

Institute of Molecular Physics, Polish Academy of Sciences  
Faculty of Physics, Adam Mickiewicz University

The European Conference  
PHYSICS OF MAGNETISM 2008

**ABSTRACTS**

Poznań 2008

The European Conference  
PHYSICS OF MAGNETISM 2008  
June 24-27, 2008  
Poznań Poland  
**Abstracts**

Edited by: F. Stobiecki, R. Micnas, A. Szajek, R.J. Wojciechowski

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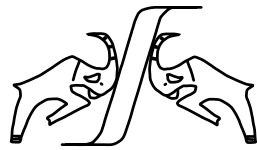
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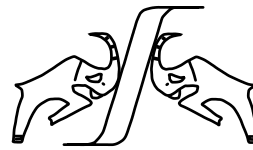
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# The European Conference PHYSICS OF MAGNETISM 2008



June 24-27, 2008  
Poznań, POLAND



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**S.3 EMERGENT BEHAVIOUR IN CORRELATED MATTER  
- COST P-16 SESSION (cont.)**

Chairman: E. Bauer

- 12<sup>15</sup>-12<sup>45</sup> **P. PRELOVŠEK** Jozef Stefan Institute, Ljubljana, Slovenia  
*Anomalous normal-state and resonant magnetic response in cuprates*
- 12<sup>45</sup>-13<sup>15</sup> **V. ZLATIC** Institute of Physics, Zagreb, Croatia  
*Enhancement of thermal transport in the degenerate periodic Anderson model*
- 13<sup>15</sup>-13<sup>45</sup> **B. COQLIN** Lab. Physique des Solides, Universite Paris-Sud, Orsay, France  
*Kondo lattice and magnetic properties in strongly correlated electron systems*
- 12<sup>15</sup>-13<sup>45</sup> **S.4 MAGNETIC STRUCTURE OF THIN FILM SYSTEMS**  
Chairman: S. Robaszkiewicz
- T. ŚLĘZAK** AGH University of Science and Technology, Kraków, Poland  
*Magnetism of ultra-thin iron films seen by the nuclear resonant scattering of synchrotron radiation*
- Short presentations: O-5-06, O-5-09, O-5-12, O-3-08

- 13<sup>45</sup>-15<sup>00</sup> lunch break and **MC meeting of COST action P-16**

**S.5 EMERGENT BEHAVIOUR IN CORRELATED MATTER  
- COST P-16 SESSION (cont.)**

Chairman: B. Idzikowski

- 15<sup>00</sup>-15<sup>30</sup> **J.C. GÓMEZ-SAL** Universidad de Cantabria, Santander, Spain  
*Overview on the physics of the complex phase diagram of CeNi<sub>1-x</sub>Cu<sub>x</sub>*
- 15<sup>30</sup>-16<sup>00</sup> **M. REIFFERS** Institute of Experimental Physics,  
Slovak Academy of Sciences, Kosice, Slovakia  
*Heat capacity of the melt-spun cubic RCu<sub>5</sub> compounds (R - heavy rare earths)*
- 16<sup>00</sup>-16<sup>30</sup> **J. SPALEK** M. Smoluchowski Institute of Physics,  
Jagiellonian University, Kraków, Poland  
*Fulde-Ferrel-Larkin-Ovchinnikov superconducting phase for paired quasiparticles with spin-dependent masses and their distinguishability*
- 16<sup>30</sup>-17<sup>00</sup> **M.C. MUÑOZ** Instituto de Ciencia de Materiales de Madrid (CSIC),  
Madrid, Spain  
*Ferromagnetic states at the o surfaces of ZnO and Co-ZnO*

15<sup>00</sup>-17<sup>00</sup>

## **S.6 MOSTLY SPIN POLARIZED TRANSPORT**

Chairman: S. Krompiewski

**M. ZWIERZYCKI** Institute of Molecular Physics, Polish Academy  
of Sciences, Poznań, Poland

*Spin polarized transport from first principles. From magnetic multilayers to  
graphene*

Short presentations: O-4-01, O-4-03, O-4-06, O-4-09, O-8-01, O-5-02

17<sup>00</sup>-17<sup>30</sup>

coffee break

17<sup>30</sup>-19<sup>00</sup>

## **ORAL SESSIONS**

### **O.1 MOSTLY CORRELATED ELECTRON SYSTEMS AND HTS**

Chairman: A. Ślebarski

Short presentations: O-1-04, O-1-02, O-1-01, O-1-06, O-1-05, O-5-07

### **O.2 MAGNETIC STRUCTURE AND DYNAMICS**

Chairman: A. Szytuła

Short presentations: O-3-09, O-3-06, O-3-02, O-5-01, O-3-01, O-1-07

19<sup>15</sup>-

## **WELCOME PARTY**

Wednesday, June 25

### S.7 REALISTIC MODELING OF MATERIALS

Chairman: J. Slonczewski

9<sup>00</sup>- 9<sup>30</sup>

**D. VOLLHARDT** Institute for Physics, University of Augsburg,  
Augsburg, Germany

*Realistic modelling of materials with strong electronic correlations*

9<sup>30</sup>-10<sup>00</sup>

**D. KHOMSKII** University of Cologne, Faculty of Mathematics and  
Natural Sciences, Köln, Germany

*Spin-driven spontaneous currents and polarization in Mott insulators:  
are electrons really localized?*

10<sup>00</sup>-10<sup>30</sup>

**M. FIEBIG** HISKP, Universität Bonn, Germany

*Magnetoelectric interaction phenomena in multiferroics and the role of  
space-time symmetry violation*

10<sup>30</sup>-11<sup>00</sup>

**C. VAN HAESSENDONCK** Katholieke Universiteit Leuven,  
Leuven, Belgium

*Resistance of domain walls induced by spatial modulation of exchange bias  
and surface roughness*

11<sup>00</sup>-11<sup>30</sup>

coffee break

11<sup>30</sup>-13<sup>30</sup>

### PARALLEL SESSIONS

#### S.8 SUPERCONDUCTIVITY, METAL-INSULATOR TRANSITION

Chairman: R. Troć

**K. BYCZUK** Institute of Theoretical Physics, Warsaw University, Warsaw,  
Poland and Institute for Physics, University of Augsburg,  
Augsburg, Germany

*Ferromagnetism and metal-insulator transitions in correlated electron systems  
with alloy disorder*

Short presentations: O-1-03, O-1-14, O-1-12, O-1-11, O-1-08, O-1-10

#### S.9 NANOSTRUCTURES

Chairman: J. Sznajd

**J. WRÓBEL** Institute of Physics, Polish Acad. of Sci., Warsaw, Poland  
*Controlling electron spin in non-magnetic nanostructures*

Short presentations: O-5-03, O-5-05, O-5-10, O-5-11, O-5-13, O-2-07

13<sup>30</sup>-15<sup>00</sup>

lunch break



- 15<sup>00</sup>-17<sup>15</sup> **S.10 SPINTRONICS**  
Chairman: K. Maki
- 15<sup>00</sup>-15<sup>30</sup> **V. CROS** CNRS, Palaiseau, France  
*Microwave generation in nanopillars induced by a spin transfer torque: a new paradigm of high frequency oscillators*
- 15<sup>30</sup>-16<sup>00</sup> **M. KLÄUI** Dept. of Physics, University of Konstanz, Konstanz, Germany  
*Interactions between domain walls and spin-polarized currents*  
Short presentations: O-6-01, O-4-08, O-4-10, O-4-04, O-3-05
- 17<sup>15</sup>-17<sup>30</sup> coffee break
- 17<sup>30</sup>-19<sup>00</sup> **POSTER SESSION I** (categories: 1, 3, 7, 8)  
Chairman: B. Buřka

## Thursday, June 26

### S.11 SPIN DYNAMICS IN NANOSCALE

Chairman: A. Ehresmann

- 9<sup>00</sup>- 9<sup>30</sup> **B. HEINRICH** Department of Physics, Simon Fraser University,  
Burnaby, Canada  
*Spin dynamics in nanoscale systems*
- 9<sup>30</sup>-10<sup>00</sup> **M. FARLE** Universität Duisburg-Essen, Fachbereich Physik,  
Experimentalphysik, Duisburg, Germany  
*Magnetic nanohybrids: status and challenges*
- 10<sup>00</sup>-10<sup>30</sup> **H. ZABEL** Lehrstuhl für Experimentalphysik/Festkörperphysik,  
Ruhr-Universität Bochum, Bochum, Germany  
*Ordering and frustration in artificial magnetic patterns*
- 10<sup>30</sup>-11<sup>00</sup> **B. RELINGHAUS** Leibniz Institute for Solid State and Materials Research  
Dresden, Dresden, Germany  
*Tailoring the properties of magnetic nanoparticles from the gas phase*
- 11<sup>00</sup>-11<sup>30</sup> coffee break
- 11<sup>30</sup>-13<sup>30</sup> **PARALLEL ORAL SESSIONS**  
**O.3 MOSTLY THEORY**  
Chairman: A. Jezierski  
Short presentations: O-4-07, O-5-04, O-3-12, O-2-03, O-2-05, O-3-04, O-3-03,  
O-2-09
- O.4 QUANTUM AND CLASSICAL MAGNETIC SYSTEMS**  
Chairman: H. Puszkarski  
Short presentations: O-2-01, O-2-02, O-3-07, O-2-04, O-3-10, O-2-06, O-2-08,  
O-2-10
- 13<sup>30</sup>-14<sup>45</sup> lunch break
- 14<sup>45</sup>-16<sup>15</sup> **POSTER SESSION II** (categories: 2, 4, 5, 6)  
Chairman: S. Lipiński
- 16<sup>20</sup>-17<sup>00</sup> TRANSPORTATION TO THE KÓRNIK PALACE
- 18<sup>00</sup>- 21<sup>30</sup> **BANQUET**
- 21<sup>45</sup> TRANSPORTATION TO HOTEL

**Friday, June 27**

**S.12 STRONGLY CORRELATED ELECTRONS**

Chairman: J.A. Morkowski

- 9<sup>00</sup>- 9<sup>30</sup> **T. MITO** Graduate School of Material Science, University of Hyogo, Japan  
*High pressure studies on Yb based strongly correlated electron systems*
- 9<sup>30</sup>-10<sup>00</sup> **R.A. COWLEY** Department of Physics, Oxford University, Oxford, U.K.  
*Dynamics of the two-dimensional Heisenberg model: experiment, computation and theory*
- 10<sup>00</sup>-10<sup>30</sup> **V. JANIŠ** Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic  
*Magnetic properties of metallic impurities with strongly correlated electrons*
- 10<sup>30</sup>-11<sup>00</sup> **O. ERIKSSON** Dept. of Physics, Uppsala University, Uppsala, Sweden  
*First principles spin-dynamics simulations, theory and applications*
- 11<sup>00</sup>-11<sup>30</sup> coffee break

**S.13 MOSTLY MAGNETIC OXIDES**

**Session in Honor of Professor Leon Kowalewski's 80-th Birthday**

Chairmen: R. Micnas, F. Stobiecki

- 11<sup>30</sup>-11<sup>45</sup> **R.J. Wojciechowski** Faculty of Physics, Adam Mickiewicz University, Poznań, Poland  
*Laudation*  
Chairman: L. Kowalewski
- 11<sup>45</sup>-12<sup>15</sup> **A.M. OLEŚ** Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland  
*Spin-orbital physics in transition metal oxides*
- 12<sup>15</sup>-12<sup>45</sup> **P. THALMEIER** Max-Planck-Institut für Chemische Physik fester Stoffe (CPFS), Dresden, Germany  
*Frustrated magnetism in vanadium oxides*
- 12<sup>45</sup>-13<sup>15</sup> **S. SANVITO** University of Dublin, Trinity College, Physics Department, Dublin, Ireland  
*Density functional theory for spin-transport*
- 13<sup>15</sup>-13<sup>45</sup> **SUMMARY and CLOSING**
- 13<sup>45</sup>-15<sup>00</sup> lunch



## INVITED LECTURES

## SWITCHING OF MOLECULAR MAGNETS

**J. Barnaś<sup>1,2</sup> and M. Misiorny<sup>1</sup>**

<sup>1</sup> Department of Physics, A. Mickiewicz University, Poznań, Poland

<sup>2</sup> Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Single-molecule magnets draw attention as potential candidates for applications in hybrid spintronics devices and information processing/storage technology. Consequently, the key question arises how to effectively manipulate the molecule in order to write a bit of information on it. One possibility of switching the molecule's moment is external magnetic field. The other one is due to the macroscopic quantum tunnelling phenomenon. However, the current-induced switching seems to be most promising for future applications.

There are, however, several challenging aspects of the current-induced manipulation of the molecule's spin. First, one can hardly control the relative orientation of the molecule's easy axis and leads' magnetizations. Second, intrinsic spin-relaxation time of the molecule significantly influences the switching parameters and also is hardly controllable.

When the energy of the lowest unoccupied orbital (LUMO) level of the molecule is sufficiently low, electronic transport takes place owing to tunneling between the electrodes and the LUMO level. The molecule's switching then occurs when the LUMO level is exchange coupled to the molecule's spin. When the energy of the LUMO level is large enough, electron tunneling to the molecule is energetically forbidden at bias voltages of interest. However, current still can flow due to higher order processes, e.g. cotunneling ones, and switching of the molecule's spin is still possible.

**OCCURRENCE OF TWO QUANTUM CRITICAL POINTS IN  
Yb<sub>2</sub>Pd<sub>2</sub>Sn OR, Yb SYSTEMS DO NOT BEHAVE MIRROR-LIKE  
TO Ce COMPOUNDS**

**E. Bauer<sup>a</sup>, R.T. Khan<sup>a</sup>, H. Michor<sup>a</sup>, T. Muramatsu<sup>b</sup>,  
T. Kanemasa<sup>b</sup>, T. Kagayama<sup>b</sup>, K. Shimizu<sup>b</sup>, Y. Aoki<sup>c</sup>,  
H. Sato<sup>c</sup>, M. Giovannini<sup>d</sup>, P. Bonville<sup>e</sup>**

<sup>a</sup>Institute of Solid State Physics, Vienna Univ. of Technology, A-1040 Wien, Austria;

<sup>b</sup>Kyokugen, Center for Quantum Science and Technology under Extreme Conditions,  
Osaka University, Toyonaka, Osaka 560-8531;

<sup>c</sup>Department of Physics, Tokyo Metropolitan University, Tokyo 192-0397, Japan;

<sup>d</sup>Dipartimento di Chimica e Chimica Industriale, Univ. of Genova, I-16146 Genova;

<sup>e</sup>CEA, Centre de Saclay, DSM/IRAMIS/SPEC 91191 Gif-sur-Yvette, France

Ce and Yb compounds have been proven as ideal playground to explore the principal features of competing electronic ground states and peculiarities associated with a quantum critical point (QCP). Here, we report on the first discovery of *two* consecutive, pressure driven QCP's. They emerge in a non-Fermi liquid environment at the origins of a dome-like, single magnetic phase in Yb<sub>2</sub>Pd<sub>2</sub>Sn at pressures  $p_{c1} \approx 1$  GPa and  $p_{c2} \approx 4$  GPa. This unique behavior of Yb compounds is supposed to result from mutually competing, pressure modified energy scales, which in case of Yb<sub>2</sub>Pd<sub>2</sub>Sn cause a sign change of the pressure dependence of the Kondo temperature  $T_K$  and magnetic ordering temperature  $T_N$ . Our finding turns out to be inimitable for Yb compounds, unlikely occurring in any Ce system. We present a variety of temperature, field and pressure dependencies of bulk properties, substantiating this conclusion.

**FERROMAGNETISM AND METAL-INSULATOR TRANSITIONS  
IN CORRELATED ELECTRON SYSTEMS WITH ALLOY  
DISORDER**

**K. Byczuk<sup>a,b</sup>**

<sup>a</sup>Center for Electronic Correlations and Magnetism, University of Augsburg,  
Augsburg, Germany

<sup>b</sup>Institute of Theoretical Physics, Warsaw University, Warsaw, Poland

Effects of an alloy disorder on ferromagnetism and metal-insulator transitions will be discussed in the frameworks of the Hubbard and the periodic Anderson models and the dynamical mean-field theory. The alloy disorder can lead to increasing of the Curie temperature, as compared to non-disordered systems, and also yield novel Mott or Kondo insulators with fractional densities of electrons.



# KONDO LATTICE AND MAGNETIC PROPERTIES IN STRONGLY CORRELATED ELECTRON SYSTEMS.

**B. Coqblin**

Laboratoire de Physique des Solides, UMR 8502, Université Paris-Sud,  
91405-Orsay, France

Recent works on the Kondo lattice and magnetism in heavy fermion systems are briefly reviewed here. First, the underscreened Kondo lattice model, which describes the case of a number of f-electrons larger than 1, gives a coexistence between the ferromagnetic order and the Kondo effect and explains the behavior of Uranium compounds, such as UTe, which present both a Kondo effect and a ferromagnetic order with a large Curie temperature of order 100K; this behavior is different from the classical Kondo lattice where there is a strong competition between the Kondo effect and the magnetic order, as observed in Cerium or Ytterbium systems. Second, the competition between Kondo, spin glass and magnetically ordered phases has been extensively studied within the Sherrington-Kirkpatrick and the Mattis models and some important results are presented here, in order to account for the peculiar phase diagrams, such as that of  $Ce(Ni, Cu)$  disordered alloys. Finally, we present a brief analysis of thermal transport properties, like the thermoelectric power and the thermal conductivity of Cerium or other anomalous rare-earth systems.

# **DYNAMICS OF THE TWO-DIMENSIONAL HEISENBERG MODEL: EXPERIMENT, COMPUTATION AND THEORY**

**R.A. Cowley**

Oxford Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, U.K.

The excitations of the 2D Heisenberg antiferromagnet,  $\text{Rb}_2\text{MnF}_4$ , have been studied using neutron scattering techniques with the MAPS spectrometer at the ISIS facility of RAL. Measurements were made of the magnetic excitations over the whole of the 2D Brillouin zone at 4 temperatures below the ordering temperature of 38K and 6 temperatures above. It was found that the excitations were well defined if their wave vectors were larger than the inverse correlation length and were overdamped if the wave vectors of the excitations were smaller than the inverse correlation length. In more detail we have compared our experimental results with the results of classical simulations and the calculations gave a very adequate description of the experimental results except at the lowest temperature where the form of the dispersion relation was correct but the energies of the excitations were in error. Nevertheless, classical simulations do provide an efficient and easily implemented methodology for modelling the excitations in Heisenberg magnets. Random phase calculations gave a good description of the energy of the excitations at low temperatures. The damping of the excitations was experimentally found to follow a  $T^2$  behaviour over all wave vector and energy scales. This is in agreement with the classical simulations but inconsistent with analytic theories of the damping for the 2D Heisenberg model and in particular does not agree with hydrodynamic behaviour or dynamic scaling. The result is similar to that found in 3D Heisenberg systems and suggests that more analytic theory is needed to explain the experimental results. For both 2D and 3D Heisenberg magnets.

# MICROWAVE GENERATION IN NANOPILLARS INDUCED BY A SPIN TRANSFER TORQUE: A NEW PARADIGM OF HIGH FREQUENCY OSCILLATORS

V. Cros<sup>1</sup>, B. Georges<sup>1</sup>, O. Boulle<sup>1</sup>, M. Darques<sup>1</sup>, J. Grollier<sup>1</sup>,  
B. Marcilhac<sup>1</sup>, C. Deranlot<sup>1</sup>, G. Faini<sup>2</sup>, J. Barnas<sup>3</sup>, A. Fert<sup>1</sup>

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<sup>2</sup> Phynano team, Laboratoire de Photonique et de Nanostructures LPN-CNRS,  
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<sup>3</sup> Faculty of Physics, A. Mickiewicz Univ., Umultowska 85, 61-614 Poznań, Poland

STNOs (Spin Transfer NanOscillators) are non-linear oscillators [1, 2]. The study of their dynamics implies new problems and new physics. The characteristics of STNOs in terms of integration and agility are very promising for applications in next generation telecommunication devices. In view of the state of the art, two main problems have first to be addressed: the large applied field and the very low emitted power.

First, I will show that in nanopillars with specific magnetic stacks, microwave emission might be generated without any applied field. This is obtained by tuning the angular dependence of the spin torque through the choice of appropriate spin dependent transport parameters. This results into a cancellation of the torque at an angle  $\varphi_c$  (different from 0 or  $\pi$ ) leading to sustain magnetization oscillations at zero (or very low) field. I will show some recent experimental results for which we have performed transport and high frequency measurements on ‘wavy’ nanopillars [3]. These experiments not only represent a good test of the theoretical models of spin transfer but also open an interesting path for spin transfer oscillators without the need of applying a magnetic field.

In the second part, I will address the question of the enhancement of the output power since the emitted power by a single STO (nanopillar or nanocontact) is far too weak (of the order of a few pW). The only solution to overcome this problem is to achieve the synchronization of an assembly of STOs, that should result in an increase the output power and a decrease the linewidth of the emitted signals [4, 5, 6]. We have recently proposed a scheme for synchronization of several STOs by connecting them in series or parallel [6]. Furthermore, in order to investigate the prerequisites to lock-in of large networks of STOs, we have studied the phase locking of a single STO with an external microwave source in various conditions of applied field and dc current. From the analysis, we can correlate the locking efficiency with the intrinsic characteristics of the STO: linewidth, emitted power, agility of the free-running oscillations. The collected information allow us to propose some optimized conditions needed for successful synchronization through the stimulated microwave current of a large amount of STOs [7].

*This work was partly supported by the French National Agency of Research ANR through the PNANO program (NANOMASER PNANO-06-067-04) and the EU network SPINSWITCH (MRTN-CT-2006-035327)*

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# **FIRST PRINCIPLES SPIN-DYNAMICS SIMULATIONS, THEORY AND APPLICATIONS**

**Olle Eriksson**

Department of Physics, Uppsala University, Uppsala, Sweden

We present a theoretical background for first principles, atomistic spin dynamic simulations. A comprehensive summary of all pertinent details for performing the simulations such as equations of motions, models for including temperature, methods of extracting data and numerical schemes for performing the simulations is given. Areas of potential applications to different magnetic questions are also discussed., e.g. spin-glass materials, ultrafast switching phenomena, diluted magnetic semiconductors as well as materials for where a macrospin model breaks down.

# MAGNETIC NANOHYBRIDS: STATUS AND CHALLENGES

**M. Farle**

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Lotharstr. 1, 47048 Duisburg, Germany

Composite magnetic nanostructure consisting of different materials offer many functionalities for applications ranging from medical diagnostics and therapy to water waste treatment and magnetic sensors. Examples for the synthesis of magnetic capsules, magnetic luminescent particles and core-shell structures with tunable magnetic properties [1,2] will be presented. Using recent work on FePt nanoparticles [3,4,5] as examples it will be demonstrated that the crystalline structure as well as the magnetic composition of objects with diameters of less than 10 nm is not uniform and that special techniques are required to identify structural relaxations at the surface and the element-specific magnetism of nanoparticles.

In collaboration with V. Salgueirino-Maceira, M. Spasova and partners from the EU research training network "SyntOrbMag".

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# **MAGNETOELECTRIC INTERACTION PHENOMENA IN MULTIFERROICS AND THE ROLE OF SPACE-TIME SYMMETRY VIOLATION**

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Recently, an enormous interest in multiferroics – compounds uniting two or more forms of primary ferroic ordering in one phase – is observed. Aside from technological aspects the interplay of different forms of (anti-) ferroic ordering is a rich source for exploring the fundamental science of phase control. Magnetic ferroelectrics may constitute the most interesting type of multiferroics because they may exhibit an unusually strong, so-called magnetoelectric (ME), coupling of magnetic and electric properties which is useful for controlling magnetic order with electric fields and vice versa. In my talk I will discuss the relation between space-time symmetry violation and the ME properties multiferroics. Two examples based on the nonlinear optical experiments done in our group will be given. On the one hand, space-time symmetry violation can lead to ferrotoroidicity, a fourth form of ferroic order characterized by long-range ordering of magnetic vortices inherently displaying the ME effect. On the other hand, space-time symmetry violation by the formation of magnetic spirals can lead to magnetically induced ferroelectricity with strong coupling of the spontaneous polarization to the magnetic order parameter.

# OVERVIEW ON THE PHYSICS OF THE COMPLEX PHASE DIAGRAM OF $\text{CeNi}_{1-x}\text{Cu}_x$

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Intrinsic disorder in Strongly Correlated Electrics Systems has been since many years a strong point to discussion, giving rise to several theories considering such disorder to understanding non Fermi liquids, magnetic clusters, etc.

During last years we have performed intensive work in order to characterise and try to understand the complex physics underlying on the  $\text{CeNi}_{1-x}\text{Cu}_x$  system. In this system, the existence of magnetic clusters has been evidenced and the ferromagnetism is established at low temperature by means of a percolative processes.

We will focus in this paper on a detailed discussion of the phase diagram, analysing the different situations depending on the composition. In this way we describe the situation of the Ce rich side, where pure AF structure are present, and no magnetic clusters are detected. Increasing the Ni content, ferromagnetism appears at very low temperature, while increasing temperature a cluster glass state appears just below the paramagnetic region. In the Ni rich side, the long range ordering has disappeared. We discuss the validity of the general scheme for the different situations, depending on the strength of the magnetic interactions involved.

A special emphasis is made on the evolution to the non magnetic Ce state found in CeNi, as well as on recent theoretical models on phase diagrams with spin glass and hysteresis cycles with steps related to the existence of magnetic clusters.

The phase diagram is also analysed from the point of view of quantum critical point or non Fermi liquid behaviour.

**RESISTANCE OF DOMAIN WALLS INDUCED BY  
SPATIAL MODULATION OF EXCHANGE BIAS  
AND SURFACE ROUGHNESS**

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We present two different approaches that can be used to artificially induce domain walls in a thin ferromagnetic film and to determine the corresponding intrinsic domain wall resistance (DWR). In a first approach, we induce domain walls in ferromagnetic Co and Fe films by bringing the Co and Fe in contact with an antiferromagnetic CoO film that is patterned into micrometer wide parallel lines to create a spatially modulated exchange bias coupling. This causes a local enhancement of the coercive field and allows us to achieve a periodic domain configuration with  $180^\circ$  Néel walls. The intrinsic DWR can be determined by using rotating magnetic fields that result in a reversible creation and annihilation of the Néel walls. For Co as well as for Fe the intrinsic DWR is positive and in agreement with models that are based on the giant magnetoresistance effect. In a second approach, a periodic configuration with  $180^\circ$  Néel walls can be created due to the spatial modulation of the roughness of an Fe film. This is achieved by depositing the Fe on top of a pattern consisting of micrometer wide parallel rough Ag lines, resulting in a local enhancement of the coercive field. In this case the determination of the intrinsic DWR becomes complicated by non-perfect anti-parallel alignment of the magnetization and uncontrolled formation of additional domain walls at submicrometer scale.



