is a crucial contribution from the different generation mechanisms, which has been largely disregarded till date. A. Pfeiffer et al., Appl. Phys. Lett. 107, 082401 (2015)

MA 35.4 Wed 15:45 H33

Room temperature operation of n-type Si spin MOSFET — •Masashi Shiraishi[1], Takayuki Tahara[1], Hayato Koike[2], Sasaki Tomoyuki[2], Yuichiro Ando[1], Makoto Kameno[1,3], Kazuyuki Tanaka[3], Shinji Miwa[3], and Yoshishige Suzuki[3] — [1]Kyoto University, Japan — [2]TDK Corporation, Japan — [3]Osaka University, Japan

Si spintronics has been collecting tremendous attention, because of its long spin lifetime and achievement of spin transport at room temperature (RT) [1,2]. In 2014, we have demonstrated the room temperature spin transport in non-degenerate Si [3], and the next milestone was set to be realization of Si spin MOSFET. In this presentation, we report on our experimental demonstration of Si spin MOSFET with high on/off ratio of spin signals. The on/off ratio is greater than 103, whereas on/off ratio in a conventional MOSFET operation is ca. 105. More importantly, the gate voltage dependence of the spin signals and the MOSFET signals are in good agreement [4]. This achievement can pave the way to a practical application of Si spin MOSFETs.

References : [1] T. Suzuki, M. Shiraishi et al., Appl. Phys. Express 4, 023003 (2011). [2] E. Shikoh, M. Shiraishi et al., Phys. Rev. Lett. 110, 127201 (2013). [3] T. Sasaki, M. Shiraishi et al., Phys. Rev. Applied 2, 034005 (2014). [4] T. Tahara, M. Shiraishi, et al., Appl. Phys. Express 8, 113004 (2015) (selected as Spotlight Paper).

MA 35.5 Wed 16:00 H33

***Ab initio* investigations on the magneto-thermoelectric properties of the Co_2TiZ (Z = Si, Ge, Sn) Heusler alloys** — •Voicu Popescu[1], Peter Kratzer[1], Diemo Ködderitzsch[2], and Hubert Ebert[2] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Department Chemie/Physikalische Chemie, Ludwig Maximilian University, 81377 Munich, Germany

The half-metallic ferromagnetic full Heusler alloys Co_2TiZ (Z = Si, Ge, Sn) have been experimentally reported to exhibit a negative Seebeck coefficient with a large absolute value for a metal. Moreover, the temperature dependence of both the resistivity and the Seebeck coefficient display a cusp at the magnetic Curie temperature, a behavior that was so far insufficiently explained by standard band structure approaches.

We investigate, by means of *ab initio* calculations performed within the framework of the full potential spin-polarized relativistic Korringa-Kohn-Rostoker Green function method, to what extent yet unexplored effects are influencing the magneto-transport properties in these systems. We account for electron correlations (GGA+U), substitutional disorder and temperature dependent scattering of the charge carriers by lattice vibrations and spin fluctuations. Among these, we show that only the last two factors are considerably improving the qualitative and quantitative agreement between the calculated and the reported experimental results.

MA 35.6 Wed 16:15 H33

Molecular Anisotropic Magnetoresistance — •Fabian Otte[1], Stefan Heinze[1], and Yuriy Mokrousov[2] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Using density functional theory calculations, we study ballistic transport in metal-benzene complexes contacted by $3d$ transition-metal wires. The electronic structure is obtained using the one-dimensional version of the full-potential linearized augmented plane-wave method as implemented in `FLEUR` [1], and is further projected onto the set of maximally-localized Wannier functions. In terms of this localized basis a tight-binding like Hamiltonian is constructed, which is treated in

a Green's function formalism to obtain the transmission function [2]. We demonstrate that the anisotropic magnetoresistance (AMR) can be enhanced by orders of magnitude with respect to conventional bulk ferromagnets in junctions containing molecules sandwiched between ferromagnetic leads [3]. We attribute this effect to the orbital-symmetry filtering of the molecules, which drastically enhance the AMR arising from spin-orbit coupling effects in the leads. We further show that such molecular anisotropic magnetoresistance can be tuned by proper choice of materials and their electronic properties.

[1] Y. Mokrousov *et al.*, Phys. Rev. B **72**, 045402 (2005).
[2] B. Hardrat, N.-P. Wang *et al.*, Phys. Rev. B **85**, 245412 (2012).
[3] F. Otte, S. Heinze, and Y. Mokrousov, arXiv:1510.06632.