## SPIN DYNAMICS IN NANOSCALE SYSTEMS

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Research interest in magnetic nanostructures and spintronics has shifted increasingly towards dynamic properties. This is motivated by the fact that the switching time of magnetic hybrid multilayers used in mass data storage devices, magnetic random access memories (MRAM), and spintronics devices is a real technological issue. Spin relaxation processes in metallic structures will be summarized and demonstrated on several ultrathin film structures. It will be shown that the intrinsic Gilbert damping in metallic films is caused by noise in the spin orbit interaction. In ultrathin films the Gilbert damping is affected by interface electron band contributions resulting in inverse dependence on the film thickness. In multilayer films involving FM/NM/FM structures (FM-ferromagnet, NM-normal spacer) the spin dynamics becomes affected by non-local spin transport. A gyrating magnetic moment creates a spin current in surrounding normal metal layers and leads to non-local interface spin damping. Landau-Lifshitz-Gilbert (LLG) equations of motion are modified by spin pumping and spin sink effects. Time Resolved Magneto-Optical Kerr effect (TRMOKE) allows one to investigate propagation of spin currents. The stroboscopic time-resolved measurements (with the time resolution of 1 ps and sub micron spatial resolution) were carried out using Fe/Au/Fe/GaAs(001) structures which were in proximity of a co-planar transmission line driven by a CW microwave signal which was synchronized with the TRMOKE fs wide laser pulses. Spin currents generated by spin pumping at the Au/Fe interface were investigated from the ballistic to spin diffusion limit by using the Fe/Au interface as a spin detector.

Ultrathin films are often accompanied by lattice defects resulting in extrinsic contributions to magnetic relaxation processes. It will be shown that one can distinguish the intrinsic and extrinsic contributions by studying the ferromagnetic resonance (FMR) linewidth as a function of microwave frequency and angle of the magnetization with respect to the film surface. The role of extrinsic damping will be demonstrated in crystalline epitaxial GaAs/Fe/Pd(001) and MnSbNi(001) Heusler alloy structures. The Pd lattice has a large lattice mismatch with respect to Fe. The lattice strain was partially released by a self-assembled rectangular network of misfit dislocations. Stacking faults in Heusler alloys lead to bulk ordered lattice defects. It will be shown that these nano-networks of lattice defects can lead to a strong extrinsic magnetic damping which is described by two magnon scattering mechanism. The two magnon scattering can surpass significantly the intrinsic Gilbert damping. FMR measurements on Fe/Pd(001) and MnSbNi(001) Heusler alloy structures were carried out from 4 GHz to 73 GHz. The contribution of two magnon scattering to the FMR linewidth was found strongly anisotropic following the symmetry of crystallographic defects. This suggests that the scattered spin waves propagated mostly along the planes of crystallographic defects.

This work was done in collaboration with the following groups:  
Simon Fraser University: B. Heinrich, B. Kardasz, and O. Mosendz  
University Regensburg: W. Woltersdorf and Ch. Back  
University of Wuerzburg: G. Schmidt and L. Molenkamp

# MAGNETIC PROPERTIES OF METALLIC IMPURITIES WITH STRONGLY CORRELATED ELECTRONS

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We study the single impurity Anderson model in an external magnetic field. There is no exact solution for this situation and hence only approximate schemes can be employed. We demonstrate that the strong coupling regime is Kondo-like with a quasiparticle resonant peak that with magnetic field splits into two. The Kondo behavior is controlled by two Kondo scales (temperatures), one for transverse and one for longitudinal spin fluctuations. The two scales coincide at zero field, but in nonzero fields the former dominates. We show that the salient features of the spectral function in the Kondo regime can be seen already within an extended random phase approximation. To reveal the dependence of the Kondo scales on the bare electron interaction, however, one has to use a two-particle self-consistency with renormalized vertices. The Kondo temperatures in nonzero fields derived within the parquet approach are not so simply related to the density of states at the Fermi energy as in the the spin-symmetric case.

# ON THE SEARCH FOR QUANTUM CRITICALITY IN A FERROMAGNETIC SYSTEM $\text{UNi}_{1-x}\text{Co}_x\text{Si}_2$

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The orthorhombic compound  $\text{UNiSi}_2$  is a ferromagnetically ordered ( $T_C = 95$  K) Kondo lattice with rather well localized  $5f$  electrons, whereas the isostructural phase  $\text{UCoSi}_2$  exhibits a spin-fluctuation behavior. Here, we report on our systematic study of the solid solution  $\text{UNi}_{1-x}\text{Co}_x\text{Si}_2$  ( $0 \leq x \leq 1$ ) with the main focus on the alloys being close to a ferromagnetic instability, which might be expected to occur for a certain Co-content  $x_c$ . Measurements of the magnetic susceptibility, the electrical resistivity and the heat capacity were performed down to 0.35 K in magnetic fields up to 9 T on single crystals of the terminal compounds, i.e.  $\text{UNiSi}_2$  and  $\text{UCoSi}_2$ , and polycrystalline samples of the mixed alloys. The experimental data have revealed an evolution from strongly anisotropic ferromagnetism with pronounced Kondo effect, observed for the alloys with  $x < 0.98$  and being gradually suppressed with rising Co-content, to spin-glass-like states with dominant spin fluctuations seen for the samples with  $0.98 < x < 1$ . Most interestingly, clear non-Fermi liquid features manifesting the proximity to a ferromagnetic quantum critical point have been found for single-crystalline  $\text{UCoSi}_2$ . The low-temperature behavior of this pure stoichiometric system seems being governed by collective excitations of heavy quasiparticles in the vicinity of spin-density-wave transition.

**SPIN-DRIVEN SPONTANEOUS CURRENTS AND POLARIZATION  
IN MOTT INSULATORS:  
ARE ELECTRONS REALLY LOCALIZED?**

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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. We demonstrate that in general this is not true [1]: 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 as building blocks. We 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*. We discuss also some dynamic consequences of the effects discovered, such as dipole-active "ESR" transitions, rotation of electric polarization by magnetic field, and possibility to get negative refraction.

[1] arXiv: 0709.0575 (cond-mat)

# INTERACTIONS BETWEEN DOMAIN WALLS AND SPIN-POLARIZED CURRENTS

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Rather than using conventional field-induced reversal, a promising approach for switching magnetic nanostructures is current-induced domain wall motion (CIDM), where due to a spin torque effect, electrons transfer angular momentum and thereby push a domain wall [1-4]. Since this interaction is strongly dependent on the wall spin structure, we have imaged domain walls in NiFe and Cobalt nanostructures and correlate the above mentioned effects with the imaged spin structure [1-4].

We find that both domain walls types can be moved due to the spin torque effect in the direction of the electron flow [2]. In addition to wall movement, changes in the wall spin structure have been observed yielding insights into the relation between the non-adiabaticity and the damping [2].

Temperature dependent measurements of field- and current-induced wall motion have shown that the critical fields for field-induced wall motion decrease with increasing temperature, which can be attributed to thermal excitations. The critical current densities for current-induced motion though have been found to increase with increasing temperature, which is opposite to the behaviour due to thermal excitations [3], and might be due to the influence of thermally activated spin waves [3]. Using constrictions, we have been able to probe the interplay between current-induced motion and the attractive potential wells that the constrictions generate [4].

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# HIGH PRESSURE STUDIES ON Yb BASED STRONGLY CORRELATED ELECTRON SYSTEMS

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Ytterbium based compounds display a rich variety of physical properties. We have studied the pressure effect on  $\text{YbXCu}_4$  ( $X = \text{In}$  and  $\text{Cu}$ ).  $\text{YbInCu}_4$  undergoes first-order valence transitions as functions of temperature and pressure: the valence transition at 42K from the well localized ( $\text{Yb}^{3+}$ ) high-temperature state to the mixed-valence phase, and the magnetic transition around 2.4 GPa from the mixed-valence to the ferromagnetic ordered ground states. On the other hand,  $\text{YbCu}_5$  shows substantially large electronic specific heat coefficient  $\gamma \sim 550 \text{ mJ/mol K}^2$  at ambient pressure, and it approaches the localized-delocalized phase boundary with increasing pressure. We present the detailed studies of the pressure dependence on these materials by NMR/NQR (nuclear magnetic/quadrupole resonance), resistivity and magnetic susceptibility measurements.

# SPIN-ORBITAL PHYSICS IN TRANSITION METAL OXIDES

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Spin-orbital superexchange models provide a theoretical framework for describing magnetic properties and optical spectra of Mott (charge-transfer) insulators with orbital degrees of freedom [1]. Here we review recent results obtained for perovskite vanadates with  $t_{2g}$  orbital degrees of freedom. Although finite Hund's exchange suppresses spin-orbital entanglement [2] at  $T = 0$ , joint spin-orbital fluctuations are important at finite temperature. Recently we have shown that the spin-orbital superexchange model provides a satisfactory description of both orbital and magnetic transition observed in the  $RVO_3$  perovskites [3]. Thereby the orbital-lattice coupling due to the  $GdFeO_3$ -like rotations of the  $VO_6$  octahedra and the orthorhombic lattice distortion  $u$  which increase with decreasing ionic radius  $r_R$  suppress orbital fluctuations and thus modify the magnetic properties. Finally, we demonstrate that an unexpected quasi-one-dimensional hole propagation occurs in the orbital  $t$ - $J$  model with Ising-like superexchange [4], suggesting that hole self-localization is excluded in models with purely electronic interactions.

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# ANOMALOUS NORMAL-STATE AND RESONANT MAGNETIC RESPONSE IN CUPRATES

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Magnetic spin response in hole-doped cuprates, as measured by inelastic neutron scattering (INS) experiments, reveals an anomalous non-Fermi-liquid  $\omega/T$  scaling in the normal state (NS) and a dispersive resonant peak in the superconducting (SC) phase. A theory unifying the NS and SC spin dynamics based on the memory-function approach will be presented. A phenomenological damping function combined with a  $T$ -independent sum rule is used to describe the NS scaling. The emphasis is on the doping dependence of the response and on the analysis of recent INS experiments of underdoped  $\text{YBa}_2\text{CuO}_{6+x}$  (YBCO). Within the SC phase the SC gap induces a resonant mode, which shows an hour-glass-like dispersion at intermediate doping and a spin-wave dispersion at higher energies at low doping. The intensity and position of the resonant peak will be analysed in relation with the NS response. Existence of resonant mode in heavily underdoped YBCO and electron-doped cuprates will be also discussed.



## HEAT CAPACITY OF THE MELT-SPUN CUBIC $RECu_5$ COMPOUNDS ( $RE$ - HEAVY RARE EARTHS)

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Very few experimental data on physical properties and crystalline electric field (CEF) are available for the cubic intermetallic compounds of the  $RECu_5$  ( $RE$  - heavy rare earths) series, because of the difficulty in obtaining single phase samples, due to the proximity of the congruently melting  $RECu_5$  phase. Previously we have studied the electron-quasiparticle interaction (EQI) by point-contact spectroscopy. We have determined the crystalline electric field contributions to EQI. Therefore, we have performed a systematic study of the heat capacity, transport, and magnetic properties of this class of compounds. The polycrystalline samples have been prepared in ribbon shape by low temperature melt-spun and subsequent annealing. We have performed the heat capacity measurements by commercial device PPMS of QUANTUM DESIGN in the applied magnetic field up to 9 T and in the temperature range 0.4 - 300 K. We have observed the phase transition into the magnetic ordered states. First we observed the magnetic ordering in  $TmCu_5$  at 1.2 K. We determine the magnetic contribution and entropy in all compounds.

# DENSITY FUNCTIONAL THEORY FOR SPIN-TRANSPORT

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Density functional theory has revolutionarized our way to do materials science and it is now a fundamental asset for research in Physics, Chemistry, Biology and Nanoscience. This is mainly due to a combination of conceptual simplicity, rigorous theoretical foundation and efficient numerical algorithms. The Smeagol [1,2] project ([www.smeagol.tcd.ie](http://www.smeagol.tcd.ie)) has the ambitious goal of setting the same revolution in the field of ab initio quantum transport.

In this talk I will present our recent results for the bias-dependent transport of various spin-devices. I will first start from Fe/MgO (001) tunnel junctions and demonstrate how the magnetoresistance depends on the presence of resonant tunneling through surface states, how it is affected by bias and how it is reduced by FeO allowing at the interfaces. I will then move to discuss spin-effects in organic materials, and demonstrate that molecules offer the unique possibility to engineer the magneto-transport response of spin-valves. Finally I will present some very recent results on electron transport across Mn<sub>12</sub> magnetic molecules and demonstrate that the magnetic state of the molecule can be inferred by a detailed analysis of the I-V characteristics.

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# FERROMAGNETIC STATES AT THE O SURFACES OF ZnO AND Co-ZnO

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The nature of the observed high-temperature ferromagnetism (FM) in dilute magnetic oxides remains controversial since FM is strongly dependent on the preparation conditions. Ferromagnetic order is mainly observed in low-dimensional structures, with multiple surfaces and interfaces. Even more important, ZnO doped by non-magnetic elements and undoped films and nanoparticles are ferromagnetic.

We present a first-principles study of the local magnetic order at the (0001) and (000-1) Oxygen surfaces of wurzite Co-doped ZnO, which shows that the presence of the surface enhances the spin polarization induced by Co atoms. Substitutional Co ions develop large magnetic moments,  $\sim 3\mu_B$ , and induce local spin polarization at the neighbouring Oxygens. The induced magnetic moments are three times larger at the surface than at the bulk, and even for an antiferromagnetic alignment of Co atoms there is an uncompensated ferromagnetic contribution from the surface. Moreover, even in the absence of magnetic ions, a robust ferromagnetic state is predicted for the O-terminated (0001) surface, due to the occurrence of  $p$ -holes in the valence band of the oxide.  $p$ -holes mainly reside in the minority spin orbitals perpendicular to the surface and therefore, the magnetic charge distribution is highly anisotropic. Thus, besides the indirect magnetic interaction between Co atoms, low-dimensional structures of Co-doped ZnO may present additional spin polarization associated to uncompensated local Oxygen charge. This result is a general phenomena occurring in simple oxides when local charge compensation is violated.

## **TAILORING THE PROPERTIES OF MAGNETIC NANOPARTICLES FROM THE GAS PHASE**

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To a largely growing extend, the physical properties of advanced functional materials are tailored by controlling their size and/or the size of their constituents on the nanometer scale. Inert gas condensation in combination with size fractionation and in-flight thermal annealing has proven to allow for the preparation of very clean nanoparticles, since no chemical additions are involved in the synthesis process. The method provides substantial control over the particle morphology and crystal structure and thereby over the particles' physical properties. In the present talk, the versatility of this method is highlighted with some examples of our recent work which comprises

- (i) the investigation of the  $L1_0$  ordering kinetics in FePt nanoparticles close to the stoichiometric composition [1],
- (ii) the potential and challenges of using bio-templates for the regular arrangement of nanoparticles from the gas phase on a substrate [2],
- (iii) the tailoring of both the diameter and the number of walls in catalytically grown carbon nanotubes [3], and
- (iv) the possibility to control the size and the density of pinning centers for flux vortices in thin film high temperature superconductors towards an improvement of the critical current density.

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# MAGNETISM OF ULTRA-THIN IRON FILMS SEEN BY THE NUCLEAR RESONANT SCATTERING OF SYNCHROTRON RADIATION

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Conversion electron Mössbauer spectroscopy proved in the past to be very useful in studying surface and ultrathin film magnetism with monolayer resolution. Twenty years later, its time-domain analogue, the nuclear resonant scattering (NRS) of synchrotron radiation, showed up to be by orders of magnitude faster and more efficient. It will be shown how the isotopic sensitivity of NRS, combined with the <sup>57</sup>Fe probe layer concept, was explored to study influence of the interlayer exchange coupling to FeAu monoatomic superlattices on the magnetic properties of the iron monolayer on Au(001). In the second example, combination of UHV conditions and the high brilliance of the third generation synchrotron source is used to probe the evolution of spin structure in epitaxial Fe films on W(110) via the accumulation of high quality time spectra directly during the <sup>57</sup>Fe film growth. In this way the scenario of the in-plane spin reorientation transition (SRT) occurring for Fe/W(110) system could be followed. The analysis of NRS data clearly shows that the SRT consists in the formation of the unexpected, non-collinear magnetic structure which mimics the planar domain wall.

# ELECTRONIC MECHANISM OF CONDUCTANCE AND SPIN-TRANSFER TORQUE IN MAGNETIC TUNNELING JUNCTIONS

**John Slonczewski**

IBM Research Division, USA

The reading of stored information by means of magnetic tunneling junctions (MTJs) having composition FeCoB/MgO/FeCoB lies at the cutting edge of commercial magnetic storage technology. Also, both reading and writing with such junctions dominate advanced laboratory exploration of magnetic random access memory. I will show how a coherent theory explains the results of experimental measurements of magnetoresistance and current-driven spin transfer torque.

The torque measurements, performed by an IBM/Cornell collaboration, use the method of spin-transfer-excited ferromagnetic resonance. It measures well spin-transfer torque versus angle without requiring large-amplitude excitation of the free magnet. My theory mutually relating the torque to magnetoresistance requires little mathematics and no computation. It expresses both differential conductance and differential in-plane torque together in terms of one set of 4 voltage-dependent parameters which embrace both elastic and inelastic tunneling terms. It explains quantitatively why the anti-parallel differential conductance  $G_{\text{ap}}$  increases strongly with voltage  $V$ , while the corresponding torque effect is constant, for  $|V| < 400$  mV. A qualitative argument explains how inelastic tunneling due to Coulomb correlations may explain this voltage-dependence of  $G_{\text{ap}}$ .

**FULDE-FERREL-LARKIN-OVCHINNIKOV  
SUPERCONDUCTING PHASE FOR PAIRED QUASIPARTICLES  
WITH SPIN-DEPENDENT MASSES AND THEIR  
DISTINGUISHABILITY**

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Spin dependence of quasiparticle mass has been observed recently in CeCoIn<sub>5</sub> and other systems. It emerges from strong electronic correlations in a magnetically polarized state and was predicted earlier. Additionally, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase has also been discovered in CeCoIn<sub>5</sub> and therefore, the question arises as to what extent these two basic phenomena are interconnected, as it appears in theory. Here we show that the appearance of the spin-split masses essentially extends the regime of temperature and applied magnetic field, in which FFLO state is stable, and thus, it is claimed to be very important for the phase detectability. Furthermore, in the situation when the value of the spin quantum number  $\sigma = \pm 1$  differentiates masses of the particles, the fundamental question is to what extent the two mutually bound particles are indistinguishable quantum mechanically? By considering first the Cooper-pair state we show explicitly that the antisymmetry of the spin-pair wave function in the ground state may be broken when the magnetic field is applied.

# QUANTUM CRITICALITY IN SLIGHTLY Ir- AND Co-DOPED $\text{YbRh}_2\text{Si}_2$

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The heavy fermion compound  $\text{YbRh}_2\text{Si}_2$  shows antiferromagnetic (AFM) order below  $T_N = 70\text{mK}$ . It can be suppressed by a critical magnetic field  $B_c = 0.05\text{T}$  where a quantum critical point (QCP) is approached. Recent results point to the presence of multiple vanishing energy scales,  $T_N(B)$ ,  $T_{LFL}(B)$  and  $T^*(B)$ , at the magnetic-field-driven QCP. These scales can directly be observed in thermodynamic, transport and magnetic measurements, among them the dc-magnetization  $M$ , the AC susceptibility  $\chi$  and the resistivity  $\rho$  versus the magnetic field  $B$ . Slight doping with isoelectronic Co as well as with Ir on the Rh site leads to a volume change, which tunes the strength of the magnetic interaction; this shifts the  $T_N(B)$  line in the  $T - B$  phase diagram without introducing much disorder in the single crystals. However, little is known about the behavior of the  $T^*(B)$  line in the doped compounds. We present a systematic analysis of the  $M$ ,  $\chi$  and  $\rho$  measurements for the stoichiometric, Co- (7%) and Ir-doped (6%) samples to observe whether the two energy scales are still approaching zero at the same point in the doped compounds. These surprising results provide new information about the nature of the AFM state and the character of the quantum critical fluctuations at the QCP.



# FRUSTRATED MAGNETISM IN VANADIUM OXIDES

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In magnetic compounds competing exchange interactions or their geometric frustration tend to suppress long range order by enhancing the effect of quantum fluctuations. This may even result in formation of spin liquid or exotic hidden order ground states.

A prime example is the 2D square lattice frustrated  $J_1$ - $J_2$  Heisenberg antiferromagnet [1]. Various quasi-2D layered vanadium oxide compounds have now been found which are described by this model. We discuss its basic thermodynamic, high-field and magnetocaloric properties and its phase diagram. We use both analytical and numerical exact diagonalisation methods for finite clusters. It is found that high field magnetisation is strongly nonlinear close to the spin nematic hidden order phase.

The geometrically frustrated vanadium oxide  $\text{LiV}_2\text{O}_4$  is the first example of a 3d heavy fermion compound. We show that geometric frustration leads to nearly critical low energy spin fluctuations in a large part of momentum space [2], contrary to common magnets. They lead to a large mass renormalisation and heavy fermion characteristics. Furthermore, within self consistent renormalisation theory we explain the momentum and temperature dependence of low energy magnetic response from inelastic neutron scattering. In addition the NMR results will be discussed.

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# REALISTIC MODELLING OF MATERIALS WITH STRONG ELECTRONIC CORRELATIONS

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Various electronic and structural properties of materials with strongly correlated electrons will be discussed and explained which were computed within LDA+DMFT, a combination of ab initio band structure methods and the dynamical mean-field theory. In particular, I will present recent results on (i) the correlated band structure of the charge-transfer insulator NiO, (ii) the magnetic moment collapse-driven Mott transition in MnO, (iii) the correlation-induced structural relaxation in the paramagnetic Jahn-Teller system  $\text{KCuF}_3$ , and (iv) kinks in the effective dispersion of correlated electron materials such as  $\text{SrVO}_3$ .

# CONTROLLING ELECTRON SPIN IN NON-MAGNETIC NANOSTRUCTURES

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Spin-related degrees of freedom are already applied in data storage technology, and semiconductor based spintronic devices have the potential to outperform conventional electronic and communication systems. It is essential, however, to develop methods for creation and detection of coherent carriers with polarized internal magnetic moments in non-magnetic matrix of conventional semiconductors. In this contribution I review the results of our recent theoretical and experimental works devoted to controlling the electron spins by spin-orbit interaction and by application of local magnetic fields in semiconductor devices of reduced dimensionality. First, I will focus on the influence of bulk inversion asymmetry on model spin field effect transistor and show that the conductance depends significantly on subband index and on the crystallographic orientation of the GaAs and InAs device channel.

Next, I will present the experimental data obtained for GaAs/GaAlAs quantum wires of length  $L=0.6, 10$  and  $15$  micrometers. Results confirmed that the so-called "0.7 anomaly" is related to spontaneous spin polarization of one-dimensional electron gas and that this effect is very robust against the disorder. Furthermore, I will describe the new method of the g-factor determination for such quantum wires which is based on the splitting of the transmission vs width oscillations observed when the in-plane external magnetic field is applied.

Finally, I will consider theoretically the asymmetric redistribution of spins across the width of GaAs and GaN quantum wires, which may be induced by the external in-plane magnetic field gradient of  $10^6$  T/m. This study is motivated by our recent experimental work on the electronic spin separator based on the Stern-Gerlach effect. The analysis of results indicates that exchange interaction enhances strongly (up to 400 times) the effective magnetic field gradient at the center of 1D-channel. This causes the substantial spin polarization of electron liquid along the opposite wire edges for both materials, even if the bulk g-factors are assumed for GaAs and GaN.

# ORDERING AND FRUSTRATION IN ARTIFICIAL MAGNETIC PATTERNS

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We have recently investigated patterned magnetic nanostructures with different shapes and symmetries for the exploration of magnetization reversal mechanisms and of correlation effects via dipolar or exchange interaction. With the choice of materials and shapes a complete control is possible over the remanent state, the coercivity, and the type of reversal via domain wall motion or coherent rotation. Nanostructures were prepared by e-beam lithography and by ion beam modification of interfaces between ferro- and antiferromagnetic layers. The magnetic patterns investigated include magnetic stripes and dipolar arrays, triangular structures, open and closed window structures, islands, spirals, and Kagomé lattices. The magnetization reversal was studied by longitudinal vector MOKE in specular geometry as well as in Bragg MOKE geometry, using the diffraction spots from the grating for hysteresis measurements. In addition, we have carried out polarized neutron scattering (PNR) and soft x-ray resonant magnetic scattering (XRMS) to determine correlation effects during the magnetization reversal. The measurements are compared with results of micromagnetic simulation, which allows a detailed interpretation of the experimental data. An overview will be given and recent results will be discussed.

\*Work performed together with M.-S. Lee, A. Westphalen, A. Remhof, A. Schumann, K. Theis-Bröhl, B. P. Toperverg

# ENHANCEMENT OF THERMAL TRANSPORT IN THE DEGENERATE PERIODIC ANDERSON MODEL

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The low-temperature transport coefficients of the degenerate periodic  $SU(N)$  Anderson model are calculated in the limit of infinite correlation between  $f$  electrons, within the framework of dynamical mean-field theory. We establish the Fermi liquid laws, taking into account the quasiparticle damping. The latter yields a reduced value of the Lorenz number in the Wiedemann-Franz law. Our results indicate that the renormalization of the thermal conductivity and of the Seebeck coefficient can lead to a substantial enhancement of the electronic thermoelectric figure-of-merit at low temperature.

Taking into account the crystal field splitting, we discuss the low-temperature anomalies that show up in the electrical resistance of the intermetallic compounds with Cerium and Ytterbium ions, when studied as a function of pressure. Our calculations explain the sharp maximum of the coefficient of the  $T^2$ -term of the electrical resistance and the rapid variation of residual resistance found in a number of Ce and Yb intermetallics at some critical pressure. The anomalies are related to the pressure-induced variation of the Fermi volume.

**SPIN POLARIZED TRANSPORT FROM FIRST PRINCIPLES.  
FROM MAGNETIC MULTILAYERS TO GRAPHENE.**

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The flow of charge and spin currents in nanostructures can be conveniently related to their scattering properties expressed in terms of transmission and reflection coefficients. Wave function matching (WFM) is a transparent technique for calculating these quantities. In this talk we give an overview of first-principles implementation of WFM which is *i*) capable of taking into account complex electronic structures of magnetic transition metals commonly found in magnetoelectronic devices and *ii*) efficient so that disorder can be modeled using large lateral supercells. Additionally we discuss number of applications to systems ranging from metallic multilayers to graphene junctions. We concentrate on the analysis interface of scattering and the interplay between the effects related to the electronic structure mismatch and the disorder.

# CONTRIBUTIONS

## **ABSTRACT CATEGORIES**

### **1. Strongly Correlated Electrons and High Temperature Superconductivity**

Heavy fermions and Kondo systems; Charge, orbital, and multipole orderings and excitations; Quantum phase transitions; Metal-insulator transitions; Highly correlated metals and insulators; Itinerant electron magnetism; Organic conductors; Low dimensional conductors, Correlation effects in mesoscopic systems; Multiferroics.

### **2. Quantum and Classical Spin Systems**

Low dimensional quantum magnets; Frustrated magnets and spin liquids; Quantum phase transitions; Lattice effects and spin Peierls systems; Solitons and non-linear effects; Statistical mechanics of quantum and classical systems; Molecular magnetism; Quantum tunnelling and coherence; Quantum information; Organic and organo-metallic materials.

### **3. Magnetic Structure and Dynamics**

Crystal field and anisotropy; Magnetic structure and spin waves; Dynamic phenomena; Electronic structure; Magnetic interactions; Rare-earth and actinide magnetism; Transition metal alloys and compounds; Spin glasses; Random magnets; Magnonic crystals.

### **4. Spin Electronics and Magneto-Transport**

Magnetoresistance effects; Current induced magnetization reversal; Spin injection and accumulation; Spin Hall effect, Magnetic Semiconductors; Optical properties; Quantum computation.

### **5. Nano-structure, Surfaces, and Interfaces**

Surfaces and interfaces; Films, multilayers and superlattices; Exchange interaction and anisotropy; Spin dynamics, Patterned films; Nanoparticles; Nanowires and dots.

### **6. Soft and Hard Magnetic Materials**

Amorphous and nanocrystalline materials; Granular materials; Ferrites, garnets and microwave materials; Permanent magnets; Magnetization processes; Magneto-elastic and magnetostrictive materials; Modeling and simulations.

### **7. Applications**

Magnetic sensors; Ferromagnetic shape-memory materials; Actuators and magnetic drives; Magnetic refrigeration; Magnetic fluids; Magnetic separation and levitation.

### **8. Other Topics**

Biomagnetics, Magnetism in medicine, Measuring techniques and instruments, Magnetic recording and memories.



## O-1-01

### NOISE ANISOTROPY IN $YBa_2Cu_3O_{7-\delta}$ THIN FILMS

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The dependence of voltage noise on the direction of current flow with respect to c-axis of high- $T_C$   $YBa_2Cu_3O_{7-\delta}$  (YBCO) thin films has been investigated. The experiments were performed using vicinal (103)/(013) oriented YBCO films with c-axis tilted 45° from the direction normal to the substrate. Patterning of several strips along various angles to the substrate edges enabled us to force current flow in various directions with respect to the c-axis. It has been determined that noise in the normal state is isotropic while the noise intensity and its spectral form in the superconducting state depend on the direction of current flow. The difference stems from different origins of noise in both states. The noise in normal state is due to randomness in the motion of charge carriers while in the superconducting state it arises from fluctuations of density and/or velocity of moving magnetic flux vortices.

## O-1-02

### PHASE TRANSITIONS IN $TbBaCo_2O_{5.5}$ - SPECIFIC HEAT STUDIES

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Layered cobaltites ( $RBaCo_2O_{5+x}$ , R = a rare earth ion), promising for application in fuel cells, attract interest because of their intriguing properties, e.g., ionic conductivity and a metal-insulator transition not related to any magnetic ordering. For  $TbBaCo_2O_{5.5}$ , on cooling from 400 K, there are expected: metal-insulator, para-ferrimagnetic, ferri-antiferromagnetic, Co spin state ordering, and Tb short-range magnetic ordering phase transitions. The studies were aimed at determining orders and courses of these transitions, and investigating specific heat anomalies accompanying them. Specific heat of the single crystal was measured from 2 K to 395 K, in magnetic field up to 9 T. The metal-insulator transition was found to be of the first order and accompanied by an exceptionally high and narrow specific heat maximum, not affected by magnetic field. The two magnetic transitions are accompanied by slight, wide maxima, which smear in magnetic field. There is an indication that the ferrimagnetic-antiferromagnetic phase transition goes through the phase coexistence state. The Co spin state ordering transition is hardly noticeable on the temperature dependence of specific heat. The contribution of Tb ions to the specific heat was noticed as a shallow, Schottky-like, maximum near 3 K.

## O-1-03

### NEW PARADIGM FOR TRIPLET SUPERCONDUCTIVITY

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Since 1980 more than 10 or so triplet superconductors have been discovered. These are put into two different classes. Type A triplet superconductors consist of (TMTSF)<sub>2</sub>PF<sub>6</sub>, (TMTSF)<sub>2</sub>ClO<sub>4</sub>, UPt<sub>3</sub>, Sr<sub>2</sub>RuO<sub>4</sub>, PrOs<sub>4</sub>Sb<sub>12</sub> etc. These triplet superconductors are known to have extremely small spin orbit coupling energy  $E_{so} \ll \Delta$  (where  $\Delta$  is the superconducting energy gap). The superconducting order parameter is characterized by  $\mathbf{l}$  (the chiral vector) and  $\mathbf{d}$  (the spin vector) similar to the superfluid  ${}^3\text{He} - A$ . In these superconductors an Abrikosov's vortex splits into a pair of half quantum vortices (HQVs) at low temperatures (say at  $T < T_C/3$ ). Another class of triplet superconductors appear in noncentrosymmetric crystals. We call them type  $A_1$  in analogy to superfluid  ${}^3\text{He} - A_1$ . Type  $A_1$  triplet superconductors comprise CePt<sub>3</sub>Si, CeIrSi<sub>3</sub>, CeRhSi<sub>3</sub>, Li<sub>2</sub>Pt<sub>3</sub>B etc. They are characterized by an enormous spin orbit coupling energy  $\sim 10^3 K$ . In such a case the Fermi surface splits into the one for up-spin and another for down-spin in agreement with Frigeri et al. However contrary to Frigeri et al., the superconductivity resides only for one spin component (say up spin), while the other spin component remains the normal state. Also an Abrikosov's vortex cannot split into a pair of HQVs. All these triplet superconductors have Majorana fermion or the zero mode attached to an Abrikosov's vortex, of which implication deserves clearly further study.

## O-1-04

### OXYGEN VACANCY ORDER AND MAGNETIC PROPERTIES

OF  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3-d}$  ( $0 \geq d \geq 0.5$ )

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Manganese perovskites  $\text{AMnO}_{3-d}$  attain unique electronic and magnetic properties that depend on selection of the A-site ions, Mn valences, and orbital orderings, as well as the oxygen content and vacancy ordering. We have studied composition-structure-properties for new compositions  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3-d}$  ( $x \geq 0.5$ ). In addition to interesting mix-conducting and thermoelectric properties, the oxygen non-stoichiometric materials exhibit novel magnetic properties. The oxygen deficient  $x=0.5$  was found to form randomly distributed vacancies for  $3 > 3-d > 2.68$  and vacancy ordered antiferromagnetic phase for 2.50. No Sr/La ions ordering, in contrast to the  $\text{La}_{1-x}\text{Ba}_x\text{MnO}_{3-d}$  system, was found due to instability of  $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_{2.5}$  at  $T > 600^\circ\text{C}$ . Similar properties were found for  $x=0.3-0.6$ . For  $x=0.8-1$  we have discovered several oxygen vacancy ordered phases,  $3-d=2.714, 2.60, 2.55,$  and 2.50 that enhance magnetic interactions. Vacancy ordering was found to produce charge and orbital orderings, creating unique crystal and magnetic structures, some of which have been previously observed for parent compounds of HTSC  $(\text{La,Ba})\text{CuO}_{3-d}$ . These findings have revealed common vacancy ordering relationships in perovskites for which highly distorted, pyramidally-coordinated  $\text{Mn}^{3+}$  ( $\text{Cu}^{2+}$ ), and symmetric, octahedrally-coordinated  $\text{Mn}^{4+}$  ( $\text{Cu}^{3+}$ ) ions are present simultaneously.

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## O-1-05

### UNIDIRECTIONAL CHARGE INSTABILITY OF THE $d$ -WAVE RVB SUPERCONDUCTOR

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Recent scanning tunneling microscopy on  $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$  has revealed unidirectional modulation in local electronic density of states that coexists with  $d$ -wave superconductivity [1]. Motivated by this result we investigated in the previous studies the emergence of such modulations by assuming *out-of-phase*  $d$ -wave order parameters in neighboring domains [2]. Here we use a different strategy: starting from a uniform  $d$ -wave superconducting phase we study the energy cost due to imposed unidirectional defects with a vanishing pairing amplitude [3]. Both renormalized mean-field theory and variational Monte Carlo calculations within the  $t$ - $J$  model yield that the energies of inhomogeneous and uniform phases are very close to each other, especially in the presence of a tetragonal lattice distortion. This suggests that small perturbations in the microscopic Hamiltonian, might lead to inhomogeneous superconducting phases in real materials.

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## O-1-06

### COMPARISON OF VORTEX LATTICE PHASE DIAGRAM IN HIGH- $T_c$ SUPERCONDUCTORS AND IN $\text{MgB}_2$

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$\text{MgB}_2$  is, particularly concerning influence of thermal fluctuations on vortex lattice, intermediate compound between high- $T_c$  cuprates and low- $T_c$  superconductors. In the  $H - T$  phase diagram, lines that determine transitions between various phases of vortex matter to great extent may be modified by irradiation induced defects and/or by disorder due to chemical substitutions. The changes of superconducting properties of pure and carbon-substituted  $\text{MgB}_2$  single crystals prior to and after fast neutron irradiation will be presented. The observed changes in upper critical field, flux pinning and disorder induced phase transition between the Bragg glass and a highly disordered phase of vortex matter will be discussed in terms of the characteristic length scale of the defects in comparison with the coherence length and compared with effects observed in high- $T_c$  superconductors.

## O-1-07

### MAGNETIC AND ELECTRONIC PROPERTIES OF NpPdSn

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A new compound NpPdSn was prepared and studied by X-ray diffraction, magnetization, heat capacity, electrical resistivity, thermoelectric power and Hall effect measurements, performed in the temperature range 2-300 K and in magnetic field up to 14 T. The crystal structure [ZrNiAl-type (s.g.  $P62m$ ),  $a = 7.5076 \text{ \AA}$  and  $c = 4.0954 \text{ \AA}$ ] was determined from single-crystal X-ray data. The compound orders antiferromagnetically at 19 K and exhibits a Curie-Weiss behavior with  $\mu_{eff} = 2.66 \mu_B$  and  $\Theta_p = -47 \text{ K}$ . The total splitting of the neptunium  $^5I_4$  multiplet is of the order of 250 K with a doublet as the ground state. Below  $T_N$  the specific heat and the electrical resistivity are governed by electron-magnon scattering with a spin-waves spectrum typical of anisotropic antiferromagnetic systems. Above  $T_N$  the resistivity shows Kondo-like response to the applied magnetic field. Enhancement of the low-temperature specific heat ( $\gamma \sim 90 \text{ mJ/mol K}^2$ ) points to the presence of conduction electrons with high effective masses. The Seebeck coefficient exhibits a behaviour expected for scattering of conduction electrons on a narrow quasiparticle band near the Fermi energy. All the bulk properties show temperature variations similar to systems with strong electronic correlations. It suggests that NpPdSn may be classified as new Np-based antiferromagnetic Kondo lattice, one of the very few known amidst transuranium-based intermetallics.

## O-1-08

### MAGNETIC ORDER IN PrFe<sub>4</sub>As<sub>12</sub> FILLED SKUTTERUDITE

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We studied diffraction of polarized neutrons on single-crystal samples of filled skutterudite PrFe<sub>4</sub>As<sub>12</sub>. Earlier magnetization study has clearly shown ferromagnetic ordering below 18 K. Isotherms at 2 K have revealed saturated moment of  $2.3\mu_B/\text{f.u.}$  at 5.5 T and a change of easy axis from [100] to [111] above 0.5 T.

Refinement of magnetic structure from polarized neutron flipping ratios unambiguously revealed magnetic moments on both, Pr and Fe sites. Values of Pr moment at 2 K are: 1.55(4), 1.80(5) and 1.84(5) $\mu_B$ , in fields of 0.3, 2 and 6 T, respectively. Corresponding values of Fe moment are 0.19(1), 0.24(2) and 0.25(1) $\mu_B$ . These values were obtained assuming collinear ferromagnetic alignment of all moments in direction of applied field. Such assumption was drawn from the 2 K isotherms of magnetization and seems fully justified at least for fields of 2 and 6 T. When the directions of moments were allowed to vary as parameters of the model, the refinement was slightly better and values of the moment were smaller, e.g. for 6 T they were: 1.43(9) and 0.17(2) $\mu_B$ , for Pr and Fe, respectively, and aligned parallel to a bisection between [111] and [100]. Further releasing of constraints on moment angles (i.e. allowing some non-collinearity in the structure) did not improve the refinement and values of all angles converged very close to those corresponding to the collinear model.

## O-1-10

### INTRIGUING PHYSICAL PROPERTIES OF THE As-BASED FILLED SKUTTERUDITES

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First-ever single crystals of As-based filled skutterudites have been grown by a high-pressure Cd/As-flux method. Sufficiently large specimens enable a comprehensive research of their ground state. While low-temperature physical properties of LaRu<sub>4</sub>As<sub>12</sub> (superconductivity), CeRu<sub>4</sub>As<sub>12</sub> (non-Fermi-liquid behavior), PrFe<sub>4</sub>As<sub>12</sub> (complex ferromagnetic state), and PrOs<sub>4</sub>As<sub>12</sub> (multiple low- $T$  ordered phases) will be briefly reviewed, a magnetic-field-driven metal-insulator transition in CeOs<sub>4</sub>As<sub>12</sub> will be discussed in detail: Below about 130 K, the electrical resistivity increases by two orders of magnitude upon cooling to 65 mK. At the lowest temperatures ( $T < 3$  K), both the electrical resistivity and Hall resistivity are significantly suppressed by a magnetic field  $B \simeq 3$  T. Whereas these effects depend on the magnetic-field orientation, the further increase of  $B$  does not significantly affect the charge transport in CeOs<sub>4</sub>As<sub>12</sub>. Remarkable that its zero-field thermoelectric power displays a broad peak at around 2 K. Additionally, the Sommerfeld coefficient to the heat capacity as small as  $7 \text{ mJK}^{-2}\text{mol}^{-1}$  is barely influenced by  $B \leq 9$  T. Finally, a nonmagnetic or weakly magnetic ground state is inferred from the magnetization data. These experimental findings for CeOs<sub>4</sub>As<sub>12</sub> apparently point at an energy-gap formation due to a hybridization between  $4f$  electrons and conduction electrons.

## O-1-11

### SPIN-GAP PHASE IN SUPERCONDUCTOR Mo<sub>3</sub>Sb<sub>7</sub>: A SPECIFIC HEAT STUDY

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Several years ago, Bukowski and coworkers reported the superconductivity in an intermetallic Mo<sub>3</sub>Sb<sub>7</sub> [1]. Although with rather low  $T_C$  of 2.1 K the material is interesting in many aspects. According to the recent report, Mo<sub>3</sub>Sb<sub>7</sub> is a spin fluctuation superconductor [2]. Very recently, we have measured low-temperature specific heat on a polycrystalline sample and found a large Sommerfeld coefficient, which has been attributed to a narrow Mo-4d band pinned at the Fermi level. Furthermore, the electronic specific heat in the superconducting state has been ascribed to the presence of two BCS-like gaps with  $2\Delta_1 = 4.0k_B T_c$  and  $2\Delta_2 = 2.5k_B T_c$  [3]. In this contribution, we report measurements of high-temperature specific heat for Mo<sub>3</sub>Sb<sub>7</sub> and for phonon reference Ir<sub>3</sub>Ga<sub>3</sub>Ge<sub>4</sub>. As the measurements revealed Mo<sub>3</sub>Sb<sub>7</sub> exhibits a pronounced maximum around 50 K, for which the behavior may be interpreted as the opening of a spin gap [4], thus resembling very much the situation found in high-temperature superconductors.

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## O-1-12

### SUBGAP CURRENT THROUGH THE STRONGLY CORRELATED QUANTUM DOT HYBRIDIZED WITH THE NORMAL AND SUPERCONDUCTING LEADS

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We investigate the nonequilibrium transport through the strongly correlated quantum dot embedded between one metallic and one superconducting leads. For small voltage  $|V| \leq \Delta/e$  applied across the junction the charge flow is transmitted by the mechanism of Andreev reflections. Such anomalous current is sensitive to the proximity effect (spread onto the quantum dot from the superconducting electrode) and it is strongly dependent on the Coulomb interactions which prevent even occupancy of the quantum dot. We shall discuss their interplay, in particular analyzing the influence of particle-hole splitting on the Kondo resonance signified in the zero-bias differential conductance.

## O-1-14

### ENORMOUS ANISOTROPY OF THE HALL EFFECT AND MAGNETORESISTIVITY IN URhGe FERROMAGNET

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The orthorhombic URhGe is well known as intermetallic compound showing the co-existence of ferromagnetism ( $T_c=9.5$  K) and superconductivity ( $T_{sc}=0.25$  K). In this contribution, we report the measurements of the Hall effect  $R_H$  and magnetoresistance  $MR$  in a single crystalline sample of URhGe, grown by Czochralski method. The data obtained in the temperature range 2-300 K and magnetic fields up to  $\mu_0 H = 5.5$  T from two configurations ( $J//a, \mu_0 H//c$ ) and ( $J//c, \mu_0 H//b$ ) revealed very large anisotropy. For the first configuration, the Hall coefficient is positive in the whole temperature range studied.  $R_H$  reaches a pronounced maximum at 18.5 K with a value of  $41.3 \times 10^{-9} \text{m}^3/\text{C}$ .  $MR$ , however, is negative with a minimum at  $T_C$ . A more complex behaviour of  $R_H(T)$  was found for the second configuration. The Hall coefficient is positive down to 35 K, where it changes to negative values, attaining a minimum near  $T_C$ . At this temperature  $R_H$  amounts to  $-2.28 \times 10^{-9} \text{m}^3/\text{C}$ . Magnetoresistivity below 7 K is positive and reveals a complex field dependence. The presented data indicate a complexity and anisotropy of the band structure and scattering mechanisms in URhGe.

## **P-1-01**

### **STRUCTURAL, MAGNETIC AND TRANSPORT PROPERTIES OF NdBaCo<sub>2</sub>O<sub>5+x</sub> THIN FILMS DEPOSITED BY MAGNETRON SPUTTERING**

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For the first time, thin films of NdBaCo<sub>2</sub>O<sub>5+x</sub> have been deposited by RF magnetron sputtering on different substrates. The thin films deposited on single crystalline SLA(001) substrates exhibited highly textured structure with c-axis directed out-of-plane. Magnetic measurements  $M$  vs.  $T$  of three NdBaCo<sub>2</sub>O<sub>5+x</sub> / SLA(001) films, obtained at different substrate temperature and annealed in situ in oxygen, revealed successively PM-FM-AFM transitions with decrease in temperature. Their paramagnetic Curie – Weiss temperature were estimated to be in the range of  $T_C = 100$  K -116 K. Resistivity of the cobaltite thin film was measured in wide temperature range exhibiting insulating behavior over the entire range studied. The best fit was found for the VRH mechanism.

## **P-1-02**

### **LEVEL OCCUPANCY ANOMALIES IN A DOUBLE QUANTUM DOT SYSTEM**

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A double-dot system is considered in the presence of the electron intra-Coulomb  $U$  interactions within the dots and inter-Coulomb  $U_{12}$  interactions between them. For spinless electrons, when  $U_{12}$  is the only interaction, the double-dot Hamiltonian is formally equivalent to spin-degenerate Anderson impurity Hamiltonian embedded in the host metal and is solved within Hubbard approximation. The self-consistently calculated occupancy numbers of the dots levels vs. gate voltage show two kinds of non-monotonic behavior strongly deviating from usual level filling at Coulomb blockade: one when the levels have different widths and the second when a finite splitting between them is present. These non-monotonicities originate from dynamical correlations between electrons. For the spin-full case a two step procedure is applied to the Hamiltonian due to the different physical nature of inter- and intra-Coulomb interactions. The first one is non-local and pure electrostatic, thus treated in Hartree-Fock approximation. Then, intra-Coulomb interactions, as local and of many-body nature, are treated in Hubbard approximation. It is shown that in the spin-full case the level occupancy anomalies are also present and are caused by electrostatic interactions between the dots. Surprisingly, these interactions also modify the auto-correlators of the dots levels.

### **P-1-03**

#### **PERCOLATIVES OF LOW TEMPERATURE MAGNETIC PROPERTIES OF MANGANITE $\text{NbMnO}_3$**

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En experimental investigations of the magnetic properties of a lightly seft-doped insulating ceramic sample  $\text{NbMnO}_3$  are presented. The temperature and magnetic field dependences of magnetization of sample were carried out in temperature range 0.5-300K at external magnetic field up to 20kOe at different cooling regimes (ZFC and FC). The  $M_{ZFC}(T)$  and  $M_{FC}(T)$  curves exhibit two anomalies near 11 K and 60K. The anomaly typical for the phase transition to a ferromagnetically ordered state is observed at temperature near 60K. But difference in the curves  $M(T)$  in ZFC and FC regimes argues for phase separation (anti- and ferromagnetic phases) and spin cluster phase existence. Close 11K the competition between the antiferromagnetic exchange and ferromagnetic interaction results to phase transition in an antiferromagnetic or ferrimagnetic ordered state. This phase transition is shifted in the lower temperature in sample  $\text{NbMnO}_3$  dopped by small La concentration. The field dependences of magnetization in the wide range of temperatures from 0.5 K up to 300 K also were measured. They demonstrate rather ferromagnetic character with sophisticated hysteresis loops.

### **P-1-04**

#### **ELECTRON-PHONON INTERACTION AND BANDWIDTH IN THE THIN FILM $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ UNDER PRESSURE.**

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The magnetic and transport properties of the thin film  $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$  under pressure up to 2 GPa are studied. The temperature dependences of the resistivity  $\rho(T)$  were used to find the residual resistance  $\rho_0$ , Curie temperature  $T_C$  and  $\rho(T_C)$  as functions of the pressure. It was found the monotonous increase of  $T_C$  and decrease of both  $\rho_0$  and  $\rho(T_C)$  with increasing pressure. In the framework of the Holstein model with strongly correlated electrons, the diagrammatic method for the theory of magnetic and resistive properties of manganites has been developed. The  $\rho_0$ ,  $T_C$  and  $\rho(T_C)$  parameters as functions of the electron concentration  $n$ , bandwidth  $W$  and polaron binding energy  $\xi$  were calculated. A comparison of the calculated and experimental data gives the pressure dependence of the bandwidth and polaron binding energy. It was obtained that  $W$  is of order 1 eV and  $\xi \approx 0.2W$ . Under pressure  $W$  is increased and  $\xi$  is decreased. It correlates with similar results obtained in the two-site model study.



## **P-1-05**

### **A SUSCEPTIBILITY OF COMPLEX MAGNETIC SYSTEMS**

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The paramagnetic susceptibility of magnetic systems is calculated with the help of the microscopic theory of complex magnetic systems. Fluctuations of spin and charging density which determine behavior of system both in paramagnetic and in regular phases are investigated. The model of collectivized s, d, f-electrons which cooperate among themselves, with a crystal lattice and with a field of irregular electronic spin system, is considered. In this model distribution of spins is connected to spatial distribution of charges, thus fluctuations of spin density are directly connected to fluctuations of charging density. The formula for calculation of full density of a charge in magnetic system is obtained. The integrated ratio for inverse dielectric permeability is deduced. With the help of this ratio the paramagnetic susceptibility of system is determined. It is shown that inverse static susceptibility will comply with the Curie-Weiss law and Curie temperature is defined by exchange interaction in self-congruent approach. The experimental data for complex combinations of rare-earth metal are explained with formula for susceptibility. The value of dielectric permeability is negative one in the area of critical temperature. This fact allows to value susceptibility of the system in regular phase. In the combination  $Er_{1-x}Ho_xRh_4B_4$  ( $x=0.813$ ), when  $T < T_C$ ,  $\chi_{\text{theor}} = -0.8$  ( $\chi_{\text{theor}} = -0.9$ ). The new modes in spectrum of the spin waves are predicted in this model. It is shown that electron spins get out of the plane near by dislocation line, i.e. Neel's domain wall becomes Bloch's one. Thus, magnetic symmetry of the crystal varies near by dislocation center.

## **P-1-06**

### **STRUCTURE AND MAGNETIC CHARACTERIZATION OF BiFeO<sub>3</sub>/YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> BILAYERS**

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Complex perovskite oxides exhibit a rich spectrum of functional responses including superconductivity, magnetism, ferroelectricity etc. Combination of different oxides offers a new physical effects in structures composed of such systems. Multiferroic materials are both ferroelectric and magnetic. BFO is antiferromagnetic below Neel temperature  $T_N = 643$  K and ferroelectric below  $T_C = 1143$  K. Bilayers composed of multiferroic BiFeO<sub>3</sub> (BFO) layers and superconducting YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> (YBCO) layers were fabricated using high pressure sputtering on (100) LSAT substrates. X-ray diffraction analysis confirms epitaxial growth of BFO layers on YBCO buffer layers. Magnetization measurements indicate both superconducting state and weak ferromagnetism. Such epitaxial coupling could create a new way of obtaining a magnetoelectric effect between magnetization of BFO layer with screening currents in superconducting YBCO layer.

### ***P-1-07***

## **THE ROLE OF THE EXCHANGE INTERACTION IN THE ONE-DIMENSIONAL $n$ -COMPONENT HUBBARD MODEL**

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The commensurate  $p/q$ -filled  $n$ -component Hubbard chain was investigated by bosonization and high-precision density-matrix renormalization-group analysis. It was found that depending on the relation between the number of components,  $n$ , and the filling parameter,  $q$ , the system shows metallic or insulator behavior, and for special fillings bond ordered (dimerized, trimerized, tetramerized etc.) ground state develops in the insulating phase [1]. In the sense of the applied mean-field approximation one can conclude that this bond ordering is a direct consequence of the spin-exchange interaction, which plays a crucial role in the one-parameter Hubbard model — not only for infinite Coulomb repulsion, but for intermediate values as well.

[1] Phys. Rev. B **77**, 045106 (2008).

### ***P-1-08***

## **THE GROUND STATE PHASE DIAGRAM OF THE KONDO-LATTICE MODEL**

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We present the ground state ( $T=0$ ) phase diagram of the 2D and 3D (ferromagnetic) Kondo-lattice model. By using a moment conserving decoupling approach for the electronic self-energy we have calculated the inner energies of different phases explicitly. The phase diagram is then constructed by comparing the energies for the different phases. For low coupling  $J$  we find that depending on the band filling different anti-ferromagnetic configurations are favored. For larger  $J$  ferromagnetism is favored except for the half-filled band case. Furthermore, regions of phase-separation are determined by an explicit Maxwell construction.