15 min. break

MA 35.7 Wed 16:45 H33

Disentangling interface and bulk contributions to the anisotropic magnetoresistance in Pt/Co/Pt sandwiches — •André Kobs[1,2] and Hans Peter Oepen[1] — [1]Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany

We present the *pure* Co thickness dependence of the anisotropic magnetoresistance (AMR) in Pt(5nm)/Co(t_{Co})/Pt(3nm) sandwiches at room temperature ($0.8 \leq t_{\mathrm{Co}} \leq 50$ nm) obtained by a detailed analysis of the experimental data that were used to prove the existence of the anisotropic interface magnetoresistance (AIMR) effect [1]. The analysis was triggered by a controversy that came up in a discussion about the properties of AIMR [2,3] and demonstrates that the interfacial AMR is also present when varying the magnetization within the film plane [4]. This interfacial in-plane AMR is two times smaller than the contribution that arises when the magnetization is varied in the plane perpendicular to the current direction. This finding is in contrast to the spin Hall MR found for ferromagnetic insulator/Pt bilayers [5] revealing the existence of different MR effects at the interfaces of Pt with conducting and insulating ferromagnets. Financial support by DFG via OE 251/7-1 and SFB 668 is gratefully acknowledged. [1] A. Kobs and H. P. Oepen *et al.*, PRL **106**, 217207 (2011). [2] A. Kobs, A. Frauen, and H. P. Oepen, PRB **90**, 016401 (2014). [3] S. Y. Huang *et al.*, Phys. Rev. B **90**, 016402 (2014).[4] A. Kobs and H. P. Oepen, submitted to PRB. [5] H. Nakayama *et al.*, PRL **110**, 206601 (2013).

MA 35.8 Wed 17:00 H33

Giant spin Nernst effect induced by resonant scattering at surfaces of metallic films — •N. H. Long, P. Mavropoulos, B. Zimmermann, S. Blügel, and Y. Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The spin Nernst effect (SNE), where a transverse spin current is generated in a metal by an applied temperature gradient, is expected to open new possibilities in the field of spin caloric transport. However, due to limitations on the magnitude of temperature gradients in metals, the magnitude of SNE observed in experiments is rather small.

In this work, a new concept for engineering a giant SNE in metallic films is proposed by means of resonant impurity scattering. Extending the Fert and Levy model [1] for the spin Hall effect to the case of SNE, we found that scattering off sharp resonant impurity states leads to a strong asymmetric energy-dependence of charge and spin conductivities, as well as of the spin Hall angle. As a result, the spin Nernst conductivity (SNC) is predicted to be gigantic in a wide range of temperatures. By employing the first-principles relativistic full-potential Korringa-Kohn-Rostoker Green function method, we demonstrate that the SNC in Ag(111) films with 1% covarage of Pb or Cr adatom impurities can reach up to 200 (A/K m) at 300 K, exceeding up to one order of magnitude the values of the SNE reported so far.

We acknowledge funding from SPP 1538 SpinCaT programme and HGF-YIG Programme VH-NG-513.

[1] A. Fert and P. M. Levy, Phys. Rev. Lett. **106**, 157208 (2011).

MA 35.9 Wed 17:15 H33

Material analysis of the spin and anomalous Hall efffect in dilute magnetic alloys — •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

The spin Hall effect (SHE) [1] and anomalous Hall effect (AHE) [2] are two allied transport phenomena caused by spin-orbit coupling. For dilute alloys, the dominant contribution to these effects is given by the skew-scattering mechanism. For relatively light hosts with heavy p scatterers, this mechanism causes the so-called giant SHE, as was obtained for Bi impurities in copper [3-5].

Here, we explore the strength of the skew-scattering mechanism in various dilute alloys based on Fe, Co, and Ni crystals by means of *ab initio* calculations performed within a semiclassical approach of Refs. [6,7]. Considering the SHE and the AHE in the investigated systems, an extensive study is presented uncovering trends and underlying microscopic processes.

[1] Sinova *et al.*, Rev. Mod. Phys. **87**, 1213 (2015); [2] Nagaosa *et al.*, Rev. Mod. Phys. **82**, 1539 (2010); [3] Gradhand *et al.*, Phys. Rev. B **81**, 245109 (2010); [4] Niimi *et al.*, Phys. Rev. Lett. **109**, 156602 (2012); [5] Fedorov *et al.*, Phys. Rev. B **88**, 085116 (2013); [6] Gradhand *et al.*, Phys. Rev. Lett. **104**, 186403 (2010); [7] Zimmermann *et al.*, Phys. Rev. B **90**, 220403(R) (2014).