## **P-1-09**

### **GROUND STATES OF THE SPIN-ONE-HALF FALICOV-KIMBALL MODEL WITH HUND COUPLING IN TWO DIMENSIONS**

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The spin-one-half Falicov-Kimball model with spin-dependent on-site interaction between localized ( $f$ ) and itinerant ( $d$ ) electrons is studied by small-cluster exact-diagonalization calculations and a well-controlled approximative method in two dimensions. The results obtained are used to categorize the ground-state configurations according to common features (charge and spin ordering) for all  $f$  and  $d$  electron concentrations ( $n_f$  and  $n_d$ ) on finite square lattices. It is shown that only a few configuration types form the basic structure of the charge phase diagram in the  $n_f - n_d$  plane. In particular, the largest regions of stability correspond to the phase segregated configurations, the axial striped configurations and configurations that can be considered as mixtures of chess-board configurations and the full (empty) lattice. Since the magnetic phase diagram is much richer than the charge phase diagram, the magnetic superstructures are examined only at selected values of  $f$  and  $d$  electron concentrations.

## **P-1-10**

### **THERMODYNAMICS OF THE GENERALIZED SPIN-ONE-HALF FALICOV-KIMBALL MODEL IN TWO DIMENSIONS**

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The extrapolation of small-cluster exact-diagonalization calculations and the Monte-Carlo method is used to study the spin-one-half Falicov-Kimball model extended by the spin-dependent Coulomb interaction ( $J$ ) between the localized  $f$  and itinerant  $d$  electrons as well as the on-site Coulomb interaction ( $U_{ff}$ ) between the localized  $f$  electrons. It is shown that in the symmetric case, when the chemical potential  $\mu$  equals to  $U$  (where  $U$  is the spin-independent on-site Coulomb interaction between the  $f$  and  $d$  electrons) the ground-state phase diagram of the model has an extremely simple structure that consists of only two phases, and namely, the charge-density-wave (CDW) phase (with local  $f$ -electron pairs on one of the two sublattices of a bipartite lattice) and the spin-density-wave (SDW) phase. The nonzero temperature studies of the specific heat showed that these phases persist also at finite temperatures. The critical temperature  $T_c$  for a transition from the low-temperature ordered phases to the high-temperature disordered one is calculated numerically for various values of  $J$  and  $U_{ff}$ . It was found that in the CDW area the maximum value of the critical temperature is for  $J = 0$  and in the SDW area for  $J \sim U$ .

## **P-1-11**

### **RULES OF FORMATION OF CHARGE AND MAGNETIC ORDER IN THE GENERALIZED FALICOV-KIMBALL MODEL WITH HUND COUPLING**

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Charge and spin ordering are studied on the simplest 1D and 2D square lattice within the generalized Falicov-Kimball model with Hund coupling between localized and itinerant electrons and Coulomb type repulsion between localized electrons. Using the restricted phase diagrams method (RPDM) a number of simple rules of formation of various sorts of ground state phases have been detected. It appears that both a period and a kind of arrangement of charge and spin inside a unit cell are primarily determined by the density of moving electrons. In 2D in the mixed valence regime only axial stripes (vertical or horizontal) have been found for intermediate values of the coupling constants. They are composed of ferromagnetic or antiferromagnetic chains interchanged with non-magnetic ones. And phases located along the diagonal  $\rho_f = 1 - \rho_d/2$  have the most homogenous distribution of charge. After including the Coulomb type coupling between localized electrons located on neighboring sites the distribution of phases appearing in the phase diagram changes in that way, that more periodic phases occur on the right hand side of the line  $\rho_f = \frac{1}{2}\rho_d$  and less on the left hand side of that line.

## **P-1-12**

### **MAGNETIC PHASE DIAGRAMS AND RESISTIVITY IN AN EXTENDED TWO-BAND KONDO LATTICE MODEL WITH RESPECT TO CMR-MATERIALS**

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We use an extended two-band Kondo Lattice Model (KLM) to investigate the occurrence of different (anti-)ferromagnetic phases depending on several model parameters. With regard to CMR-materials like the manganites we have added a Jahn-Teller term, direct antiferromagnetic coupling and Coulomb interaction to the KLM. The electronic properties are calculated in an interpolating self-energy approach with no restriction to classical spins. We present zero-temperature phase diagrams which show a strong influence of the important parameters (Hund's coupling, direct antiferromagnetic exchange, Jahn-Teller distortion) and of the type of Coulomb interaction (intra-band, inter-band). Some of these calculations can be extended to finite temperatures using a modified RKKY treatment. This makes the calculation self-consistent in the electronic and magnetic part. The results are in very good agreement with experimental measurements for different manganites.

## P-1-13

### MAGNETISM IN CaRuO<sub>3</sub>

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CaRuO<sub>3</sub> is a narrow-band metal with strong electronic correlations that is expected to be influenced in many respects by quantum criticality. From magnetic point of view it is considered a quantum paramagnet very close to ferromagnetic instability; nevertheless, a unified and integrated picture on magnetism of this material is still missing.

In this article we present the results of specific heat and magnetization measurements on very high quality and purity polycrystalline CaRuO<sub>3</sub> pellets at temperatures from 2 to 300 K. We found a strong logarithmic upturn of specific heat over temperature  $C/T$  below 13 K, its sensitivity to magnetic field indicates the magnetic origin of this anomaly. This observation gives further evidence of non-Fermi liquid electronic behavior in this material [1]. Magnetic susceptibility measurements have confirmed the large negative Weiss temperature (around -200 K) in this system. Low-field susceptibility measurements revealed hysteresis in ZFC and FC magnetization curves with bifurcation at 85 K, what signalizes the existence of magnetic clusters. Moreover, at lowest measuring magnetic fields of 5 and 10 mT a new feature, a broad bump has been observed around 20 K on the ZFC curves, indicating further possible ordering. The small hysteresis loop evidenced at 2 K supports the idea of ferromagnetic correlations in the system.

[1] A. Zorkovská, *et al.*, *Acta Physica Polonica A* **113**, 351, (2008).

## P-1-14

### MODELLING CHARGE, ORBITAL AND MAGNETIC ORDER IN La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>4</sub> MONOLAYER MANGANITES

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The model which describes correlated  $e_g$  electrons in doped, monolayer manganites [1] was recently studied by using correlated wave functions [2]. The effective Hamiltonian [3] takes into account: the kinetic energy of  $e_g$  electrons, the crystal-field splitting between  $x^2 - y^2$  and  $3z^2 - r^2$  orbitals, on-site Coulomb interactions, the interaction between  $e_g$  electrons and core  $S = 3/2$  spins due to  $t_{2g}$  electrons, antiferromagnetic superexchange interaction between core spins, and finally the coupling between  $e_g$  electrons and Jahn-Teller modes. We have demonstrated that this model is in general capable of reproducing the phase situation in monolayer manganites [3]. Quite recently, it was found [4] that the splitting between the occupied and empty  $e_g$  states at every site is quite large in La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>4</sub> (exceeding by far any previous estimates) and here we investigate the reasons and physical consequences of this large splitting.

[1] M. Daghofer, W. von der Linden, and A.M. Oleś, *Phys. Rev. B* **70**, 184430 (2004).

[2] D. Góra, K. Rościszewski and A.M. Oleś, *Phys. Rev. B* **60**, 7429 (1999).

[3] K. Rościszewski and A.M. Oleś, *J. Phys.: Condens. Matter* **19**, 186223 (2007).

[4] A. Gössling *et al.*, *Phys. Rev. B* **77**, 035109 (2008).

## **P-1-15**

### **REITER'S WAVEFUNCTION OF THE POLARON IN THE $t$ - $J$ MODEL WITH $t_{2g}$ ORBITAL DEGENERACY**

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Recently, using self-consistent Born approximation (SCBA), we showed that a single hole introduced into the undoped ground state of an orbital  $t$ - $J$  model with  $t_{2g}$  orbital degeneracy is mobile [1]. This striking result contradicts the naive expectations which suggest that a hole should be trapped in this Ising-like ordered ground state. However, we demonstrated in Ref. [1] that the motion of a single hole is due to the frequently neglected three-site terms and showed that this new mechanism of hole movement is fundamentally different from the hole motion via quantum fluctuations in the standard spin  $t$ - $J$  model. Though, a more detailed understanding of this novel mechanism is needed. Hence, instead of considering the Green's function as in Ref. [1] we investigate the corresponding Reiter's wavefunction [2] calculated in the SCBA. In particular, we show how the number of orbitons associated with a hole motion depends on the superexchange parameter  $J$  and compare this result to the one obtained for the spin model.

[1] M. Daghofer *et al.*, Phys. Rev. Lett. **100**, 066403 (2008).

[2] G. F. Reiter, Phys. Rev. B **49**, 1536 (1994).

## **P-1-16**

### **OPTIMIZED WANNIER FUNCTIONS FOR HUBBARD CHAIN WITH VARIABLE-RANGE HOPPING**

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One-dimensional Hubbard model (Hubbard chain) with a variable-range hopping is described within the extended Hubbard model. The Gutzwiller-ansatz approximation is used to determine the optimized single-particle (Wannier) wave functions in the correlated state. Hopping integral up to the third neighbors is taken into account and the result is compared with those for the infinite-range hopping limit. Ground state energy of the system is calculated with that making use of the rigorous Lieb-Wu solution with the optimized wave functions [1]. The evolution of the properties as a function of interatomic distance is carried out.

[1] J.Kurzyk, J.Spałek, W.Wójcik, Acta Phys. Pol. A, **111**, 603 (2007); arXiv:0706.1266 (2007).

**P-1-17**  
**CURRENTS CORRELATIONS IN THE SYSTEM OF COUPLED  
QUANTUM DOTS**

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Extensive research of the shot noise in mesoscopic systems have shown, that a negative correlation between the conducting electrons is responsible for the reduction of the shot noise below Poissonian value. However, in some cases positive correlations can arise and shot noise is enhanced much above Poissonian value. The recent theory and experiment have been focused on the sign reversal of noise cross correlations [1]. In the paper we study current noise correlations in a device composed of two large quantum dots capacitively coupled in parallel. Stationary currents, charge accumulations and polarization are calculated in the limit of sequential tunnelling. Fluctuations in the system are analyzed by means of an extended generation-recombination approach for multi-electron channels. We show that the Coulomb interactions of charges accumulated on the both quantum dots can lead to the dynamical Coulomb blockade effect. The effect can be controlled by the applied bias and the gate voltages. In the regions of the dynamical Coulomb blockade the positive noise cross correlations can induce super-Poissonian noise, while besides these regions the noise cross correlations are negative. Our theoretical results show, that the dynamical Coulomb blockade is responsible for bunching of electrons and enhancement of the current noise seen in recent experiment [1].

[1] D.T. McClure, L. DiCarlo, Y. Zhang, H.-A. Engel, C.M. Marcus, M.P. Hanson, A.C. Gossard, PRL **98**, 056801 (2007)

**P-1-18**  
**d-WAVE SUPERCONDUCTOR WITH ANDERSON IMPURITIES**  
 $T \ll T_c$

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I study the model of a  $d$ -wave superconductor interacting with finite concentration of Anderson impurities. The interaction of the impurity with conduction electrons is taken into account within the mean field slave boson approximation. I discuss the obtained phase diagram and its dependence on the main energy scales.

## **P-1-19**

### **HEAT CAPACITY OF HEAVY FERMION COMPOUND CeCu<sub>4</sub>Ga IN HIGH MAGNETIC FIELDS**

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The heat capacity in the applied magnetic field up to 9 T, susceptibility and magnetization of polycrystalline CeCu<sub>4</sub>Ga are presented. Magnetic ordering was not observed down to 2 K. For temperature  $T < 200$  K a Curie-Weiss behavior is observed giving an effective magnetic moment  $\mu_{\text{eff}} = 2.53\mu_{\text{B}}/\text{f.u.}$ . The experimental value of  $\mu_{\text{eff}}$  is close to the calculated one for a free Ce<sup>3+</sup> ion  $\mu_{\text{eff}} = g(j(j+1))^{1/2} = 2.54\mu_{\text{B}}$ , thus indicating the presence of well localized magnetic moments carried by the stable Ce<sup>3+</sup> ions. At low temperatures the electronic heat capacity coefficient  $\gamma$  value depends strongly on the temperature range used for the extrapolation and applied magnetic field. We observe a typical heavy fermion behavior with  $\gamma$  value of about 380 mJmol<sup>-1</sup>K<sup>-2</sup> obtained from extrapolation to  $T = 0$  K of the temperature range above 4 K. However, extrapolation of the lowest temperatures range yields the  $\gamma$  value of 1.1 Jmol<sup>-1</sup>K<sup>-2</sup>. The observed behavior is in a qualitative agreement with Refs. [1,2]. The effects of magnetic field on low-temperature heat capacity of CeCu<sub>4</sub>Ga are presented.

[1] E. Bauer et al., J. Magn. Magn. Mat. 69 (1987) 158

[2] E. Bauer et al., Solid State Commun. 63 (1987) 271

## **P-1-20**

### **HEAT CAPACITY STUDIES OF THE NdNi<sub>4</sub>Si COMPOUND**

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The study of the heat capacity of the intermetallic compound NdNi<sub>4</sub>Si and the influence of magnetic fields up to 4 T is presented. This compound crystallizes in the hexagonal CaCu<sub>5</sub>-type structure, space group P6/mmm. Nd atoms occupy the (1a) site, Ni(1) the 2c site and Ni(2) and Si are statistically distributed on the 3g positions. NdNi<sub>4</sub>Si is ferromagnetic with  $T_{\text{C}} = 8$  K and saturation moment of 1.5 $\mu_{\text{B}}/\text{f.u.}$  at 4.2 K (in  $H = 9$  T). The heat capacity has been analyzed considering the electronic contribution, the Schottky anomaly, and the lattice contributions in frames of the Debye model. The scheme of the energy levels created by the crystal electric field split is determined from Schottky contribution to the specific heat. Zero field heat capacity reveals a peak close to the magnetic ordering temperature. The maximum is shifting to higher temperatures with increasing magnetic fields. The ferromagnetic NdNi<sub>4</sub>Si was characterized by the electronic heat capacity coefficient  $\gamma = 85$  mJmol<sup>-1</sup>K<sup>-2</sup> and the Debye temperature  $\Theta_{\text{D}} = 325$  K.



## **P-1-21**

### **ELECTRON PHASE SEPARATIONS INVOLVING CHARGE ORDERINGS IN ITINERANT FERMION SYSTEMS**

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We study two effective models for description of charge orderings (CO) in narrow band materials: the spinless fermion model with repulsive intersite interaction and the Holstein model in the static limit. The cases of  $d$ -dimensional hypercubic lattices are investigated for arbitrary particle concentration  $n$ . The analysis is concentrated on the problem of electron phase separations and the effects of next-nearest neighbor hopping  $t_2$  on the charge ordered states in these systems. The ground state phase diagrams and the phase diagrams at finite temperatures are evaluated for several representative cases as a function of both the electron concentration  $n$  and the chemical potential  $\mu$ . The evolution of basic characteristics of the systems in the CO states with the increasing interaction and a change of  $n$  are discussed.

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## **P-1-22**

### **MAGNETIC DICHROISM, PHOTOEMISSION AND MAGNETOMETRIC STUDIES ON CeNi<sub>4</sub>B**

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The CeNi<sub>4</sub>B compound is a mixed-valence system [1,2]. It is a paramagnet with  $\mu_{\text{eff}} = 0.52\mu_B/\text{f.u.}$  and the paramagnetic Curie temperature  $\theta = -10.7$  K. In the present research we complete our previous magnetic susceptibility and x-ray photoemission (XPS) measurements with new studies by the x-ray magnetic circular dichroism (XMCD) method. The observation of the Ce- $M_{4,5}$  edges carried out with XMCD confirms the mixed-valence state deduced previously from XPS, which revealed the f-states occupancy  $n_f = 0.83$  and hybridization between the f-states and the conduction electrons  $\Delta = 85$  meV. Moreover, we report on the measurements of the Ni- $L_{2,3}$  edges, which enable verification of the Ni contribution to the magnetism of this compound.

[1] T. Toliński, A. Kowalczyk, M. Pugaczowa-Michalska, G. Chelkowska, J. Phys.: Condens. Matter 15, 1397 (2003).

[2] C. Mazumdar, Z. Hu, G. Kaindl, Physica B 259-261, 89 (1999).

## **P-1-23**

### **MAGNETIC ORDERINGS IN THE HUBBARD MODEL WITH ANISOTROPIC SPIN-EXCHANGE INTERACTIONS IN THE ZERO-BANDWIDTH LIMIT**

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We discuss the phase diagrams and thermodynamics properties of the extended Hubbard models with anisotropic intersite spin-exchange interactions ( $J_{\perp}$ ,  $J_{\parallel}$ ) in the zero-bandwidth limit. The cases of ferromagnetic ( $J_{\alpha} > 0$ ) and antiferromagnetic ( $J_{\alpha} < 0$ ) exchange couplings are considered for arbitrary electron concentration ( $0 < n < 2$ ). The analysis of these  $U - J_{\perp} - J_{\parallel}$  models has been performed for  $d$ -dimensional hypercubic lattices by means of a variational approach which treats the  $U$  term exactly. Some rigorous results derived for  $d = 1$  and  $d = \infty$  cases are also presented. Depending on the interaction parameters and  $n$  the systems are found to exhibit several various phases with uniaxial and planar magnetic orderings as well as the phase separated states and the nonordered states. The effects of intersite Coulomb interactions and external fields on the phase diagrams are also concluded.

One shows that the systems considered can exhibit very interesting multicritical behaviors, including among others bicritical, tricritical, tetracritical and critical end points. The ground state phase diagrams of the zero-bandwidth model at half filling are compared with the corresponding diagrams derived recently for the case of finite bandwidth.

## **P-1-24**

### **CHARGE ORDERINGS, SUPERCONDUCTIVITY AND PHASE SEPARATIONS IN A ZERO-BANDWIDTH EXTENDED HUBBARD MODEL**

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A simple effective model of charge ordered insulators and superconducting systems with very short coherence length is studied. The tight binding Hamiltonian consists of the effective on-site interaction  $U$ , the intersite density - density interaction  $W_{ij}$  (both: nearest - neighbor (nn) and next - nearest - neighbor (nnn) and the intersite charge exchange term  $I_{ij}$ , determining hopping of electron pairs. In the analysis of the phase diagrams and thermodynamic properties of this model we have adopted the variational approach, which treats the on-site interaction term exactly and the intersite interactions ( $W_{ij}$  and  $I_{ij}$ ) within the mean - field approximation. Within such an approach, only the particular cases, (i)  $U - W_{ij}$  ( $I_{ij} = 0$ ,  $W_{ij}$  restricted to nn) and (ii)  $U - I_{ij}$  ( $W_{ij} = 0$ ), have been studied till now. Moreover, the phase separated (PS) states have not been taken into account in those analyses.

Our investigation of the general case shows that, depending on the values of interaction parameters and electron concentration  $n$ , the system can exhibit not only several homogeneous phases: charge ordered (CO), superconducting (SS), mixed (SS/CO), nonordered (NO), but also various phase separated states (CO - NO, CO - SS, particle droplets, etc). We will also present some rigorous results obtained for the ground state at  $n = 1$  and point out the effects of intersite magnetic exchange interactions on the phase diagrams for  $0 < n < 2$  and  $U \rightarrow \infty$ .

## **P-1-25**

### **STUDY OF NI-PD SUBSTITUTION IN $\text{UNi}_x\text{Pd}_{2-x}\text{Al}_3$ SYSTEM**

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$\text{UNi}_2\text{Al}_3$  and  $\text{UPd}_2\text{Al}_3$  have the same crystal structure belonging to the space group  $P6/mmm$  and are 'isoelectronic' in the sense that Ni and Pd lie in the same column of the periodic table. These heavy fermion systems behave differently on a microscopic level as regards their magnetism, while the superconducting properties are qualitatively similar.  $\text{UPd}_2\text{Al}_3$  orders into a simple antiferromagnetic structure with a substantial magnetic moment  $\sim 0.8 \mu_B/\text{U}$  below  $T_N \sim 14.3\text{K}$  and then exhibits superconductivity below  $T_c \sim 2\text{K}$ .  $\text{UNi}_2\text{Al}_3$  enters an incommensurate spin-density-wave state with magnetic moment  $\sim 0.2 \mu_B/\text{U}$  below  $T_N \sim 4.5\text{K}$  and becomes superconducting below  $T_c \sim 1\text{K}$ . Comparative studies of the electronic structures in the two compounds may help elucidate where these differences come from. It was anticipated that only because of small differences in the band structures between the Pd and the Ni compounds is the magnetic ground state incommensurably ordered in  $\text{UNi}_2\text{Al}_3$ , while it is commensurate in  $\text{UPd}_2\text{Al}_3$ . A tuning of the electronic structure by substitution Pd with Ni and subsequent study of magnetic and electronic properties of  $\text{UNi}_x\text{Pd}_{2-x}\text{Al}_3$  system is main goal of our study performed on polycrystalline samples with  $x = 0.5$  and  $1.5$ .

## **P-1-26**

### **DESIGNING OF A ROTATION SENSOR USING MICROMAGNETIC SIMULATIONS**

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In this paper we show the good sensitivity of the Planar Hall Effect (PHE) signal which can be, together with MR measurements, a useful technique not only for the characterization of thin films but, also for building low cost rotation sensors for microcompass or contactless potentiometer applications. Measurements for field and angular dependencies of the PHE were made on Permalloy based thin films and multilayered structures. At low magnetic fields, i.e., less than 200 Oe, we observed distortions from the expected sinusoidal shape of the PHE angular dependence. In order to have a better understanding of this behaviour, micromagnetic simulations were performed for square, circular and ring-shape thin film structures used as rotation sensors. Finally, a method to improve the quality of the output signal regarding the angular dependence of the PHE voltage is presented. The resolution of the rotation sensor is better than 0.5 degrees.

## **P-1-27**

### **SPIN-GLASS BEHAVIOUR IN A METAL-ORGANIC [Co(C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>)<sub>2</sub>]<sub>n</sub> POLYMER**

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The magnetic behavior of a metal-organic [Co(C<sub>3</sub>H<sub>3</sub>N<sub>2</sub>)<sub>2</sub>]<sub>n</sub> polymer has been investigated by magnetization and specific heat measurements. Low-field magnetic susceptibility shows the presence of two maxima at  $\sim 8$  and 4 K, respectively. The first maximum of a broad feature was attributed to a short-range low-dimensional antiferro-magnetic behavior and the second with a more sharp structure the existence of a spin-glass-like state. This state was evidenced by magnetic irreversibility observed in the zero-field cooled and field-cooled data, and confirmed by specific heat measurements. The magnetic specific heat ( $C_{mag}$ ) shows a lack of any long-range-ordered peak. Instead, a broad maximum near  $T_f$  was observed in the  $C_{mag}/T(T)$ -curve. Below  $T_f$ , the  $C_{mag}/T$  data follow a relation:  $C_{mag}/T = \gamma + AT$ . We suggest that the competition of antiferromagnetic (AF) intra-chain and ferromagnetic (F) inter-chain interactions in a low-dimensional arrangement of magnetic Co<sup>2+</sup> ions can produce the spin-glass behavior in the sample. The susceptibility data analyzed in terms of a spin  $S = 3/2$  Heisenberg linear-chain model with small exchange energy are consistent with the presence of F and AF interactions. Splitting of the energy levels of the Co<sup>2+</sup> ions in the crystal field causes a Schottky-type specific heat anomaly around 60 K.

## **P-1-28**

### **STRIPES AND CANTED PHASES IN CHARGE-ORDERED SYSTEM**

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Analysis of the extended Hubbard model with additional nearest-neighbour Coulomb repulsion leads to the appearance of separated states including charge-ordered phase. The new grand canonical Monte Carlo simulations have shown a complex and highly nontrivial structure of the phase diagrams comprising the orderings with alternating charge density for the bipartite lattice in a wide range of electron concentrations. The most interesting findings have indicated the presence of stripes or canted domains of different charge-ordered phases and domain ordering of the Mott phase. The phase transitions observed have occurred in finite temperature range for finite-size systems on a square lattice [1]. The results show a possible classical nature of the phase separation and striped states for orders considered.

[1] G.Pawłowski, T.Kazmierczak, "Phase separation and critical phenomena in the charge ordered system", Sol. Stat. Commun. 145, 109 (2008);

## **P-1-29**

### **THERMOELECTRIC POWER OF $\text{Ce}_2\text{RhSi}_3$**

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$\text{Ce}_2\text{RhSi}_3$  crystallizes with a hexagonal structure of the  $\text{AlB}_2$  type. The compound was found to order antiferromagnetically at  $T_N = 4.5 \text{ K}$  with the magnetic moments confined to the hexagonal basal plane. The metamagnetic-like transition occurs in the field  $6 \text{ T}$ . In the paramagnetic region the magnetic susceptibility follows a Curie-Weiss law with the effective magnetic moments close to the free  $\text{Ce}^{3+}$  ion value and the paramagnetic Curie temperature being strongly negative. Above  $T_N$  the electrical resistivity and magnetoresistivity variations show behaviour characteristic of single ion Kondo systems. We present here for the first time the results of thermoelectric power measurements performed down to  $2 \text{ K}$  in magnetic fields up to  $13 \text{ T}$  on the oriented single-crystals of  $\text{Ce}_2\text{RhSi}_3$ . The Seebeck coefficient measured with the temperature gradient set along two main crystallographic directions exhibits distinct anisotropy. The values of the thermopower are rather small (of about several  $\mu\text{V}/\text{K}$  at room temperature). The overall temperature behaviour of the Seebeck coefficient down to  $50 \text{ K}$  can be properly described in the framework of the two band approach that originates from the Hirst model. Then, with decreasing temperature the thermoelectric power changes sign, shows a negative minimum and start to increase giving maximum near  $T_N$ , which is depressed upon applying external magnetic field along a-axis (easy magnetic direction). On the contrary, magnetic field applied along c-axis (hard magnetic direction) does not effect the overall shape of the thermoelectric power curves.

## **P-1-30**

### **POLARIZATION DEPENDENCE XANES STUDY ON**

*$\text{Bi}_{2-y}\text{Pb}_y\text{Sr}_{2-x}\text{La}_x\text{Cu}_{6+\delta}$*  SINGLE CRYSTALS

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X-ray absorption spectroscopy (XAS) has been used to determine the hole concentration for high  $T_C$  polycrystalline materials. However, until yet some difficulties with single crystals appeared. By considering the geometrical differences between single- and polycrystals, polarization dependent XAS measurements on  *$\text{Bi}_{2-y}\text{Pb}_y\text{Sr}_{2-x}\text{La}_x\text{Cu}_{6+\delta}$*  single crystals was done to evaluate the hole concentration on single crystals. The  $\text{Cu}L_{III}$  edge is evaluated for a quantitative investigation. The satellite peak of the  $\text{Cu}L_{III}$  edge displays the overlap of Cu states with oxygen hole states localized in the  $\text{CuO}_2$  planes. Besides measuring the carrier concentration, it can be used to study the distribution of carriers residing in the  $\text{CuO}_2$  planes. The specificity to holes solely of the  $\text{CuO}_2$  planes is due to the fact that XAS is a local probe and therefore detects only holes near O sites. We had observed an interesting small variation of the absorption strength with respect to the angle of the incoming linearly polarized light on a scale of 10-15%. Thus, this may give an insight on the distribution of hole states in the  $\text{CuO}_2$  planes. By proper incorporation of a geometry factor and 10-15% modulation, we found that the hole concentration decreases systematically with increasing La content for single crystals.