MA 35.10 Wed 17:30 H33

Longitudinal and transverse transport in Gadolinium at finite temperatures — •Kristina Chadova[1], Sergiy Mankovsky[1], Svitlana Polesya[1], Jan Minar[1,2], Diemo Ködderitzsch[1], and Hubert Ebert[1] — [1]Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München — [2]New Technologies-Research Centre, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic

Finite temperature effects have a pronounced impact on the transport properties of the solids. In magnetic systems, besides the scattering of conduction electrons by impurities and phonons, an additional scattering source coming from the magnetic degrees of freedom must be taken into account. A first-principle scheme which treats all these scattering effects on equal footing was recently implemented within the framework of the multiple scattering formalism [1]. Employing the alloy analogy model treated by means of the CPA, the thermal lattice vibrations and spin fluctuations are effectively taken into account. The calculation of the transport properties is based on the Kubo-Středa equation. The computational scheme is implemented using the fully relativistic KKR Green function method. As an example, we consider the temperature dependence of the longitudinal resistivity and the anomalous Hall effect in the strongly correlated metal Gd. The comparison with experiments demonstrates that the proposed numerical scheme does, indeed, provide an adequate description of the DC electronic transport coefficients at finite temperatures.

[1] H. Ebert *et al.*, PRB **91**, 165132 (2015).

MA 35.11 Wed 17:45 H33

Interfacial spin-orbit fields in ferromagnet/normal metal (FN) and ferromagnet/superconductor (FS) systems — •Petra Högl[1], Alex Matos-Abiague[2], Igor Zutic[2], and Jaroslav Fabian[1] — [1]University of Regensburg, Germany — [2]University at Buffalo, State University of New York, USA

Breaking of space-inversion symmetry at interfaces induces spin-orbit fields as an emergent phenomenon. Interfacial spin-orbit fields are believed to enable a wealth of new phenomena, not existent or fragile in the bulk, such as the tunneling anisotropic magnetoresistance (TAMR), interfacial spin-orbit torques, Skyrmions, or possible realization of topological superconductors. We theoretically investigate spin-polarized transport in FN and FS junctions in the presence of Rashba and Dresselhaus interfacial spin-orbit fields. The interplay of magnetism and spin-orbit fields leads to a marked magnetoanisotropy of the conductances. Remarkably, the anisotropy in FS systems–magnetoanisotropic Andreev reflection (MAAR)–is giant compared to TAMR, its normal-state counterpart in FN junctions [1]. We further report on the dependence of spin-flip probability currents on characteristic system parameters [2]. This work has been supported by DFG SFB 689, Int. Doct. Prog. Top. Insulators of Elite Network of Bavaria, DOE-BES Grant No. DE-SC0004890, and ONR N000141310754.

[1] P. Högl, A. Matos-Abiague, I. Žutić, J. Fabian, Phys. Rev. Lett. **115**, 116601 (2015)
[2] A. M. Kamerbeek, P. Högl, J. Fabian, T. Banerjee, Phys. Rev. Lett. **115**, 136601 (2015)

MA 35.12 Wed 18:00 H33

Investigation of ac currents and spin excitations triggered by dynamical Hall effects — •Filipe Souza Mendes Guimarães[1], Manuel dos Santos Dias[1], Antonio Tavares da Costa Jr[2],

Roberto Bechara Muniz[2], and Samir Lounis[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Universidade Federal Fluminense, Niterói, Brazil

Hall effects involving the interchange of charge, spin and orbital angular momentum may be used to excite and measure properties of nanostructures. Present theoretical descriptions of these effects ignore the dynamical character of the transport and excitation processes. We demonstrate, in a fully quantum mechanical and dynamical approach, how ferromagnetic and antiferromagnetic resonances can be excited by dynamical spin accumulations induced by the ac spin Hall effect in Fe/W bilayers and Fe/W/Fe trilayers. [1] Moreover, focusing on Co/Pt bilayers, we explore how intrinsic dynamical anomalous Hall effect, planar Hall effect and anisotropic magnetoresistance can be seen in a unified picture.

We acknowledge funding from CAPES (Brazil), Alexander von Humboldt foundation (Germany) and HGF-YIG Programme VH-NG-717 (Funsilab).

[1] F. S. M. Guimarães, S. Lounis, A. T. Costa, and R. B. Muniz, accepted in PRB: Rapid Communications, (2015). [arXiv:1509.04599]