### **P-1-31**

#### **PHASE SEPARATION IN t-J MODEL**

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A t-U-J and t-U-J-V models in  $U=\infty$  limit are examined within renormalized mean-field theory. These models exhibit proper low density limits (known from the exact calculations for the two-electron bound states), unlike t-J model. The phase diagrams for arbitrary electron density are calculated, including not only pure superconducting phases but also the phase-separated areas.

### **P-1-32**

#### **THE PROPERTIES OF THE ANISOTROPIC KONDO LATTICE MODEL**

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The study of the properties of the magnetic Kondo lattice model with anisotropic exchange interactions  $J_{XY}$  and  $J_Z$  has been performed. In our investigations we have used an extended mean-field approximation, analogous to that used in the treatments of the isotropic Kondo model. We have made analysis of the phase diagrams and ground state characteristics of this model for arbitrary, positive and negative  $J_{XY}$  and  $J_Z$ , and the interaction with external magnetic field  $H$ .

### **P-1-33**

#### **NUMERICAL ANALYSIS OF THE ORBITAL EFFECTS WITHIN THE DYNAMICAL MEAN FIELD APPROACH**

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We investigate the electronic structure of the strongly correlated electron systems with an orbital degeneracy within the framework of the iterated-perturbation theory (*IPT*) [1, 2] of the dynamical mean field method. We consider the multi-orbital Hubbard model in the limit of infinite lattice spatial dimensions. Our motivation comes from recent studies of the orbital effects in strongly correlated electron systems such as transition metal oxides, strontium ruthenates, manganites, and organic metals. Almost all of these materials consist of valence bands coming from d shells, where intra- and inter-orbital Coulomb interactions are equally important. The important part of the paper is a detailed discussion on the problem of the analytical continuation of the complex frequency Matsubara Green function from the Matsubara points to the real frequency axis. The analytical continuation is a necessary step in the numerical calculations if we are interested in calculating the physical quantities such as the density of states or transport quantities.

[1] H. Kajueter and G. Kotliar, Phys. Rev. Lett. 77, 131 (1996)

[2] T. Fujiwara, S. Yamamoto and Y. Ishii, J. Phys. Soc. Jpn. 72, 777 (2003)

### **P-1-34**

#### **INTERBAND PAIRING IN CUPRATE SUPERCONDUCTIVITY**

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The nonrigid electron spectrum of a cuprate superconductor is modelled by an itinerant band and nodal and antinodal defect subbands created by doping. In the case of hole doping the region near the top of the oxygen band is involved, for electron doping near the bottom of the UHB. It is supposed that the leading pair transfer channel works between itinerant and defect states. Bare gaps between these subsystems are expected to be quenched by doping and are sources of pseudogaps. Band overlap conditions determine the phase diagram special points. Illustrative mean-field calculations have been made with a plausible parameter set. Self-consistent results\* demonstrate that the elaborated approach is able to reproduce the behaviour of cuprate basic superconducting characteristics as e.g. the doping dependence of  $T_c$ , superconducting gaps and pseudogaps, supercarrier density and effective mass, coherence lengths and the penetration depth, critical magnetic fields and some other properties. Interband pairing scheme is suggested to be an essential aspect of cuprate multiband superconductivity.

\*N.Kristoffel et al., Physica C 402, 257 (2004); 437-438, 168 (2006); 460-462, 977 (2007)

## **P-1-35**

### **SUPERCONDUCTING PROPERTIES OF THE SPIN-POLARIZED ATTRACTIVE HUBBARD MODEL**

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Spin-polarized superfluidity in the context of the cold atomic Fermi gases and unconventional superconductivity with a nontrivial Cooper pairing have recently been investigated both theoretically and experimentally. In the presence of a magnetic field, the numbers of particles with spin down and spin up are different. This makes the formation of Cooper pairs across the spin-split Fermi surface with non-zero total momentum ( $\vec{k} \uparrow$ ,  $-\vec{k} + \vec{q} \downarrow$ ) (Fulde and Ferrell, and Larkin and Ovchinnikov state) possible.

In this work the influence of a pure Zeeman effect on the superfluid characteristics has been investigated within the spin-polarized attractive Hubbard model. The ground state and temperature phase diagrams have been obtained both for a fixed number of particles and a fixed chemical potential. For sufficiently high magnetic fields the finite temperature transition between the superconducting and the normal state changes from the second to the first order. Two critical magnetic fields have been found for a fixed number of particles. The two critical fields define the phase separation region between the superfluid phase with the particle density  $n_s$  and the normal state with the density of particles  $n_n$ . Moreover, the behaviour of the order parameter and the spin polarization has been investigated at  $T = 0$  as well as at finite temperature. Finally, the BCS-BEC crossover with increasing attraction in the ground state has been discussed.

## **P-1-36**

### **COEXISTENCE OF FERROMAGNETISM WITH SPIN TRIPLET SUPERCONDUCTIVITY**

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The experimental results for  $\text{ZrZn}_2$ ,  $\text{URhGe}$ , and partly also for  $\text{UGe}_2$  have shown that the ferromagnetic superconductors are weak itinerant ferromagnets. We describe the phenomenon of coexistence between equal spin triplet pairing superconductivity and ferromagnetism using the extended Stoner model, which includes in Hamiltonian the on-site Coulomb interaction,  $U$ , and occupation dependent hopping integral,  $t_{ij}^\sigma$ . This occupation dependence of hopping integral 'produces' the additional terms in Hamiltonian, i.e. assisted hopping,  $\Delta t$ , and exchange-hopping,  $t_{ex}$ , interaction. We use Hartree-Fock (H-F) approximation and the Green functions technique. In the H-F approximation the on-site Coulomb interaction plays the role of the on-site exchange (Hund's) field. All inter-site interactions will have included the inter-site kinetic correlation,  $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$ , within the H-F approximation. We introduce the pressure-dependence to the hopping integral. We compare the numerical results with experimental data for  $\text{ZrZn}_2$ . The kinetic correlation creates the superconductivity without the help of negative values of Coulomb interactions. The model can explain stimulation of triplet SC by the weak itinerant ferromagnetism. This effect was observed experimentally in  $\text{ZrZn}_2$ . The numerical analysis also confirms the experimental effect of decreasing of the critical temperatures (Curie and superconducting) with increasing external pressure.



## **P-1-37**

### **HIGH MAGNETIC POINT-CONTACT PROPERTIES OF YbCu<sub>3.5-x</sub>Al<sub>x</sub> ( $x = 1.3 - 1.75$ ) IN THE VICINITY OF QCP**

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The non-Fermi liquid system YbCu<sub>5-x</sub>Al<sub>x</sub> ( $x = 1.3 - 1.75$ ) has been investigated by point-contact spectroscopy (PCS). The observed  $dV/dI(V)$  characteristics do not agree with the model of thermal contact heating, at least close to zero-bias voltage. In the case of a hetero-contact arrangement we have observed a maximum at only one voltage polarity at about 1.3 mV (for  $x = 1.5$ ). We have observed asymmetric shape of  $dV/dI(V)$  of current-voltage characteristics for hetero-contact arrangement. Application of magnetic field destroys NFL state in sample and restores normal FL state. In high magnetic fields the asymmetry is suppressed. We suppose, that the asymmetry has origin in the NFL state of the sample. Moreover, the observed maximum near zero-bias voltage is in contradiction to the thermal regime. We observed new kind of asymmetry. We suppose that in our heterocontacts some intermediate regime between diffusive and thermal is present.

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## **P-1-38**

### **WE HAVE FOUND ATOMIC-SCALE DESCRIPTION OF NiO!**

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We have solved an old and fundamental problem of NiO - why it is insulator having incomplete 3d shell. Our solution is in agreement with a Sir Mott's suggestion (for it NiO is regarded as the exemplary Mott insulator) that the insulating ground state is caused by strong electron correlations. However, the nature of strong correlations was discussed by last 50 years and is still a subject of a hot debate in most prestigious physical journals. According to the Quantum Atomistic Solid-State Theory (QUASST) the strong correlations are predominantly related with the charge transfer during the formation of the compound and with the intra-atomic correlations. We have proved that the many-electron crystal-field approach is an approach with inherently incorporated strong electron correlations. We provide consistent description of monoxide NiO, which reconciles its insulating ground state and a strong magnetism related to 3d electrons, in a number of eight, in the incomplete 3d shell. We have evaluated the real multipole potential, in the atomic scale, in contrary to generally introduced pseudopotentials. For the low-energy electronic structure and for the formation of the magnetically-ordered state the spin-orbit coupling is fundamentally important. We have reproduced values of the magnetic moment and its direction in the *NaCl* structure. We have found that small lattice distortions determine the direction of the magnetic moment. We have revealed a quite substantial orbital magnetic moment, of 0.54  $\mu_B$ .

## **P-1-40**

### **QUANTUM MONTE CARLO STUDY OF THE REPULSIVE HUBBARD MODEL ON A SIERPINSKI GASKET**

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We employ the Determinant Quantum Monte Carlo method to analyze the thermodynamic properties of the repulsive Hubbard model on a Sierpinski gasket. We calculate the temperature dependence of energy, specific heat and various magnetic properties. The electron concentration at a constant value of chemical potential varies strongly with temperature. Therefore, to obtain the temperature dependences for a fixed electron concentration, the chemical potential that leads to the desired concentration is computed. In addition, we discuss the fermion sign problem for this system.

## **P-1-41**

### **TRANSPORT PROPERTIES OF THE FILLED SKUTTERUDITES LnFe<sub>4</sub>As<sub>12</sub> (Ln = La, Ce, Pr)**

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Electrical resistivity, thermoelectric power, and thermal conductivity are presented for single crystals of the arsenide filled skutterudites LnFe<sub>4</sub>As<sub>12</sub> (where Ln = La, Ce, Pr). Whereas an itinerant-electron weak ferromagnetism below  $T_C = 5.3$  K was recently reported for LaFe<sub>4</sub>As<sub>12</sub> [1], a long-range ferromagnetic order ( $T_C = 18$  K) exists in PrFe<sub>4</sub>As<sub>12</sub>. The latter leads to e.g., a sharp drop of the electrical resistivity and a slope change of the thermoelectric power. Furthermore, magnetization isotherms at  $T = 2$  K revealed a change in the easy axis from [100] to [111] for  $B > 0.5$  T. Additionally, Pr-based compound displays the dimensionless figure of merit equal to 0.015 at low temperatures. On the other hand, two different types of the low-temperature dependency of the electrical resistivity was found for CeFe<sub>4</sub>As<sub>12</sub>. This holds especially true for a pronounced negative coefficient of the resistivity for some of the single crystals investigated. Down to about 160 K, all the CeFe<sub>4</sub>As<sub>12</sub> samples display virtually the same metallic character. [1] S. Tatsuoka et al., J. Phys. Soc. of Japan, 77, No. 3 (2008) 033701.

## **P-1-42**

### **NANOSTRUCTURE FORMATION DURING RAPID SOLIDIFICATION PROCESS IN $\text{Ce}_{100-x}\text{Al}_x$ ( $x=45, 50$ ) ALLOYS**

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The heavy-fermion behavior in some compounds with Ce or Yb could be strongly enhanced by granular structure. The nanocrystalline state formation, crystallization processes, crystal structure of 10-30 nm particles in  $\text{Ce}_{100-x}\text{Al}_x$  are investigated. The master alloys with  $x=45, 50$  were prepared by arc-melting and subsequent melt-spinning. The XRD patterns for both compositions show AlCe nanocrystalline phase with the ClCs-type structure (Pm-3m space group) embedded in an amorphous matrix. This crystalline AlCe phase is known as a metastable one, without unequivocally distribution of Ce and Al atoms in the lattice cell. The  $\text{Ce}_{100-x}\text{Al}_x$  ( $x=45, 50$ ) ribbons due to differences in Ce/Al ratio solidify to different nanocrystalline states, what suggests that amount of nanocrystals could be roughly controlled by wheel velocity during rapid quenching process. The constant-heating DSC curves for  $\text{Ce}_{50}\text{Al}_{50}$  and  $\text{Ce}_{55}\text{Al}_{45}$  show two exothermal crystallization peaks. For  $\text{Ce}_{55}\text{Al}_{45}$  third small feature is observed at about 350°C, which is not visible for  $\text{Ce}_{50}\text{Al}_{50}$  at this heating rate. Total enthalpy  $\Delta H$  of first two peaks is about 20 J/g for both alloys. Additionally, effective activation energies were determined by the means of Kissinger approximation.

## **P-1-43**

### **CRYSTALLIZATION PROCESSES IN AMORPHOUS $\text{Y}_x\text{Ce}_{50-x}\text{Cu}_{42}\text{Al}_8$ ( $x = 0, 25$ ) ALLOYS**

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Not only in a selected crystalline compounds but also in amorphous and nanocrystalline metals the heavy-fermion (HF) behavior was found. This effect could be strongly enhanced by topological disorder, lattice defects or granular structure. The influence of structural disorder and interaction between electrons can be successfully studied as a function of number and size of nanocrystalline grains embedded in an amorphous matrix. The best suited for such investigation are cerium-based alloys because of unstable valence character of Ce atoms that is a prerequisite for the occurrence of strongly correlated electron phenomena.

Ribbons of amorphous  $\text{Y}_x\text{Ce}_{50-x}\text{Cu}_{42}\text{Al}_8$  were produced by one wheel melt-spinning method. The produced materials were studied by X-ray diffractometry (XRD) and differential scanning calorimetry (DSC) with different heating rates from 10 to 50 K/min. There are two stages of crystallization observed in both samples, but in  $\text{Y}_{50}\text{Cu}_{42}\text{Al}_8$  second peak is not significant. Characteristic temperatures and enthalpies of crystallization process were determined. Effective activation energies were calculated from the Kissinger relation and are equal  $247 \pm 18$  kJ/mol and  $569 \pm 107$  kJ/mol for  $\text{Y}_{25}\text{Ce}_{25}\text{Cu}_{42}\text{Al}_8$  and  $\text{Y}_{50}\text{Cu}_{42}\text{Al}_8$ , respectively.



## O-2-01

### LOCALIZATION BY FRUSTRATION: FROM MAGNONS TO ELECTRONS

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For antiferromagnetic spin systems as well as for Hubbard electrons on various frustrated lattices a class of exact eigenstates can be constructed. Such eigenstates can be found, e.g., for the 1D sawtooth chain, the 2D kagomé and checkerboard, and the 3D pyrochlore lattices. The exact many-particle eigenstates consist of independent magnons/electrons localized on finite areas of the lattice. Important structural elements of the relevant systems are triangles being attached to polygons or lines. Then the magnons/electrons can be trapped on these polygons/lines. For electrons the scenario of localized eigenstates is related to the so-called flat-band ferromagnetism.

The correlated systems having localized eigenstates exhibit a highly degenerate ground-state manifold at the saturation field  $h_{sat}$  (at a characteristic value of the chemical potential  $\mu_0$ ) for magnons (electrons). The degeneracy grows exponentially with the system size and leads to a finite residual entropy. By mapping the localized magnon (electron) degrees of freedom onto a hard-core lattice gas one may find explicit analytical expressions for the low-temperature thermodynamics in the vicinity of  $h_{sat}$  ( $\mu_0$ ). Though the scenario of localized eigenstates is similar for spin and electron systems, the different statistics of spins and electrons leads to different construction rules for the localized eigenstates and, as a result, to a different hard-core lattice gas description.

## O-2-02

### AN ANALYTICALLY EXACT DERIVATION OF THE $g$ -FACTOR OF THE ELECTRON IN THE HYDROGEN ATOM

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In his famous 1933-paper “the Lagrangean in Quantum Mechanics”, Paul Dirac has linked Quantum Mechanics with Hamilton-Jacobi classical mechanics. The 2-particle problem of an electron bound to a proton, the hydrogen atom H, is the only system that one may be able to exactly solve classically. The Lagrangean is a non-relativistic approximation, and here we report a study, using modern computer algebra, of a fully relativistic calculation. The results of our analysis indicate the existence of stable orbits, resulting from a competition of the Coulomb force (attracting as  $1/r^2$ ) and the magnetic interaction between the proton- and electron-spins (repulsive at short distances as  $1/r^{5/2}$ ). We view the result as classically-derived “quantum mechanics”.

The analysis also provides a simple geometric explanation for the  $g$ -factor of the electron to 6 digits. By including an applied magnetic field, the Zeeman effect of the two spin systems could be evaluated in the spherically symmetric, orbital  $S$  ground state: hence we can derive the effective magnetic moments (i.e.  $\mu_B$ ) of electron and proton from first principles. The outcome of the analysis is that we can construct a calculable standard for the magnetic field, and in an experiment fix the strength of the magnetic field in terms of fundamental constants with uncertainties much less than 1 ppm. This could provide a Euromet standard for the SI-Tesla, easily transferred using NMR probes, ensuring magnetic field measurement traceability up to 7 digits or an uncertainty of 0.1 ppm.

## O-2-03

### MAGNETIC ANISOTROPY OF HOMONUCLEAR TRANSITION METAL DIMERS

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Calculated structural and magnetic properties of transition metal dimers are reported. All calculations have been performed using the full-potential local-orbital program package FPLO [1] for the solution of the Kohn-Sham-Dirac equations within the local spin density approximation (LSDA). The structural properties, such as ground state spin multiplicity, bond length, and harmonic vibrational frequency, are obtained by scalar-relativistic calculations. The fixed-spin moment method is applied to stabilise the convergence and to single out the ground state spin state. In the next step, orbital magnetic properties are obtained from spin polarised full-relativistic calculations. Since orbital moments are usually underestimated in such calculations, we have additionally studied the influence of orbital polarisation corrections (OPC, [2]). The results will be compared with available experimental data and other theoretical investigations.

[1] K. Koepnik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999); <http://www.fplo.de>.

[2] L. Nordström, M. S. S. Brooks, and B. Johansson, J. Phys.: Condens. Matter **4**, 3261 (1992).

## O-2-04

### TWO-DIMENSIONAL ISING MODEL WITH COMPETING INTERACTIONS AS A MODEL FOR INTERACTING $\pi$ -RINGS

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A chain or a planar array of electrically isolated  $\pi$ -rings could be treated as a set of magnetic moments oriented perpendicular to the plane (i.e. as Ising spins) and interacting via magnetic dipole forces. Due to this dipole character of the interaction between the orbital moments, it is necessary to include the next-nearest neighbor interactions in addition to those between the nearest neighbors.

We propose a two-dimensional Ising model with competing nearest-neighbor and diagonal interactions on a square lattice as a model for interacting  $\pi$ -rings. It is now well accepted that such a model with nearest-neighbor ( $J$ ) and next-nearest neighbor ( $J'$ ) interactions on the 2D square lattice exhibits two phases with magnetic long-range order; a semi-classical Néel-like magnetic order at small  $J'$  and a antiferromagnetically coupled ferromagnetic chains (vertical or horizontal stripes) large  $J'$ . These two ordered phases are separated by an intermediate quantum paramagnetic phase without the long-range order, the nature of which is still under discussion.

We show that this model exhibits an additional low temperature disordered phase due to the proximity of the lowest energy excited states to the ground state. Exact diagonalisation is used for small lattices and Monte Carlo simulations is used for larger lattices where we measure several potential order parameters for the model. We compare the results from exact diagonalisation and Monte Carlo simulations with experimental results.

## O-2-05

### AB INITIO STUDY OF MOLECULAR MAGNETISM OF m-SrN

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Magnetic properties of solids typically originate in the presence of ions with partially filled  $d$  or  $f$  shells. Recently, observations of ferromagnetism in organic materials [1] and in ZnO:C [2] have stimulated interest in magnetism in systems without magnetic ions. Moreover, theory indicates that ferromagnetism can exist in II-V nitrides (SrN and CaN) in the metastable NaCl structure [3].

The experimental structure of SrN is monoclinic (m), in which there are two types of nitrogen ions with different coordinations [4]: one half on N ions form  $N_2$  dimers, while the remaining ions are "isolated", i.e., surrounded by 6 Sr neighbors. Magnetic and electronic structure of m-SrN was analyzed within the density functional theory. We find that m-SrN is a molecular antiferromagnet.  $N_2$  dimers are in 2- charge state with two electrons occupying antibonding  $\pi$  orbitals that carry magnetic moments of about  $1 \mu_B$  per dimer. The high-spin configuration of  $N_2$  is stable because the strong exchange-induced spin polarization of the compact  $\pi$  orbitals dominates the relatively weak hybridization effects with Sr neighbors. Thus, this configuration is similar to that of  $O_2$  in molecular magnet  $Rb_2O_6$  [5].

[1].H. Ohldag et al., *ibid.* 98, 187204 (2007).

[2] H. Pan et al., *Phys. Rev. Lett.* 99, 127201 (2007).

[3] O.Volnianska and P. Boguslawski, *Phys. Rev. B* 75, 224418 (2007).

[4] G. Auffermann et al., *Angew. Chem. Int. Ed.* 40, 547 (2001).

[5] J. Winterlink et al., *J. Am. Chem. Soc.* 129, 6990 (2007).

## O-2-06

### SPIN TRANSITION IN A CORRELATED LIQUID OF COMPOSITE FERMIONS

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Fractional quantum Hall (FQH) effect occurs when 2D electrons fill a (specific) fraction  $\nu$  of the lowest Landau level (LL) in a high magnetic field. This macroscopic phenomenon involves a new state of matter – incompressible electron liquid with fractionally charged quasiparticles (QPs), the most prominent example being the Laughlin  $\nu = 1/3$  state. An elegant model of the FQH effect is the composite fermion (CF) picture, employing a concept of electrons capturing some of the external magnetic field and thus transforming themselves into nearly noninteracting CFs moving in a reduced (mean) field. New FQH states were found recently at LL fillings  $\nu$  corresponding to several simple partial fillings  $\nu^*$  of the 2nd CF LL. The importance of these "second generation" liquids relies on their incompressibility depending on the (distinct) interaction and correlation of CFs.

In this work we study spin transition of the most prominent 2nd-generation FQH state at  $\nu^* = 1/3$ . The complexity of the spin dynamics of CFs is caused by the fact that the two spin states of a CF represent distinct many-electron excitations (with different creation energies and interaction pseudopotentials). Therefore, the spin transition occurs between a pair of CF liquids with distinct CF–CF correlations (and thus different microscopic mechanisms of incompressibility). We have used numerical exact-diagonalization of representative few-body hamiltonians in spherical geometry to compare single-particle and correlation energies of the competing CF spin phases. The main result is a phase diagram in experimental parameters and prediction of a transition in realistic conditions.

## O-2-07

### 2D FALICOV-KIMBALL MODEL IN THE PERTURBATIVE REGIME AT FINITE-TEMPERATURES

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Finite-temperature properties of the Falicov-Kimball model have been studied in the perturbative regime, i.e. for  $t/U \ll 1$ , where  $t = 1$  is the hopping constant and  $U = 10$  denotes the Coulomb interaction strength. In our study, we have determined the phase diagram of the model in the second-order of the perturbation theory, where the antiferromagnetic Ising model in the magnetic field emerges. In the fourth-order, where our model constitutes the Ising model with more complicated frustrated antiferromagnetic interactions, the phase diagram was established. The Monte Carlo method was employed to investigate the phase transition lines. The existence of stripe ordering at finite temperatures is proved.

## O-2-08

### PHENOMENOLOGICAL MODELLING OF MOLECULAR-BASED ANTIFERROMAGNETIC RINGS

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Two non-perturbative approaches: the direct exact diagonalization and quantum transfer matrix (QTM) techniques, applicable to Heisenberg spin systems modelling molecular rings, are described. The models include the single-ion anisotropy, alternating nearest-neighbour bilinear exchange coupling and the biquadratic term. Using these techniques and exploiting the Hamiltonian symmetry, we have performed calculations beyond the strong exchange limit for relatively large spin systems: (i) twelve spins  $s = 1$  ( $\text{Ni}_{12}$ ) and (ii) eight spins  $s = 3/2$  ( $\text{Cr}_8$ ). In both cases, the energy spectra in the presence of single-ion anisotropy, biquadratic exchange and magnetic field have been calculated using the direct exact diagonalization. The anisotropy-dependent splitting and spin-mixing as well as the field-dependent crossing of energy levels is presented and analysed. The efficiency and flexibility of QTM method is demonstrated for the spin  $s = 3/2$  ring, including the exact magnetic torque calculations. The susceptibility and specific heat have been found to depend mainly on the mean value of the alternating couplings.



## O-2-09

### BETHE ANSATZ AND GEOMETRY OF CLASSICAL CONFIGURATION SPACE

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We demonstrate that the seminal one-dim model of the Heisenberg magnet, consisting of  $N$  spins  $1/2$  with the nearest neighbour isotropic interaction, solved exactly by Bethe Ansatz, admits an interpretation of a system of  $r = N/2 - M$  pseudoparticles (spin deviations) which are indistinguishable, have hard cores, and move on the chain by local hoppings. Such an approach allows us to construct a manifold with some boundaries, which is generically  $r$ -dimensional, and whose  $F$ -dimensional regions,  $0 < F < N$ , point out all  $l$ -strings. The latter classify, in terms of rigged string configurations of Kerov, Kirillov and Reshetikhin, all exact Bethe eigenfunctions. In this way, we interpret these eigenfunctions in terms of the classical configuration space, in particular on the structure of islands of adjacent spin deviations, in a way independent on the size  $N$ .

## O-2-10

### SKYRMION STATES IN CHIRAL MAGNETS

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Chiral interactions stabilize smooth “Skyrmion” textures in ordered condensed matter systems. In noncentrosymmetric magnetic crystals, such chiral couplings are realized as Dzyaloshinskii-Moriya exchange. Unconventional Skyrmion states may be observable in magnetic nanostructures, where the chiral Dzyaloshinskii-Moriya exchange arises owing to reduced dimensionality and modifications of the electronic properties on surfaces [1]. We develop a phenomenological theory for modulated and localized states in thin films of noncentrosymmetric ferromagnets and chiral liquid crystals. In such systems, strong surface anisotropy or anchoring stabilizes collinearly ordered states where Skyrmions can exist as localized and topologically stable excitations. The solutions for these two-dimensional “Baby-Skyrmions” in magnetic films are related to well-known spherulitic or bubble domains in chiral nematic films. The theory for magnetic films describes Skyrmions with a great variety of shapes. This variety is determined by the nature of the chiral coupling, which may arise due to broken inversion symmetry at surfaces or due to noncentrosymmetric lattice structures as in the chiral ferromagnets MnSi or FeGe [2].

[1] C. Pfeiderer, U.K. Röbller, Nature 447 157 (2007)

[2] U.K. Röbller, A. N. Bogdanov, C. Pfeiderer, Nature 442, 797 (2006)

## **P-2-01**

### **MAGNETIC PROPERTIES OF A BILAYER SYSTEM WITH ANISOTROPIC HEISENBERG INTERACTION**

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A magnetic bilayer system with spin  $S = 1/2$ , the coordination number  $z = 5$  and anisotropic Heisenberg ferromagnetic interactions is studied by the cluster variational method in the pair approximation. The anisotropy parameter defined as  $J^{x,y}/J^z$  ratio varies from zero value, which is characteristic for the pure Ising model, until unity - corresponding to the isotropic Heisenberg interactions. The complete and self-consistent thermodynamic description based on the Gibbs free-energy expression is given. All relevant thermodynamic properties such as spontaneous magnetization, pair correlation function (both quantum and classical), entropy, isothermal susceptibility and magnetic specific heat are calculated. The influence of anisotropy on all the thermal characteristics is discussed. In particular, the analytical expression for the phase transition temperature vs. anisotropy is obtained, and the numerical calculations are compared with those for  $2D$  and  $3D$  systems. It is shown how the Curie temperature increases when the anisotropy parameter decreases from unity to zero value. It is also found that the Gibbs energy at absolute zero temperature does not depend on the anisotropy parameter. However, for the isotropic Heisenberg interactions at  $T = 0$  the residual entropy remains, which reduces the spontaneous magnetization. In such a case, the possibility of occurrence of quantum phase transition is predicted.

## **P-2-02**

### **DISCRETE AND CONTINUOUS SCHEMES IN SHERRINGTON-KIRKPATRICK MODEL**

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We calculate a solution of Sherrington-Kirkpatrick model in a nonzero magnetic field. The solution is first calculated near the de Almeida-Thouless instability line in the framework of N-RSB as well as directly in the continuous limit. We discuss how the N-RSB solution approaches the continuous one in the limit of large  $N$ . The equations of the continuous limit are formulated in a novel way via T-ordered evolution operators. We study polynomial and discrete approximations to these operators. The aim is to find a reliable approximate solution in the entire spin glass phase.

## **P-2-03**

### **MAGNETIC ORDERING OF IRON IONS IN TWO KINDS OF Fe-CHITOSAN COMPLEXES**

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We report on the results of magnetic measurements for two different Fe-chitosan complexes with different structure and Fe-content: iron-crosslinked chitosan (Ch-Fe-CL) and iron-N-carboxymethyl chitosan (N-CM-Ch-Fe), with Fe-content 118 mg/g and 7 mg/g, respectively. The detailed analysis of the magnetic behaviour of Ch-Fe-CL have already been presented in [1] and demonstrates that iron ions in this material do not form superparamagnetic clusters, but exhibits features of a glassy state. New data obtained from the Mössbauer spectrometry reveal ferric ions in a high-spin state and in two different sites. Moreover these data confirm a noncollinear magnetic structure in Ch-Fe-CL and suggest the sperimagnetic ordering of  $\text{Fe}^{3+}$  magnetic moments. The static magnetic and Mössbauer measurements of N-CM-Ch-Fe show an inhomogeneous magnetic structure: a part of Fe-ions are antiferromagnetically coupled and the rest remain in a paramagnetic state. The iron ions in N-CM-Ch-Fe are in two states –  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$ . A mixed paramagnetic-antiferromagnetic behaviour of N-CM-Ch-Fe indicate that some of Fe ions are not distributed randomly within the polymer but rather forms Fe-chains.

[1] N. Nedelko *et al.*, phys. stat. sol. (c), **3**, 126 (2006)

## **P-2-04**

### **QUANTUM PHASE TRANSITION IN GENERALIZED ONE-DIMENSIONAL XZ MODEL**

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We introduce a one-dimensional (1D) anisotropic XZ model with different interactions on even and odd bonds. As a special case the interactions interpolate between the 1D Ising model and the 1D quantum compass model with frustrated pseudospin interactions  $\sigma_i^z \sigma_{i+1}^z$  and  $\sigma_i^x \sigma_{i+1}^x$ , alternating between even/odd bonds [1]. We present an exact solution which employs the mapping to fermions with spin  $S = 1/2$  and demonstrate that the pseudospin correlation functions undergo in general the second order quantum phase transition, while for particular choice of interactions this transition is first order. The properties of the compass model are investigated and we prove its disordered ground state with degeneracy  $2^{N-1}$  for the chains of length  $2N$  ( $N \geq 2$ ), while for  $N \rightarrow \infty$  the degeneracy is  $2 \times 2^N$ . The nearest neighbor pseudospin correlation functions are identical to those of the 1D XZ model for the interacting pairs of pseudospins. The results obtained for long-range correlation functions indicate divergent correlation length when the point of quantum phase transition is approached. Possible extensions to the ladder geometry will also be discussed.

[1] W. Brzezicki, J. Dziarmaga and A. M. Oleś, Phys. Rev. B **75**, 134415 (2007).

## **P-2-05**

### **MAGNETIC PROPERTIES OF S=1/2 TWO-DIMENSIONAL QUANTUM ANTIFERROMAGNET $\text{Cu}(\text{D}_2\text{O})_2(\text{C}_2\text{H}_6\text{D}_2\text{N}_2)\text{SO}_4$**

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The partial deuteration of  $\text{Cu}(\text{H}_2\text{O})_2(\text{C}_2\text{H}_8\text{N}_2)\text{SO}_4$  has been performed with the aim to tune ground state properties of the compound which was previously identified as a representative of an S=1/2 spatially anisotropic triangular antiferromagnet [1]. The studies of the magneto-structural correlations in  $\text{Cu}(\text{D}_2\text{O})_2(\text{C}_2\text{H}_6\text{D}_2\text{N}_2)\text{SO}_4$  involving specific heat and susceptibility measurements in zero magnetic field revealed only slight deviations from the magnetic behaviour observed in the original compound. The origin of the observed behaviour is discussed.

[1] M. Kajňaková et al., Phys. Rev. B 71, (2005) 014435.

## **P-2-06**

### **LOW-TEMPERATURE HEAT CAPACITY OF TWO-DIMENSIONAL (N-Me-2,6-di-Me-Pz)(TCNQ)<sub>2</sub>**

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The experimental results of the low-temperature heat capacity of ARS based on TCNQ anion-radical sample (N-Me-2,6-di-Me-Pz)(TCNQ)<sub>2</sub> in the temperature range from 100 mK to 10 K are presented. In the heat capacity lattice and magnetic contributions can be distinguished and interpreted: the first in terms of low-dimensional Debye model, the latter with spin-ladder model. Below T = 1 K a hint of  $\lambda$ -anomaly is observed. This  $\lambda$ -anomaly could indicate the three-dimensional magnetic ordering closely linked to the complicated crystal structure in which three different types of TCNQ anions figure.

## **P-2-07**

### **CHARGE TRANSPORT IN CUPRATES BY MAGNETIC TOPOLOGICAL EXCITATIONS: TOPOLOGICAL EXCITATIONS IN FRUSTRATED BACKGROUND.**

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The magnetic phase of Nd doped  $La_{2-x}Sr_xCuO_4$  ( $0.02 < x < 0.05$ ) (LSCO) is a spiral spins phase, where a fraction of spirals form the collinear ordered, incommensurate superstructure making a spins system highly anisotropic without violation of homogeneous charge distribution. Essential for the charge transport in cuprates are the spin topological excitations (TE) with finite mass (they can move) since it is natural to assume that the charge carriers are attached to them.

We claim that the relevant finite mass spin TE in LSCO are separated  $Z_2$  non-Abelian vortices which fields are screened in the frustrated background making their energy (mass) finite. In the framework of the non-Abelian Higgs model, where the frustrations are represented by a gauge field of SO(3) group but the matter field by the order parameter of spiral spins phase, we have found finite mass non-Abelian  $Z_2$  vortex solution. We argue that the motion of those vortices is diffusive and we have evaluated the vortex damping coefficient which enabled us, using Drude model of conductivity, to evaluate the temperature dependence of the cuprates resistivity  $\rho$  ( $\rho \sim T$ , at high temperature, in agreement with experiments). The presented model indicates the possibility of mechanism (based on spins degree of freedom) of formation of a strong conductivity anisotropy in cuprates without breaking the homogeneity of charge distribution.

## **P-2-08**

### **SPIN HAMILTONIAN OF THE TRIANGULAR LAYERED $\alpha$ -NaMnO<sub>2</sub> SYSTEM**

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Magnetization and electron spin resonance (ESR) measurements have been performed on  $\alpha$ -NaMnO<sub>2</sub> polycrystalline sample, a quantum spin-2 system on a frustrated triangular lattice with spatially anisotropic Heisenberg exchange. From the susceptibility curve, we have determined the antiferromagnetic exchange couplings by employing the finite-temperature Lanczos (FTL) method: in the preferably coupled spin chains,  $J_1 = 65$  K, and perpendicular to them,  $J_2/J_1 = 0.44$ . The FTL calculations on finite  $m \times n$  clusters show rapid convergence already for  $n = 2$  unit cells in  $J_2$  bond direction, indicating that the behaviour of  $\alpha$ -NaMnO<sub>2</sub> system may be described within a quasi-1D model. This is furthermore supported by FTL calculations of 2D static spin correlations at finite temperatures. From the ESR linewidth we also evaluate the dominant magnetic anisotropy term of the single-ion type,  $D = -4.1$  K, which establishes an easy-axis direction.

## **P-2-09**

### **SPECIFIC HEAT OF THE POLYDOMAIN $\text{Yb}_4\text{As}_3$ SYSTEM: AGREEMENT BETWEEN SPIN - 1/2 MODELLING AND EXPERIMENT**

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New experimental values of specific heat of a polydomain  $\text{Yb}_4\text{As}_3$  sample in a zero magnetic field are presented. They have been used for estimation of the lattice specific heat and taking into account the Bethe ansatz results, a new value of the exchange integral  $J/k_B = -28$  K has been obtained for the Heisenberg model of the antiferromagnetic spin chain  $S = 1/2$ . A quantitative agreement has been achieved between the experimental specific heat data for a polydomain sample of  $\text{Yb}_4\text{As}_3$  in magnetic field of different intensities and the numerical results obtained by the transfer-matrix simulation technique. Taking into regard the composition of the sample, 25% of the domains have been assumed to be aligned along the field and 75% perpendicular to it. The perpendicular component generates the staggered magnetic field following from the Dzyaloshinskii-Moriya interactions and the energy gap. The energy gap size has been reanalyzed as a function of the magnetic field, leading to experimental verification of the scaling law following from the sine-Gordon model.

## **P-2-10**

### **APPLICATION OF A FRUSTRATED ISING MODEL IN AN ANALYSIS OF LOW-TEMPERATURE PHASE TRANSITIONS IN $\text{LiCsSO}_4$**

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Empirical data, concerning three successive low-temperature structural transformations in  $\text{LiCsSO}_4$ , are reported. The data indicate existence of incommensurate modulations, which appear as intermediate phases at the transitions and are most possibly associated with planar rotations of  $\text{SO}_4$  tetrahedrons. This kind of behaviour is characteristic for the family of  $A'A''BX_4$  compounds. A new interpretation of the phenomenon is proposed, based on the Kurzyński and Halawa model of structural phase transitions in  $A'A''BX_4$  compounds [1,2] which, in the low-temperature region, can be effectively reduced to the one-spin frustrated Ising (ANNI) model[3]. The originally three-dimensional model is mapped onto (010) axis, perpendicular to the basal hexagonal planes. The incommensurate (010) modulation turns out to be a result of the frustrating competition between in-plane  $nn$  and out-plane  $nnn$  vs.  $nnnn$  interactions.

[1] M. Kurzyński, Phase Transitions 52,1-56(1994)

[2] M.Kurzyński and M.Halawa Phys.Rev.B34,4846(1986)

[3] I. Luk'yanchuk, A.Jorio, M.A.Pimenta, Phys.Rev.B57(9)5086(1998)

## **P-2-11**

### **DFT STUDY ON A CHAIN MODEL OF THE CHROMIUM-BASED MOLECULAR MAGNETS**

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We present a density functional theory (DFT) study of the electronic and magnetic properties of the chromium-based molecular rings. The all-electron linearized augmented plane wave method (LAPW) implemented in the Wien2k package [1] is used to calculate the electronic states, exchange coupling parameters and magnetic anisotropy of a infinite chain model system of Cr<sub>8</sub>. We demonstrate how the chain model mimics with good approximation the electronic and magnetic properties of the original Cr<sub>8</sub> molecule [2], and offers an unique opportunity, in virtue of the reduced computational effort, for carrying out extensive investigations of molecules belonging to the Cr-based molecular rings family [3].

[1] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (see [www.wien2k.at](http://www.wien2k.at) for details).

[2] V. Bellini, A. Olivieri and F. Manghi, Phys. Rev. B **73**, 184431 (2006).

[3] D. M. Tomecka, V. Bellini, F. Troiani, F. Manghi, G. Kamieniarz, and M. Affronte (to be submitted).

## **P-2-13**

### **QUANTUM MOLECULAR-BASED CHAINS: A DENSITY MATRIX RENORMALIZATION APPROACH<sup>1</sup>**

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Molecule-based nanostructures manifesting magnetic hysteresis in the absence of long-ranged magnetic order are polynuclear clusters or one-dimensional structures based on an interplay between antiferromagnetic and ferromagnetic interactions along a chain. Recently it has been shown that such a behavior can be also found for canted antiferromagnetic chains, where only one type of spins and one type of interactions are present. In order to study thermodynamic properties of such systems a quantum Heisenberg model is considered by means of the density-matrix renormalization technique.

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## **P-2-14**

### **CONDUCTANCE QUANTIZATION IN THE MELT-SPUN CUBIC HoCu<sub>5</sub>**

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We present experimental results on the electrical conductance quantization in point contact between metallic (W) wire and binary compound HoCu<sub>5</sub> sample. A description of the quantization phenomena is presented in terms of the Landauer formalism for the current flowing through a small nanoconstruction. The conductance histogram were built up using consecutive conductance curves at room temperature. In all cases, the individual conductance traces clearly showed more or less pronounced conductance plateaus. We measured 3000 nanowires, formed between W and HoCu<sub>5</sub>. In this case gently break a metallic contact, the corresponding conductance histogram, showed clear peak corresponding to the conductance step. For over 2500 conductance traces we found the conductance peak at  $G = 0.95 G_0$  ( $G_0 = 2e^2/h$ ) which corresponds to the conductance quantum associated with free propagation of the valence s electrons in the quantum channels. The quantum properties of conducting nanowires are dominantly determined by the nature of atomic structure, and we discuss the results in the context of related physical developments.

## **P-2-15**

### **TOWARDS SPIN-WAVE LIKE APPROACH TO THE $J$ - $J'$ HEISENBERG ANTIFERROMAGNET IN TERMS OF COMPOSITE SPINS**

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Conventional spin-wave approach relies on an expansion around a relevant classical (un-entangled) ground state or equivalently the ground state in the mean field approximation (MFA) for the quantum model. However for systems which may admit valence bond ground states, such as the staggered  $J$ - $J'$  Heisenberg antiferromagnet, single site MFA is obviously an incorrect zeroth order approximation. In this paper, we introduce a MFA for clusters consisting of two spins connected by a strong bond in the afore-mentioned model. We identify the quantum critical point and calculate the ground state magnetization within this cluster MFA in one and two dimensions. Furthermore, since each chosen cluster can be viewed as a composite spin- $\frac{3}{2}$ , we discuss the possibility of a spin-wave like expansion around the cluster MFA ground state.



## **P-2-16**

### **Heisenberg Model of a Ferromagnetic Monolayer Deposited on a Non-magnetic Bulk Substrate**

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A model describing a Heisenberg ferromagnetic monolayer (in a magnetic field) interacting with its non-magnetic bulk substrate is formulated. We use reduced-density operators to show that physical properties of the monolayer are affected by its interaction with the environment. Particularly the influence of the substrate lattice vibrations on the monolayer exchange parameter is examined. The Gaussian-type orbitals were used to calculate the distance dependence of the exchange parameter and the many-body Green's functions to calculate the temperature dependence of the magnetization. Finally, the influence of the Debye temperature of the substrate on the magnetization of the monolayer is depicted. Although the resultant effect is not prominent, we state that interaction of ultrathin magnetic films with their environment has to be taken into account in the construction of the reduced-density operator.

## **P-2-17**

### **FOUR-SPIN ANTIFERROMAGNETS: BEYOND THE ROTATIONAL BAND MODEL**

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Nowadays synthesized magnetic molecules comprise several ( $n > 10$ ) spins with relatively small spin number  $s \leq 3$ . In the case of antiferromagnetic couplings the rotational band model, satisfying the Landé interval rule, is frequently assumed to describe the thermodynamic properties of such a system. However, it can be shown that the *classical* Landé rule is not fulfilled in *quantum* spin systems besides some special cases. Among others, it is satisfied for four identical spins  $s$  placed in vertices of a tetrahedron, a square or a rhombus. To investigate influence of quantum effects we consider systems very close to those mentioned above: four spins  $s$  in vertices of a rectangle or an isosceles trapezium and three spins  $s$  in vertices of an equilateral triangle with a spin  $\sigma \neq s$  in its centre. Also a ring of six small spins ( $s = 1/2, 1$ ) is considered. In all these cases the thermodynamic properties can be easily determined, but we concentrate on *eigenstates* and spin-spin correlations.



## O-3-01

### CONDITIONS OF ABSOLUTE GAP OPENING IN THREE-DIMENSIONAL MAGNONIC CRYSTALS

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We use the plane wave method to determine spin wave spectra of three-dimensional magnonic crystals (the magnetic counterpart of photonic crystals) composed of two different ferromagnetic materials. The scattering centres in the magnonic crystal considered are ferromagnetic spheroids (spheres being a special case) distributed in sites of a cubic (sc, fcc or bcc) lattice embedded in a matrix of a different ferromagnetic material. We demonstrate that magnonic gaps in such structures occur at spontaneous magnetization contrast and/or exchange contrast values above a certain critical level, which depends on the lattice type. Optimum conditions for magnonic gaps to open are offered by the structure in which the scattering centres are the most densely packed (the fcc lattice). We show that in all considered lattice types the reduced width of the gap (i.e. the width referred to the gap centre) is, in good approximation, a linear function of both the exchange contrast and the magnetization contrast. Also, the gap width proves sensitive to deformation of the ellipsoidal shape of the scattering centres, and its maximum value to correspond to a scattering centre shape close to a sphere. Moreover, our numerical results seem to indicate that dipolar interactions in general result in an effective reduction of the gap width, but their impact only becomes of importance when the lattice constant of the cubic magnonic structure is greater than the ferromagnetic exchange length of the matrix material.

## O-3-02

### MAGNETIC PROPERTIES OF $\text{TbNi}_{1-x}\text{Au}_x\text{In}$ COMPOUNDS

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The work reports magnetic and neutron diffraction data of the pseudoternary  $\text{TbNi}_{1-x}\text{Au}_x\text{In}$  compounds for  $0 < x < 1$ . All these compounds crystallize in the  $\text{ZrNiAl}$ -type hexagonal structure. The hexagonal arrangement of rare earth atoms introduces geometrical frustration in case of antiferromagnetic coupling. The ternary  $\text{TbNiIn}$  and  $\text{TbAuIn}$  compounds are isostructural but have different magnetic ordering. In  $\text{TbNiIn}$  the magnetic order is described by the propagation vector  $\mathbf{k} = [\frac{1}{2}, 0, \frac{1}{2}]$  while in  $\text{TbAuIn}$  by  $\mathbf{k} = [0, 0, \frac{1}{2}]$ . In both compounds the Tb magnetic moments form a non-collinear  $120^\circ$ -type structure. In  $\text{TbNiIn}$  a change of magnetic order at 32 K is observed. The solid solutions  $\text{TbNi}_{1-x}\text{Au}_x\text{In}$  exist for all  $x$  values. Magnetic data indicate that the Néel temperature decreases with increasing  $x$  from 68 K for  $x = 0$  to 35 K for  $x = 1$ . For the sample with  $x > 0.5$  an additional phase transition below  $T_N$  at  $T_t$  is also observed. The values of  $T_t$  decrease with increasing  $x$ . Neutron diffraction data for  $x > 0.5$  indicate magnetic ordering described by the propagation vector  $\mathbf{k} = [\frac{1}{2}, 0, \frac{1}{2}]$ . The obtained data are discussed in the XY model including interactions between nearest and next-nearest magnetic moments.

### O-3-03

#### EFFECT OF DOPING ON SUPERCONDUCTIVITY IN $\text{Mo}_3\text{Sb}_7$ FROM KKR-CPA STUDY.

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$\text{Mo}_3\text{Sb}_7$  is a superconductor, with critical temperature  $T_s \simeq 2.5$  K [1]. Recently, from the experimental study it was revealed, that the relatively low value of  $T_s$  may be a result of competition of spin fluctuations with superconductivity [2]. Moreover, from our electronic structure calculations it was found that the Fermi level is located on a slope of a large DOS peak, with the DOS value close to the Stoner limit on Mo atoms, which may be the reason for enhanced spin fluctuations. In this work the results of both experimental and theoretical study of various doping of  $\text{Mo}_3\text{Sb}_7$  (e.g. with Ru, Fe) are presented. The evolution of the electronic structure and superconducting properties and the effect of spin fluctuations are discussed. The electron-phonon interactions in these alloys are studied using the rigid muffin tin approximation (RMFTA) and KKR-CPA electronic structure calculations.

This work was partly supported by the Polish Ministry of Science and Higher Education.

[1] Z. Bukowski et al., Solid State Commun. **123**, 283 (2002).

[2] C. Candolfi et al., Phys. Rev. Lett. **99**, 037006 (2007).

### O-3-04

#### ELECTRONIC BAND STRUCTURE, XPS AND BULK PHYSICAL PROPERTIES OF $\text{UCoGe}$

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The electronic structure as well as bulk physical properties of orthorhombic TiNiSi-type  $\text{UCoGe}$  have been investigated. The results of band structure calculations, employing the modern full-potential local-orbital (FPLO) code [1], are compared with experimental data of x-ray photoelectron spectroscopy (XPS), transport and magnetic properties, obtained for single crystalline samples. Based on measurements on polycrystalline samples, Huy et al. [2] have interpreted the ground state of this compound as weak itinerant ferromagnetism ( $T_C = 3$  K) coexisting with superconductivity ( $T_{SC} = 0.8$  K). In contrast, our sample does not confirm their findings but turns out to be paramagnetic and non-superconducting down to the lowest values of temperature. A ferromagnetic phase is, however, close in energy to the non-magnetic phase according to our spin- and orbital-polarized calculations. Good agreement between results of non-magnetic calculations and XPS experimental data is achieved mainly for the U 5f electrons but not as much for the Co contributions. This indicates that the real electronic structure could be different from the predicted one.

[1] FPLO 3 and 5 [improved version of the original FPLO code by K. Koepnik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999)]; [www.FPLO.de](http://www.FPLO.de);

[2] N.T. Huy et. al, Phys. Rev. Lett. **99**, 067006 (2007);

### **O-3-05**

#### **PROBING 3d-4f EXCHANGE INTERACTIONS BY HIGH-FIELD MAGNETIZATION MEASUREMENTS**

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In a 4f-3d ferrimagnet the molecular field (a net value expressing the relevant exchange interactions) can be determined from high-field magnetization measurements. If the field is high enough, it breaks the ferrimagnetic ground state and drives the system towards ferromagnetic order via non-collinear intermediate phases. Magnetization curves of Er<sub>2</sub>Fe<sub>17</sub> single crystal have been measured along the [100] and [001] crystallographic directions in magnetic fields up to 50 Tesla. An unfixed sample, free to rotate, was measured as well. The magnetization measured along the easy magnetization direction shows jumps at 37.5 and 44 Tesla. The first jump was used for the determination of the molecular field (66.4 Tesla). This agrees with the data for the unfixed sample where a kink in the magnetization at 33.5 Tesla yields a molecular field of 65.7 Tesla. The obtained values are in a good agreement with literature data.

### **O-3-06**

#### **ANISOTROPY OF MAGNETIC AND TRANSPORT PROPERTIES OF UAuSb<sub>2</sub> SINGLE CRYSTALS**

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The uranium-transition metal ditimonides UTSb<sub>2</sub> (T = transition metal) belong to a numerous family of ternary compounds crystallizing in a tetragonal structure of the HfCuSi<sub>2</sub>-type (space group P4/nmm). In the framework of our systematic investigation of this group of ternaries we have recently extended our interest to UAuSb<sub>2</sub>. Some preliminary magnetic study of this compound have shown two magnetic transitions, a ferromagnetic one at  $T_C = 31$  K and probably an antiferromagnetic one at 43 K. Previously the electronic band structure calculations and photoemission examinations of single crystalline samples UAuSb<sub>2</sub> have been reported [1]. In this paper the results of magnetic susceptibility, magnetization, electrical resistivity and thermopower measured along the main crystallographic directions are reported. The spontaneous magnetization at 1.9 K amounts about  $0.8 \mu_B$  for  $B \parallel c$ -axis. Electrical resistivity for  $J \perp c$ -axis exhibits  $aT^2$  law at low temperatures and a Kondo effect at higher temperatures. The thermopower  $S$  for both main crystallographic directions show a maximum at  $T_C$  and the lack of any anomaly at  $T_N$ .

[1] J. A. Morkowski, A. Szajek, E. Talik, and R. Troć, J. Alloys Compd. 443 (2007) 20

### **O-3-07**

#### **NONLINEAR DYNAMICS OF VORTEX-LIKE DOMAIN WALLS IN MAGNETIC UNIAXIAL MULTILAYERED FILMS WITH IN-PLANE ANISOTROPY**

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By numerical solution of Landau-Lifshitz equation, taking into account all interactions (including the dipole-dipole) we investigated the nonlinear dynamics of domain walls in multilayered magnetic films. We considered in detail the films composed of three layers differing both in their thickness and magnetic parameters. Easy axes are parallel to the film surface and each other. Apart from scientific purposes related to the study of nonlinear phenomena the motivation of such investigations is dictated by the possibility of establishing the conditions under which the nonstationary motion of the walls is suppressed and their velocity increases. Novel scenarios of dynamic rearrangement of the wall internal structure are found. In the films 100 nm thick, the rearrangement occurs via creation of two vortexes disposed over one another, while in the single-layer films of the same thickness, the rearrangement occurs by vortex tunneling from one side of a wall to the other. Application of surface layers with other magnetic parameters increases the period of rearrangement of the wall structure or even suppresses its nonstationary motion. Application of the layers with saturation induction  $B_s$  differing from the main layer most effectively suppresses nonstationary motion, however above some critical field no suppressing occurs at any induction.

### **O-3-08**

#### **CALIBRATION OF MAGNETIC FORCE MICROSCOPY PROBES MODIFICATION RESULTING FROM EXTERNAL IN-PLANE MAGNETIC FIELDS**

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Magnetic force microscopy (MFM) measurements in external in-plane magnetic fields are difficult to analyze due to the tilt of the magnetic moment of the MFM tip due to the external magnetic fields. We developed calibration samples with magnetic patterns whose magnetic state is independent on the magnetic field range to determine this tilt. For the fabrication of such topographically planar patterns we used standard lithography methods and keV He ion bombardment of exchange biased bilayers. We will present the production of calibration samples of different materials and a procedure to determine the influence of external in-plane magnetic fields on the magnetic dipole moment of commercial MFM tips.

### **O-3-09**

#### **AB INITIO CALCULATIONS OF THE MAGNETOCRYSTALLINE ANISOTROPY IN $UAuSb_2$ FERROMAGNET**

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Magnetic properties of the tetragonal uranium-transition (or noble) metal diantimonides are studied over the last decade (see [1]). Recently details of the electronic structure of  $UAuSb_2$  obtained from first-principles calculations and X-ray photoemission spectroscopy were reported [2].  $UAuSb_2$  is a strongly anisotropic ferromagnet below 36 K [1]. The present paper presents results of ab-initio calculations of the magnetocrystalline anisotropy of  $UAuSb_2$ . The total energy of the unit cell of  $UAuSb_2$  was calculated by the full potential LMTO method using the LmtART code (for references and details of computations see [1]). The computations were done for the following orientations of the magnetization vector  $\mathbf{M}$ : [1,0,0], [0,0,1], [0,1,1], [1,1,0] and [1,1,1] in the tetragonal unit cell. The differences of the values of the total energy for various pairs of directions of  $\mathbf{M}$  were fitted by the least-squares procedure to the expression for the magnetocrystalline energy suitable for tetragonal symmetry  $E_A = K(\alpha_1^4 + \alpha_2^4) + K_2\alpha_3^2$  where  $(\alpha_1, \alpha_2, \alpha_3)$  is a unit vector along the direction of magnetization  $\mathbf{M}$ . The calculated anisotropy constants at T=0 are  $K = -7.2 \text{ MJ/m}^3$ ,  $K_2 = -2.9 \text{ MJ/m}^3$ . The anisotropy appears to be very strong. The easy axis of magnetization is along [1,0,0].

[1] D. Kaczorowski et al. Phys. Rev. **B58**, 9227 (1998)

[2] J.A. Morkowski et al. J. Alloys Compd. **443**, 20 (2007)

### **O-3-10**

#### **STATICS AND DYNAMICS OF TOPOLOGICAL DEFECTS IN MAGNETIC DOTS**

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A Taylor expansion of dipole-dipole interaction in 2D systems defines a Landau-like local dipolar interaction in spin derivative field. The lowest order of this interaction gives the dipolar anisotropy. The next non zero order is responsible for the appearance of magnetic vortices and hyperbolic defects. The following non zero orders indicate the occurrence of higher topological defects such as double circle and of modulations. The arrangement of self screened topological defects is discussed in agreement with Monte-Carlo simulations and experimental observations. Excited localized modes associated with these defects are classified.

### **O-3-12**

#### **STRUCTURAL, MAGNETIC AND ELECTRONIC PROPERTIES OF STRAINED $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ (LSMO) CRYSTALS STUDIED BY *AB-INITIO* CALCULATIONS.**

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$\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) bulk under strong hydrostatic pressure and uniaxial strain has been studied with three DFT based approaches, i.e. the GGA, the GGA+U, and the PSIC (pseudo self interaction correction). As for the structural properties of the ferromagnetic (FM) phase our calculations show that under hydrostatic pressure the octahedra rotations are reduced and no Jahn-Teller distortions are present. The antiferromagnetic (AF) phases are always disfavoured at all the simulated pressure although they are strongly strengthened by the compression. The AF (metallic) phases competition vs. the FM (half metallic) phase was found to be strongly helped by the JT distortions which necessarily appear in LSMO crystals when a planar strain (corresponding to the experimental growth on  $\text{LaAlO}_3$  and  $\text{YAlO}_3$  substrates) was applied in our simulations: the AF-a order becomes favoured for a system under a planar a vertical compression, while a vertical tension stabilizes the AF-c phase. Thus, our conclusion is that under compression double exchange (DE) weakens (not strengthens, as usually believed) along the applied strain direction as a consequence of carriers depletion at the Fermi energy and of the consequent p-d hybridisation decrease. This work shows that First-Principles calculations represent a capable tool complement to the experiments fundamental in order to design manganese-based devices with improved functionalities.

### **P-3-01**

#### **THE INFLUENCE OF YB SUBSTITUTION ON THE MAGNETIC, ELECTRIC PROPERTIES AND ELECTRONIC STRUCTURE OF $\text{Yb}_x\text{Gd}_{1-x}\text{Ni}_5$ SYSTEM.**

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The crystal and electronic structure, magnetic and electric properties of intermetallic compounds  $\text{Yb}_x\text{Gd}_{1-x}\text{Ni}_5$  ( $x = 0.0, 0.2, 0.4, 0.5$ ) are presented. The change of crystal structure parameters was obtained from XRD measurements which show that all studied compounds crystallize in the hexagonal  $\text{CaCu}_5$  type of crystal structure. The ordering temperatures  $T_C$  were identified from the temperature dependence of AC magnetic susceptibility as well as from the temperature dependence of electrical resistance  $R(T)$ . The values of  $T_C$  obtained from both methods decrease with the increasing of ytterbium concentration. The same behaviour was evidenced for the effective magnetic moment estimated from the temperature dependence of DC magnetic susceptibility. The analysis of the electronic structure studied by XPS method shows that the valence band spectra near by Fermi level are dominated by Ni 3d states. The multiplet structure visible in valence bands is typical for  $\text{Yb}^{3+}$  ions. The satellite structure for Ni 2p core level lines suggest that Ni 3d band is not fully filled.



### **P-3-02**

## **EXCHANGE BIAS FOR A FERROMAGNETIC FILM COUPLED TO A SPIN GLASS**

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For a model system consisting of a ferromagnetic layer coupled to a spin glass extensive Monte Carlo simulations are performed. The spin glass is modeled as Ising system with a nearest neighbor interaction which is Gaussian distributed with zero mean. Its coupling to the ferromagnetic layer is assumed to be either random or ferromagnetic. Exchange bias and all phenomena associated with typical exchange bias systems are observed as a result of a frozen spin glass state.

A main result of our calculations is that the strength of the bias field decreases with increasing strength of the cooling field in qualitative agreement with recent experiments. This is in remarkable contrast to the conventional ferromagnetic/antiferromagnetic systems where the opposite behavior is found. We also found that for small cooling fields the bias field is much stronger for a random exchange interaction across the interface between ferromagnet and spin glass as compared to a ferromagnetic interaction. Both effects have the same origin, namely a stronger susceptibility of the spin glass to a random rather than to a homogeneous field. The coercivity decreases with increasing temperature roughly in a linear way having around the spin glass freezing temperature still about half of its zero temperature value.

### **P-3-03**

## **DIPOLAR MATRIX VS. CROSS-SECTION SHAPE AND SIZE IN MAGNETIC RODS**

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We show the dipolar matrix and the profile of the local dipolar field in nanorods strongly depend on the shape of the structure rod cross-section (structures of circular and square cross-section are compared). The effect of the cross-section shape on the local field proves especially strong (a) in smooth nanorods, in the regions close to their lateral edges, and (b) in cubical structures, in the center; it is there that the calculated values of the local field are much higher in cylindrical rods than in square cross-section ones. In thin films, on the contrary, the difference in the respective local field values is almost uniform across the structure.

### **P-3-04**

#### **DIPOLAR SURFACE UNPINNING AND SPIN-WAVE MODES VS. LATERAL SURFACE DIMENSIONS IN THIN FILMS**

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In rod samples of circular cross section (magnetized along rod's axis) the character of spatial nonhomogeneity of the demagnetization field strongly depends on the aspect ratio (the diameter to length ratio) of the rod. When the aspect ratio is large the sample can be regarded as a thin film of *finite* lateral dimensions. We show the spatial profile of the demagnetization field in a thin film evolves towards a nearly uniform distribution as the lateral dimensions of the film increase. Therefore, the Surface Inhomogeneity (SI) model, in which the value of surface anisotropy (responsible for surface dipole pinning) is assumed to depend on the lateral dimensions of the surface, can be used for description of magnetic excitations in thin films. Derived in this study, a formula for the dipolar surface anisotropy energy (including its dependence on the lateral dimensions) indicates the dipolar surface anisotropy is caused by interactions which bind a surface dipole with *all* the dipoles in the adjacent subsurface layer. Summing up the energy contributions due to these interactions leads to a surprising result: the dipolar surface energy is found to *grow as the surface lateral dimensions decrease* and in the nanometer range of lateral dimensions this energy increases even by as much as an order of magnitude.

### **P-3-05**

#### **THE RKKY INTERACTION WITH DIFFUSED CONTACT POTENTIAL**

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The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is considered when the contact potential is replaced by an arbitrary distribution, instead of the conventional Dirac's  $\delta$ -function. Such approximation describes better the physical situation where the localized spins are attributed to extended electronic orbitals. The appropriate formulas for the RKKY exchange integrals in the case of 1D, 2D and 3D systems are re-derived. In order to exemplify such modification, the three distributions are used for numerical calculations of the RKKY interaction vs. spin-spin distance, namely: gaussian, uniform (rectangular) and exponential ones. It is shown that diffusion of the contact potential removes an unphysical divergency of the RKKY integral at zero distance, and the finite value obtained depends strongly on the distribution width. Moreover, when this width increases, the first minima of the interaction become shallow and rise up towards the positive values, while the amplitude of further oscillations decreases. The strongest effect corresponds to the exponential distribution, and the weakest to the uniform one. For large distances the amplitude of oscillations is reduced by some distance-independent factor, while the period of oscillations remains unchanged and no phase shift occurs. The above generalization of the RKKY interaction is supposed to have remarkable consequences for the thermodynamic description of relevant magnetic systems.

### ***P-3-06***

## **ONE-DIMENSIONAL TIME-DEPENDENT ISING MODEL IN EXTERNAL MAGNETIC FIELD**

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A process of relaxation from the non-equilibrium state described by the Ising model to the equilibrium state has been proposed. The process is described by the action of the transition matrix on the state vector and the requirement of its normalisation. It is assumed that in the state of non-equilibrium the vector of state depend in the same way on the measurable quantities as the eigenvector of the transition matrix corresponding to the highest eigenvalue. Two cases are considered: of the cell composed of one or two sites. The calculations have been performed for a uniform initial state. For the two cases of one and two-site cells the mode of reaching the equilibrium state via magnetisation has been compared. When the external magnetic field and temperature tend to zero, both magnetisation and the correlation function of the nearest neighbours show the critical slowing down phenomenon.

### ***P-3-07***

## **FEATURES OF SH-WAVES PROPAGATION AND LOCALIZATION NEARBY THE 1D MAGNON CRYSTAL SURFACE**

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By using transfer matrix method the influence of magnetoelastic interaction on the normal SH modes spectrum of the semi-infinite 1D magnon crystal with mechanically free surface has been analyzed. In particular, the two-component magnetic superlattice with the ferro- or antiferromagnetic ordered adjacent layers similar to "easy axis ferromagnetic – nonmagnetic dielectric" and the magnetic phonon crystal similar to "easy axis antiferromagnetic - ideal superconductor" were studied. For the represented data we assumed that elastic properties of magnetic and nonmagnetic components of the magnetic phonon crystal are identical. Especially:

- i) existence conditions and dispersion relation for the three case of the surface acoustic SH-waves formation nearby a magnetic superlattice outer surface have been determined;
- ii) the criteria of a nonreflection transmission of shear bulk elastic wave through the semi-infinite 1D acoustically rigid superlattice has been formulated;
- iii) the collective shear surface acoustic wave and the condition can have a nonreciprocity relative to a direction of the SH-wave propagation along the superlattice surface.

### **P-3-08**

#### **AC MAGNETIC SUSCEPTIBILITY STUDIES OF SPIN-GLASS PHASE IN $\text{Ge}_{1-x-y}\text{Sn}_x\text{Mn}_y\text{Te}$ MIXED CRYSTALS**

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We present studies of magnetic and transport properties of  $\text{Ge}_{1-x-y}\text{Sn}_x\text{Mn}_y\text{Te}$  mixed crystals with  $0.083 \leq x \leq 0.142$  and  $0.012 \leq y \leq 0.119$ . Magnetic investigations consisted of AC magnetic susceptibility measurements including linear and harmonic susceptibilities measured as a function of temperature and of applied magnetic field amplitude and frequency. Qualitative analysis of experimental results showed appearance of a spin-glass phase at  $T < 80$  K. Moreover, measurements of AC magnetic moment  $m$  as a function of magnetic field showed hysteretic behavior characteristic of spin-glass systems. Via alloying we are able to tune spin freezing temperature in the range of 10-50 K. Transport characterization (resistivity and Hall effect measurements) of our samples was performed for temperatures between 4.2-300 K. The results showed semimetallic p-type conductivity with large carrier concentrations ( $p > 10^{21} \text{ cm}^{-3}$ ) and relatively low mobilities ( $\mu < 100 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ ). We have also observed the dependence of transport properties on the chemical composition of the sample. Thus, both magnetic and electrical properties in the investigated compound can be tuned via alloying in a wide range.

### **P-3-09**

#### **VOLUME EFFECT ON THE MAGNETISM OF $\text{Fe}_{3-x}\text{Cr}_x\text{Al}$**

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$\text{Fe}_{3-x}\text{Cr}_x\text{Al}$  alloys, in the range  $0 \leq x \leq 0.5$ , crystallise in the  $\text{DO}_3$  type structure. The decrease of the magnetic moment of iron with the increase of the chromium concentration was obtained by Mössbauer measurements [1]. However, detailed theoretical investigations [2] for the experimental values of the lattice constant [1] show a little bit different gradient of the total magnetic moment versus lattice constant. Furthermore there is quite unexpected behaviour of magnetic moment of iron atoms on one of the unequivalent positions for which the magnetic moment increases with the concentration of chromium. It is well known that magnetic moment of pure iron depends strongly on the Wigner-Seitz radii [3]. The purpose of this work is to investigate the dependence of the total and local magnetic moments on the lattice constant using the self-consistent spin-polarised TB LMTO method with changing values of the lattice constant in the range of  $\pm 15\%$  in relation to the experimental values [2].

[1] D. Satuła, et al., J. Magn. Magn. Mater. 169 (1997) 240.

[2] A. Go, et al., Molecular Physics Reports 38 (2003) 86.

[3] D. Bagayoko, J. Callaway, Phys. Rev. B 28 (1983) 5419.

### **P-3-10**

#### **EPR OF $\text{Mn}^{2+}$ IN KAGOME STAIRCASE COMPOUND**



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The electron paramagnetic resonance and magnetic susceptibility of  $\text{Mn}^{2+}$  in geometrically frustrated  $\text{Mg}_{2.97}\text{Mn}_{0.03}\text{V}_2\text{O}_8$  single crystals have reported. The studied crystals have orthorhombic symmetry and are isostructural with known kagome system  $\text{Ni}_3\text{V}_2\text{O}_8$  and  $\text{Co}_3\text{V}_2\text{O}_8$ . The EPR spectrum shows two groups of thirty resonance lines associated with two crystallographically nonequivalent Mn ions positions that are known in the kagome staircase system as "cross-tie" and "spine" sites. Additionally, a strongly anisotropic resonance lines from different  $\text{Mn}^{2+}$ - $\text{Mn}^{2+}$  pairs have observed. The values of the crystal field parameters have obtained from the spectra and the signs of the parameters were determined from the temperature dependence of the intensities of the peaks. The local symmetry of magnetic ions, main values of the hyperfine structure have determined for both manganese positions.

### **P-3-11**

#### **MODELING THERMAL EXPANSION OF $\text{Ni}_2\text{MnGe}$**

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Thermal expansion is important property in numerous applications.

In ferromagnet/semiconductor heterostructures, in which the some Heusler alloys have been recently used, stresses may be generated at the interfaces due to thermal expansion mismatch.

The present study of  $\text{Ni}_2\text{MnGe}$  is focused on describing the thermal properties of the alloy in a framework of first-principles electronic structure calculations coupled with a Debye treatment of the vibrating lattice. The presented  $\text{Ni}_2\text{MnGe}$  Heusler alloy has the cubic  $L2_1$  structure. The electronic structure of  $\text{Ni}_2\text{MnGe}$  has been studied using the full-potential nonorthogonal local-orbital minimum basis method (FPLO). The total energy of the system is found in the full-relativistic calculations based on the first-principles density of states theory (DFT) with the exchange-correlation potential of the Perdew-Wang parametrisation. The theoretical lattice parameter obtained from the dependence of the total energy on the lattice parameter is in agreement with experimental one. In order to make the prediction of the thermodynamic properties of  $\text{Ni}_2\text{MnGe}$  the Debye-Grüneisen model was chosen to account for the vibrational contribution and calculate the coefficient of linear thermal expansion. Two approximations for Grüneisen parameter  $\gamma$ , i.e. Slater's and Dugdale and MacDonald's expressions were assumed.

### **P-3-12**

#### **HYPERFINE INTERACTIONS OF $^{57}\text{Fe}$ IN $\text{Pt}_3\text{Fe}$ – AB INITIO AND MÖSSBAUER EFFECT STUDIES**

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The  $\text{Pt}_3\text{Fe}$  ordered alloy crystallizes in a cubic  $\text{Cu}_3\text{Au}$ -type of structure and shows an antiferromagnetic (AFM) phase transition at  $T_N=150$  K. In the AFM state the  $\text{Pt}_3\text{Fe}$  displays the magnetic structure of  $(1/2,1/2,0)$ -type at high and of  $(1/2,0,0)$ -type at lower temperatures. The Mössbauer measurements show that, despite cubic crystal structure the electric field gradient (EFG) is present at  $^{57}\text{Fe}$  sites. The quadrupolar splitting observed in Zeeman sextet is small and independent on the sample preparation details. The aim of the paper is to elucidate the physical mechanism responsible for the occurrence of the EFG at the  $^{57}\text{Fe}$  nucleus in antiferromagnetic  $\text{Pt}_3\text{Fe}$ . With this aim the *ab initio* electronic structure calculations for  $\text{Pt}_3\text{Fe}$  were carried out for paramagnetic, ferromagnetic and both AFM ground states. The calculations were performed applying the Full Potential version of the Linearized Augmented Plane Wave method. Basing on the results of calculations the  $^{57}\text{Fe}$  hyperfine parameters were determined and compared with the experimental data. The parameters were analyzed in relation to the electronic structure changes upon the magnetic phase transitions. Our investigations indicated that the AFM transition in  $\text{Pt}_3\text{Fe}$  forces the valence charge density reordering. The process results in the lowering of the local charge density symmetry and is responsible for the occurrence of the electric field gradient at the Fe nuclei in the AFM  $\text{Pt}_3\text{Fe}$ .

### **P-3-13**

#### **INFLUENCE OF YTTRIUM SUBSTITUTION ON THE ELECTRONIC STRUCTURE AND MAGNETIC MOMENT OF $\text{Gd}_{7-x}\text{Y}_x\text{Pd}_3$ ( $x = 0, 1, 2, 3, 4$ )**

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Materials based on gadolinium are prospective for applications in magnetic refrigeration cycles. Recently the  $\text{Gd}_5(\text{Ge}_{1-x}\text{Si}_x)_4$  alloys were widely examined [1]. The magnetic properties and temperature dependences of the lattice parameters of  $\text{Gd}_{7-x}\text{Y}_x\text{Pd}_3$  ( $x = 0, 1, 2, 4$ ) single crystals have already been reported [2, 3]. These compounds crystallized in the same type of the crystal structure ( $\text{Th}_7\text{Fe}_3$ ) with the same  $c/a$  ratio of 0.63. A strongly anisotropic behaviour of the magnetic and transport properties was found. The saturation magnetic moment per Gd ion is enhanced in relation to the theoretical value of free ion. Magnetic frustration and spin fluctuations on the palladium atoms are responsible for the complex magnetic properties of these ternary compounds. As a part of current research we present further characteristic of the  $\text{Gd}_{7-x}\text{Y}_x\text{Pd}_3$  single crystals.

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[2] E. Talik, M. Klimczak, R. Troć, J. Kusz, W. Hofmeister, A. Winiarski, J. Alloys Compd., in press.

[3] E. Talik, M. Klimczak, A. Winiarski, R. Troć, J. Crystal Growth, in press.

### **P-3-14**

#### **ANISOTROPY OF THE NEUTRON SCATTERING ON THE Mn<sub>0.71</sub>Ni<sub>0.29</sub> ALLOY**

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The subject of the present experiment is a test of the spatial anisotropy of the neutron scattering in the Mn<sub>0.71</sub>Ni<sub>0.29</sub> alloy. The earlier study of the neutron scattering in the FCC Mn<sub>0.62</sub>Ni<sub>0.38</sub> demonstrated the pronounced uniaxial anisotropy both in the static and dynamical part of the generalized susceptibility. The anisotropy axis is parallel to the scattering-vector reduced to the paramagnetic Brillouin zone. However, no significant anisotropy of the spin-wave scattering was found neither in other Mn-Ni alloys nor in FCC Mn-Fe alloys. The present extension of our study on the Mn-Ni alloys aims to find the concentration dependence of the anisotropy. Our main result for the paramagnetic phase of the Mn<sub>0.71</sub>Ni<sub>0.29</sub> alloy is that the correlation length is bigger for the direction parallel to the anisotropy axis than for the perpendicular one by a factor of 1.5. The spin-wave velocity observed at 15 K is higher for the direction parallel to the anisotropy axis than that for the perpendicular direction by a factor of 1.2. The same factors for the Mn<sub>0.62</sub>Ni<sub>0.38</sub> alloy were: 2 - for the correlation length in the paramagnetic phase and 1.4 - for the spin wave velocity. Within the Heisenberg model the spatial anisotropy is predicted to be more pronounced for the less extended magnetic interaction. Our results indicate that magnetic interactions are less extended for higher Ni concentration.

### **P-3-15**

#### **ON THE CRYSTAL AND MAGNETIC BEHAVIOUR OF ScFe<sub>4</sub>Al<sub>8</sub> SINGLE CRYSTAL**

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Nuclear and magnetic properties of the ScFe<sub>4</sub>Al<sub>8</sub> single crystal attracts our attention owing to the unparalleled complexity of nuclear and magnetic structures. Our previous neutron measurements [1] revealed presence of two modulation vectors, both along  $[\xi\xi0]$  however with different critical temperatures. Recent experiment forced us to revise our knowledge of the structural ordering in the sample. So far, the crystal structure of this alloy, being of ThMn<sub>12</sub>-type, has never been questioned. Let us remind, that the ternary compounds with the general formula MFe<sub>4</sub>Al<sub>8</sub> M=(Ac, Re, Sc) which have been ever reported as crystallizing in the body centered tetragonal I 4/mmm symmetry (no. 139) form a large family of the intermetallics with a variety of magnetic structures and in consequence physical properties. Our earlier studies carried out on crystal and magnetic structures of (U, Th)(FeAl)<sub>12</sub> samples showed identity of crystal structures and ever certain magnetic similarity in both series of actinide's systems. In case of scandium compound these rules turned out to fail.

[1] K. Rećko et al., Phase Transitions, Vol. 80, No. 6-7 (2007) 575-586.

### **P-3-16**

#### **ELECTRONIC STRUCTURE OF $Y_3Al_5O_{12}$ : V SINGLE CRYSTALS, COMPARISON WITH SINTERED CERAMICS**

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$Y_3Al_5O_{12}$  (YAG) single crystal doped with vanadium ions ( $V^{3+}$ ) is one of the few known materials, which show a nonlinear absorption effect. Such materials are especially attractive for Q-switching operation to obtain high peak power optical pulses. Single crystals of YAG: V were grown with use of the Czochralski method. A charge material was prepared on base of high purity oxides:  $Y_2O_3$  (5.0N),  $Al_2O_3$  (5.0N) and  $V_2O_5$  (4.5N) as a dopant. The concentration of  $V^{5+}$  ions was 0.80 at. %.

Recently the YAG ceramics were synthesized to replace the YAG single crystals. These ceramics, which are characterized with similar to the YAG single crystals optical properties, were obtained to increase the doping range, simplify technological process and lower costs.

X-ray photoelectron spectroscopy was used to study the chemical composition and electronic structure of the YAG: V single crystals. The XPS spectra of YAG:  $V^{3+}$  annealed in reducing atmospheres:  $H_2$ , vacuum and vacuum +  $H_2$  are presented and discussed. For comparison the ceramics were investigated. The XPS showed the dopant concentration of  $V^{3+}$  is lower than a nominal one. The aluminium deficiency and yttrium excess for the all measured samples was found. The chemical shift analysis confirmed more ionic bond of Y-O than Al-O.

### **P-3-17**

#### **BRILLOUIN LIGHT SCATTERING INVESTIGATIONS OF MAGNETOELASTIC EFFECTS IN THE MBE GROWN Mo/Co/Au SAMPLES**

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The elastic and magnetic properties of the epitaxially grown  $Al_2O_3$ /Mo(20nm)/Co(d)/Au systems, with  $d=1.2, 10, 31$  (nm), have been investigated by Brillouin light scattering (BLS) from generalized Rayleigh's elastic waves (phonons) and Damon-Eshbach spin-surface modes (magnons). For magnetic-type experiments perpendicular uniaxial anisotropy and in-plane two-fold anisotropy contributions to the energy density were distinguished and the anisotropy constants were determined. The contributions showed tendency to compete mutually. The same tendency was confirmed qualitatively in ferromagnetic resonance (FMR) experiments. For samples with higher uniaxial anisotropies, and lowered in-plane anisotropy contribution, higher BLS-magnon frequencies were observed. Obtained magnetic results were correlated with the measured phonons frequencies. Phonons results were in-plane isotropic and the uniaxial anisotropy contributions affected only the average level of the observed spin-wave frequencies. However, measured phonons frequencies were lower for samples with higher uniaxial anisotropies. Obtained results provide information useful for technology of magnetoelectronic devices.



### **P-3-18**

#### **PRESSURE INDUCED MAGNETIC PHASE TRANSITION IN RMn<sub>6</sub>Sn<sub>6-x</sub>In<sub>x</sub> SOLID SOLUTIONS (R = Y, Lu, Sc)**

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The three HfFe<sub>6</sub>Ge<sub>6</sub>-type compounds: ScMn<sub>6</sub>Sn<sub>5.45</sub>In<sub>0.55</sub>, YMn<sub>6</sub>Sn<sub>5.65</sub>In<sub>0.35</sub> and LuMn<sub>6</sub>Sn<sub>5.1</sub>In<sub>0.9</sub> are characterized by similar magnetic properties. At ambient pressure, they order ferromagnetically about the room temperature ( $293 \leq T_C \leq 356K$ ) and undergo a ferromagnetic to helimagnetic transition upon cooling ( $235 \leq T_t \leq 327K$ ). This paper reports our study on the influence of hydrostatic pressure up to 1.5 GPa on magnetic properties of these solid solutions at low temperature. Increasing hydrostatic pressure under isothermal conditions yields a phase transition from helimagnetic to ferromagnetic order. The obtained (P, T) magnetic phase diagrams are discussed and compared with the corresponding properties of the isotypic compounds RMn<sub>6</sub>Ge<sub>6-x</sub>Ga<sub>x</sub> (R = Y, Lu, Sc).

### **P-3-19**

#### **MAGNETIC PROPERTIES AND MAGNETIC ENTROPY CHANGE IN TERNARY RARE EARTH INTERMETALLICS**

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In this work the magnetic properties, magnetic phase transitions and magnetic entropy changes in polycrystalline ternary rare earth intermetallic compounds are discussed. These compounds crystallize in the tetragonal ThCr<sub>2</sub>Si<sub>2</sub>-type structure with the space group I4/mmm. It is known that the magnetic properties of these compounds are sensitive to the atomic distance and the magnetic structure can be easily modified by external pressure, temperature and magnetic field. The general magnetic phase diagrams for Sm<sub>1-x</sub>Gd<sub>x</sub>Mn<sub>2</sub>Ge<sub>2</sub> are similar to those observed for SmMn<sub>2</sub>Ge<sub>2</sub> under external pressure. For  $0.1 \leq x \leq 0.6$  a typical SmMnGe<sub>2</sub>-like magnetic behavior is observed. In this paper, we discussed the magnetic entropy change  $\Delta S_M$  and magnetic properties deduced by the magnetization and structural properties. For Sm<sub>1-x</sub>Gd<sub>x</sub>Mn<sub>2</sub>Ge<sub>2</sub> with  $x = 0, 0.1, 0.15$ , the value of relative volume  $\Delta V/V$  at magnetic phase transition is negative at T<sub>1</sub> and positive in T<sub>2</sub>. The magnetic entropy change is found to be  $|\Delta S_M(T_1)| = 0.96 \div 1.34$  JK<sup>-1</sup>mol<sup>-1</sup> at the re-entrant ferromagnetic transition and  $|\Delta S_M(T_2)| = 1.05 \div 1.24$  JK<sup>-1</sup>mol<sup>-1</sup> at the antiferro-ferromagnetic one.

### **P-3-20**

## **SYMMETRY INDUCED HALF-METALLIC ALKALINE EARTH FERROMAGNETS**

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Search for new half-metallic ferromagnetic binary compounds composed of alkaline earth and III or IV elements (like Boron or Carbon) is reported. *Ab initio* all-electron density functional theory calculations in the generalised gradient approximation indicate possibility of half-metallic ferromagnetism with Curie temperatures in the range of room temperature. These are a new type of theoretically predicted hypothetical materials without transition metal elements, not yet fabricated. Ferromagnetism is induced by the lack of four-fold crystalline symmetry for lattice constants larger than that of equilibrium for the bulk material. The predominant *s-p* electron mechanism is responsible for the formation of localised magnetic moments and their interactions.

### **P-3-21**

## **THERMODYNAMIC AND RELAXATION DYNAMICS OF THE SPIN-GLASS MODEL WITHIN CLUSTER APPROXIMATION**

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Within the two-particle cluster approximation and within the Glauber dynamics approach we study an Ising-type model with essential competing short-range interaction (first coordination sphere with distribution  $(1-x)\delta(\sigma-1) + x\delta(1+\alpha)$  of interaction and with Gaussian distribution of interaction parameter) and with weak competing long-range interactions for different lattices. The system of equations for average values of dynamic short-range field and dynamic long-range field and its dispersions is found. The linear dynamic susceptibility and  $T-x$  phase diagram are explored. It is shown that at low frequency the imaginary part of the susceptibility exhibits a low-temperature peak which corresponds to the system transition to a non-ergodic state. We demonstrate an essential smoothing of the temperature peaks of the real and imaginary parts of the susceptibility due to macroscopic fluctuations of competing interactions concentration. 1. R.R. Levitskii, S.I. Sorokov, A.S. Vdovych, Cond. Matt. Phys. 8 (2005), 603.

## **P-3-22**

### **MFM INVESTIGATIONS OF $[\text{NiFe}/\text{Au}/\text{Co}/\text{Au}]_N$ MULTILAYERS**

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It was shown that Co layers of certain thicknesses sandwiched between Au layers exhibit perpendicular magnetic anisotropy. Therefore, in sputter deposited  $[\text{NiFe}/\text{Au}/\text{Co}/\text{Au}]_N$  multilayers (MLs), in neighboring ferromagnetic layers in-plane and out-of-plane anisotropy is observed for NiFe and Co layers, respectively. It was also demonstrated that the remnant magnetic configuration of NiFe layers is strongly influenced by stray fields induced by stripe domains in Co layers. Magnetic Force Microscopy (MFM) measurements combined with computer simulations were applied to investigate the strengths of magnetic field over the sample.

All measurements were performed in air atmosphere at RT. Dimensions and density of magnetic domains were estimated. The distribution of magnetization directions was deduced from comparison of MFM with the simulation results. Some sort of modulation in stray magnetic field was observed, but till now it is of unknown origin.

## **P-3-23**

### **ELECTRONIC STRUCTURE OF $\text{Mg}_2\text{Ni}_{1-x}\text{Cu}_x$ ALLOYS**

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Magnesium-based alloys are a good material for absorb and desorb hydrogen [1]. The electronic and electrochemical properties of  $\text{Mg}_2\text{Ni}$  alloy have been investigated during the last years [1-2]. Recently Szajek et al.[2] studied the influence of Pd on the electronic structure of  $\text{Mg}_2\text{Ni}$  alloy. In this work we present the change of the electronic structure of  $\text{Mg}_2\text{Ni}_{1-x}\text{Cu}_x$  for  $0 < x < 0.3$ . The band structure was calculated by FPLO5-CPA [3] and KKR-CPA [4] methods.  $\text{Mg}_2\text{Ni}$  has the hexagonal P6<sub>2</sub>22 type structure and Ni atoms occupy two positions: (3d) and (3b) in the unit cell. In our calculations we substituted Cu atoms into Ni site located at 3d and 3b positions. We observe the change of the electronic properties in the  $\text{Mg}_2\text{Ni}$  doped by copper atoms particularly near the Fermi level.

[1] A. Gasiorowski et al., J.Alloys Compd. 364 (2004) 283.

[2] A. Szajek, I. Okonska, M. Jurczyk, Material Sciences-Poland 25 (2007) 1251.

[3] K. Koepernik, H. Eschrig, Phys. Rev.B.59 (1999) 1743.

[4] H. Akai P. Dederichs, J.Phys.C.18 (1985) 2455.

### **P-3-24**

#### **ELECTRONIC STRUCTURE OF TERNARY ANTIMONIDES PdYbSb**

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The electronic and magnetic properties of the ternary PdYbSb and Pd<sub>2</sub>YbSb Heusler alloys have been studied experimentally and theoretically in the last years. The structural analysis [1] has shown that YbPdSb has a low temperature (LT) MgAgAs-type structure and high temperature (HT) TiNiSi-type structure. In this work we present the electronic structure of YbPd<sub>2-x</sub>Sb compounds calculated by *ab-initio* method. We applied relativistic full potential FPLO7 method [2] in the local spin density approximation (LSDA). The calculations were performed for two types of crystal structures LT and HT for the experimental values of lattice parameters. We have also studied the influence of dilution on the electronic structure of Pd<sub>2-x</sub>YbSb for  $1 < x < 2$ .

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### **P-3-25**

#### **ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF GdN - BULK AND SURFACE EFFECTS**

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The GdN crystallizes in a rocksalt structure and belongs to the family of rare-earth compounds which, due to the highly localized *4f* orbitals, offer interesting magnetic properties for the field of spintronics. Although the electronic properties of GdN were studied previously the band structure of the compound is still under debate.

We present the results of the *ab initio* electronic structure calculations for bulk and surface of GdN carried out in ferromagnetic ground state with the Coulomb correlation interaction for the *4f* manifold taken into account. The calculations were performed applying the Full Potential version of the Linearized Augmented Plane Wave method.

The GdN is strongly correlated electron system and to describe its thermodynamic properties we map it on the one-band Kondo-lattice model. Our aim was to elucidate the finite temperature electrical transport properties. We calculated the self-energy solving numerically equations for the single-electron Green functions. The set of parameters for the many-body Kondo-lattice model was based on the results of single-particle *ab-initio* calculations.

### ***P-3-26***

## **MAGNETIC FIELD INFLUENCE ON CRITICAL ATTENUATION AND VELOCITY VARIATION IN FERROMAGNETS**

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The ultrasound velocity and attenuation are investigated under an application of magnetic field. In the magnetic field six different characteristic regimes are distinguished instead of traditional two (hydrodynamic and critical) found for the case of zero magnetic field. The mean-field Landau-Khalatnikov theory as well as the scaling predictions are given for each regime. Various critical exponents are identified for these regions and compared with the ultrasonic data for MnP. The shift of the ultrasonic attenuation peak under the influence of magnetic field towards higher temperatures, found in various ferromagnets, is discussed

### ***P-3-27***

## **MAGNETIC FIELD EFFECT ON SOUND PROPAGATION IN ANTIFERROMAGNETS**

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On the basis of the theory of phase transitions a model describing anomalies of sound attenuation coefficient close to the antiferromagnet-paramagnet phase transition in magnetic field has been developed. The scaling behaviour of sound velocity and attenuation coefficient was obtained. The physical origin of the two-peak structure in the field dependent ultrasound attenuation observed in a number of antiferromagnets was identified. The theoretical results have been compared with experimental measurements in terbium.

### **P-3-28**

#### **MULTI-STEP MAGNETIC PHASE TRANSITION IN CeRh<sub>3</sub>Si<sub>2</sub> STUDIED BY MEANS OF SPECIFIC HEAT MEASUREMENTS**

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High-quality single crystal of a novel cerium silicide CeRh<sub>3</sub>Si<sub>2</sub>, crystallizing in the orthorhombic ErRh<sub>3</sub>Si<sub>2</sub>-type structure, was grown by Czochralski pulling method in a tetra-arc furnace and studied by means of specific heat measurements. Previous detailed magnetic susceptibility and electrical resistivity measurements [1] have revealed that the compound exhibits strong easy-plane magnetocrystalline anisotropy, orders antiferromagnetically at  $T_N = 4.5$  K and undergoes another phase transition at  $T_t = 4.2$  K. As inferred from the temperature dependence of the specific heat of CeRh<sub>3</sub>Si<sub>2</sub>,  $C(T)$ , the magnetic ordering is very sensitive to applied magnetic field – the phase transitions at  $T_N$  and  $T_t$  split into four separate anomalies, which independently shift to lower temperatures with rising field. Above 1 T these anomalies merge into a single peak in  $C(T)$ , and finally disappear in a field of 2 T. The multi-step character of the magnetic ordering in CeRh<sub>3</sub>Si<sub>2</sub> is very similar to that reported recently for the isostructural compound CeIr<sub>3</sub>Si<sub>2</sub> [2] and may possibly be interpreted in the framework of incommensurate exchange field approach developed for CeSb [3].

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[3] M. Date, J. Phys. Soc. Jpn. 57 (1988) 3682

### **P-3-29**

#### **ELECTRONIC PROPERTIES OF TM<sub>3</sub>V<sub>2</sub>O<sub>8</sub> TM=Mn, Fe and Ni COMPOUNDS**

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Mn<sub>3</sub>V<sub>2</sub>O<sub>8</sub>, Fe<sub>3</sub>V<sub>2</sub>O<sub>8</sub> and Ni<sub>3</sub>V<sub>2</sub>O<sub>8</sub> compounds are interesting magnetic materials that have a complex magnetic order in the kagome staircase. The magnetic and optical properties of TM<sub>3</sub>V<sub>2</sub>O<sub>8</sub> compounds were studied experimentally and theoretically in the last years [1-5]. In this work we present the electronic structure and magnetic properties of TM<sub>3</sub>V<sub>2</sub>O<sub>8</sub> for TM=Mn, Fe and Ni compounds calculated by full relativistic FPLO [6] method within the local spin density approximation. In the LSD+U scheme the values of U parameters were assumed in the range from 5 eV to 7eV for TM elements. These compounds have the orthorhombic (Cmca) crystal structure [1]. The band calculations were performed for the experimental lattice parameters [1-5].

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### **P-3-30**

#### **ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $\text{Ni}_2\text{MnGa}_{1-x}\text{Ge}_x$ AND $\text{Ni}_2\text{Mn}_{1-x}\text{Sn}_x$ HEUSLER ALLOYS**

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The magnetic and electronic properties of  $\text{Ni}_2\text{MnX}$  ( $X=\text{Ga,Ge,Sn,In}$ ) Heusler alloys were studied experimentally and theoretically, recently. In this work we present the influence of atomic disorder in one sublattice on the electronic and magnetic properties of  $\text{Ni}_2\text{MnGa}_{1-x}\text{Ge}_x$  and  $\text{Ni}_2\text{Mn}_{1-x}\text{Sn}_x$  [1] Heusler alloys. Ab-initio band calculations were performed for the experimental lattice parameters. We have applied FPLO-CPA [2] and SPR KKR-CPA [3-5] methods in the local spin density approximation (LSDA).

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### **P-3-31**

#### **ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE $\text{UCoAs}_2$ COMPOUND**

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The  $\text{UCoAs}_2$  compound crystallizes in the tetragonal  $\text{HfCuSi}_2$  type structure with space group  $P4/nmm$  [1]. The compound orders ferromagnetically at 150K with a spontaneous magnetic moment of about  $1.8 \mu_B$  per formula unit. It exhibits a giant magnetic anisotropy alike in the ordered and the paramagnetic region, which has been interpreted as being caused predominantly by strong f-d hybridization and a pronounced crystal field effect [1].

We present results of fully relativistic band structure calculations based on the Full-Potential Local-Orbital Minimum-Basis Scheme (FPLO-5.10-20) [2]. An interesting problem is the magnetic behavior of the Co atoms. In this paper we compare magnetic moments obtained from calculations with and without orbital polarization correction [3].

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## P-3-32

### THE ELECTRONIC AND ELECTROCHEMICAL PROPERTIES OF THE $LaNi_5$ -BASED ALLOYS

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$LaNi_5$ -type alloys exhibit desirable electrochemical properties and are among the most promising electrode materials for nickel-metal hydride (Ni-MH<sub>x</sub>) batteries. They crystallize in the hexagonal  $CaCu_5$  structure and at room temperature can absorb up to 6 H/f.u.. Partial replacement of Ni by Al, Co, and Mn leads to an enhancement of the discharge capacity. Nanocrystalline  $LaNi_5$ -type materials have been prepared by mechanical alloying followed by annealing. The electrochemical properties have been investigated for the following materials  $LaNi_5$ ,  $LaNi_4Al$ ,  $LaNi_3CoAl$  and  $LaNi_{15/4}Mn_{3/4}Al_{1/4}Co_{1/4}$ . Changes in electronic structure are analyzed based on full-potential local-orbital minimum basis bandstructure code FPLO [1], effects of chemical disorder in occupancy of 2c and 3g sites are considered within coherent potential approximation [2]. Total energy calculations allow predicting of site preference by Al, Mn and Co atoms in the  $CaCu_5$ -type unit cell. The impurities reduce the densities of electronic states at the Fermi level comparing to pure  $LaNi_5$  compound.

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## P-3-33

### ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE $Ce_2Co_7B_3$ COMPOUND

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The rare earth compounds  $R_{n+1}Co_{3n+5}B_{2n}$  ( $R$  = rare earth atoms) are interesting as they allow systematic studies of dependence of magnetic moments on local environment, not to mention their relevance to the search for high performance permanent magnets. The compounds crystallize in hexagonal  $CaCu_5$ -type structure, belonging to the  $P6/mmm$  space group. Their structure is generated from  $RCO_5$  ( $n = 0$ ) by replacing Co atoms by B atoms, until the saturation ( $n = \infty$ ) is reached in  $RCO_3B_2$  [1]. The electronic structure of the  $R_{n+1}Co_{3n+5}B_{2n}$  ( $R = Y, Gd, Tb$ ) was studied using TB-LMTO-ASA method [2, 3]. Here we present results for  $R = Ce$  and  $n=3$ ,  $Ce_2Co_7B_3$  compound, based on the fully relativistic FPLO code [4]. The magnetic moments on Co atoms are sensitive to the number of cobalt ions in the local environment and are equal to 1.55, 0.56, and 0.06  $\mu_B/atom$  for Co(2c), Co(6i<sub>1</sub>) and Co(6i<sub>2</sub>), respectively. The density of electronic states is dominated by d-electrons.

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[4] FPLO-5.10-20 improved version of FPLO code by K. Kopernik and H. Eschrig, Phys. Rev. B 59 (1999) 1743; <http://www.fplo.de>



### **P-3-34**

#### **ELECTRONIC STRUCTURE OF THE $U_5Ge_4$ COMPOUND**

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The  $U_5Ge_4$  compound crystallizes in the hexagonal  $Ti_5Ga_4$  type structure having space group  $P6_3/mcm$  [1]. The unit cell has a complex structure containing 18 atoms: the uranium atoms occupy two inequivalent sites, 4d and 6g, and germanium ones also two sites: 6g and 2b. Following the Hill diagram [2], the magnetic properties of the uranium compounds depend on the interuranium distances, which in the case of  $U_5Ge_4$  are the following:  $U(4d) - U(4d) \approx 2.93 \text{ \AA}$ ,  $U(4d) - U(6g) \approx 3.48 \text{ \AA}$ , and  $U(6g) - U(6g) \approx 3.83 \text{ \AA}$ , below and above the Hill limit  $\sim 3.4 \text{ \AA}$ . Magnetic measurements [1] indicate nearly temperature independent paramagnetic behaviour down to 2 K. Previously reported band structure *ab-initio* calculations [3] showed that the magnetic moments can be formed on uranium atoms, and their values are dependent on the local environments. In this paper we present results of calculations obtained based on fully relativistic FPLO code [4]. The values of magnetic moments on uranium atoms are equal to 0.08 and 0.05  $\mu_B$ /atom for U(4d) and U(6g) atoms, respectively.

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### **P-3-35**

#### **MAGNETIC AND ELECTRICAL TRANSPORT PROPERTIES OF THE COMPOUNDS $PrT_2Ge_2$ , WHERE $T = Ni, Ru, Rh, Pd$ and $Ag$**

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The recent discovery of unconventional heavy-fermion superconductivity in the filled skutterudite-type compound  $PrOs_4Sb_{12}$  has ignited much new interest in studying other Pr-based materials. Here we report our results obtained on polycrystalline samples of a few germanides forming with the tetragonal  $ThCr_2Si_2$ -type crystal structure. Measurements of the magnetic susceptibility, magnetization, electrical resistivity, magnetoresistivity and specific heat were performed in wide ranges of temperature (down to 350 mK) and magnetic field (up to 9 T). They revealed antiferromagnetic ground state in  $PrPd_2Ge_2$ ,  $PrAg_2Ge_2$  and  $PrNi_2Ge_2$ , which sets in at  $T_N = 5, 12$  and  $24$  K, respectively. The compound  $PrRu_2Ge_2$  exhibits an antiferromagnetic phase transition at  $T_N = 18$  K that is followed by a ferromagnetic transition at  $T_C = 14$  K. The most complex magnetic behavior was observed for  $PrRh_2Ge_2$ . In the latter compound an antiferromagnetic state develops below as high temperature as  $T_N = 48$  K. In the ordered state the bulk characteristics exhibit some other singularities at about 38, 29 and 21 K, which probably manifest subsequent order-order phase transitions. The magnetic behavior of the entire series is discussed in terms of RKKY exchange interactions and crystal field effects.

## **P-3-36**

### **Room-Temperature ferromagnetism in CdCrTe alloy**

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Cd<sub>1-x</sub>Cr<sub>x</sub>Te solid solution seems to be prospective material for spintronics. We have performed the ferromagnetic resonance experiments on CdCrTe at room temperature. The studies were carried out on the X-band EPR spectrometer. The FMR spectra consist of one broad line with a high value of g factor. We have measured the angular dependence of the resonance field as well as the shape of the line. Magnetic anisotropy observed corresponds to the Van Vleck theory very well. The XRD studies show the CdTe sphalerite crystal structure and exclude the microscopic inclusions of other phase. We have compared FMR results with FMR spectra of CrTe which was initial material in the CdCrTe sample preparation. The nature of the ferromagnetic interactions in the material has been addressed.

## **P-3-38**

### **TO THE ORIGIN OF STRONG ELECTRON CORRELATIONS IN 3d/4f/5f COMPOUNDS**

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Strong correlations are charged to be a reason of inability of the first principles studies based on the local density approximation (LDA) to describe the insulating ground state of 3d/4f oxides causing a need to extend it by using U term (LDA+U), GGA or DMFT approaches. Also strong correlations are regarded to be a reason for heavy-fermion phenomena at low temperatures in cerium, ytterbium or actinide intermetallics. According to the Quantum Atomistic Solid-State Theory (QUASST) the strong correlations are predominantly related with the charge transfer during the formation of a compound and with the intra-atomic correlations leading to the formation of the strongly-correlated atomic like systems  $3d^n$ ,  $4f^n$  or  $5f^n$  with n being an integer number. Such quantum-mechanical object experiences in a crystal the multipolar charge potentials described customarily as the crystal field. We consistently described a monoxide NiO, reconciling its insulating ground state and a strong magnetism related to eight 3d electrons in the incomplete 3d shell, and intermetallic UPd<sub>2</sub>Al<sub>3</sub> for which neutrons confirm a low-energy structure being a fingerprint of the strongly-correlated  $5f^3$  configuration. Recently strongly-correlated  $4f^{13}$  systems have been revealed in heavy-fermion metal YbRh<sub>2</sub>Si<sub>2</sub> at 1.5 K, 15 times lower than the Kondo temperature. We claim that the crystal-field interactions should be evaluated the first for any meaningful description of magnetic and electronic properties both ionic and intermetallic compounds. The many-electron crystal-field approach has inherently incorporated strong-electron correlations.

### **P-3-39**

#### **PHASE TRANSITIONS IN MONOPNICRIDES AND MONOCHALCOGENIDES**

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We consider a wide class of antiferromagnets with a NaCl structure. This class includes binary compounds: mononictides and monochalcogenides of actinides and lanthanides; monoxides MnO, CoO, FeO, NiO; and also MnS and MnSe; and ternary compounds with partial substitution of cations and anions. These antiferromagnets possess very peculiar features that did not obtain the adequate explanation within the framework of existing theoretical models and approaches. In particular, a wide variety of changing magnetic structures with varying temperature and magnetic field, coincidence of magnetic and structural phase transitions of the first order, very strong anisotropy, very special diffuse magnetic neutron scattering above phase transition points, and so on. On the base of magnetic modified 6-state Potts model (for compounds with oblate distortion of magnetic cations) and 8-state Potts model (for compounds with prolate distortion of magnetic cations), we developed a theory of simultaneous magnetic and structural phase transitions of the first order for antiferromagnets with a NaCl structure and with a strong cubic magnetic anisotropy. Temperature evolution of diffuse magnetic scattering of neutrons is calculated and it is shown that the mechanism of the phase transition is conditioned by the high-temperature diffuse scattering transformation into magnetic Bragg reflections below Néel point.

### **P-3-40**

#### **HIGH-FIELD MAGNETISATION AND MAGNETORESISTANCE OF $U_3P_4$ AND ITS SOLID SOLUTION $U_3(P,As)_4$**

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We studied magnetisation and longitudinal magnetoresistance of single-crystal samples of two compositions: stoichiometric compound  $U_3P_4$  and its solid solution  $U_3(P,As)_4$  (with As:P ratio close to 1) in pulsed magnetic fields with strength up to 47 T, and in temperatures from 4K up to few tens of Kelvins above Curie temperatures (135 K and 150 K for both compositions, respectively). Field was applied in hard magnetic direction [100] (easy one is [111] for both compositions). Magnetisation experiments showed no sign of expected metamagnetic transition (similar to that observed for  $U_3As_4$ , at  $\approx 20$  T and 4 K) either for  $U_3P_4$  or for  $U_3(P,As)_4$  and data look quantitatively similar. On the other hand, longitudinal magnetoresistance (MR) is remarkably different for each composition. First it has opposite signs, and moreover strongly nonlinear form of MR(B) curves for  $U_3(P,As)_4$  is strikingly dissimilar to these for  $U_3P_4$ . Onset of the above mentioned transition can be held responsible for broad maxima observed in MR(B) curves for  $U_3(P,As)_4$ . Values of magnetic field strength corresponding to these maxima clearly follow a linear dependence on temperature. We assume that such a bending of MR(B) curves is due to the deformation of magnetic structure of  $U_3(P,As)_4$  in high magnetic fields.

## P-3-41

### EPR STUDY OF $\text{Cd}_4\text{Fe}_8\text{V}_{10}\text{O}_{41}$ VANADATE

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A new multicomponent vanadate  $\text{Cd}_4\text{Fe}_8\text{V}_{10}\text{O}_{41}$  has been synthesized [1] and investigated by electron paramagnetic resonance (EPR) technique. The compound  $\text{Cd}_4\text{Fe}_8\text{V}_{10}\text{O}_{41}$  is isostructural with previously studied  $\text{Mg}_3\text{Fe}_4(\text{VO}_4)_6$  [2]. According to the nominal stoichiometry of the  $\text{Cd}_4\text{Fe}_8\text{V}_{10}\text{O}_{41}$  compound the ions (excepted iron ions) are nonmagnetic. The registered EPR spectra in the 4-300 K temperature range have dominated the presence of very wide almost symmetrical resonance line which is disappeared below 20 K. The resonance line is centered at  $g_{\text{eff}}=2.017(1)$  with linewidth  $\Delta B_{\text{pp}}=77.3$  mT at room temperature. Its amplitude decreases with decreased temperature where below 40 K the linewidth strongly depends from temperature. Below 60 K the resonance line shifts essential with decreasing temperature towards lower magnetic fields. It is suggested the strong magnetic interaction leads to magnetically ordering state. Replacing non-magnetic cations ions by divalent cadmium ions seems to intensify the magnetic ordering processes in the low temperatures region [2].

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## P-3-42

### ELECTRONIC AND MAGNETIC PROPERTIES OF $\text{La}_{1-x}\text{Pr}_x\text{Pb}_3$ ALLOYS

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The low-temperature properties of  $\text{La}_{1-x}\text{Pr}_x\text{Pb}_3$  alloys were studied experimentally in the last years [1-2]. For low concentration of Pr the quadrupolar Kondo effect was observed [2-3]. These systems have  $\text{AuCu}_3$  type cubic crystal structure. In this work we have studied the electronic and magnetic properties of  $\text{La}_{1-x}\text{Pr}_x\text{Pb}_3$  alloys for  $0 < x < 1.0$ . The band structure was calculated by ab-initio FPLO-CPA [4-5] method in the local spin density approximation. The spin polarised band calculations were performed for the experimental lattice parameters. We have applied the full relativistic mode for  $\text{LaPb}_3$  and  $\text{PrPb}_3$  alloys, however in the case of the disordered systems we used the coherent potential approximation in the scalar-relativistic mode. The exchange correlation potential was assumed in the form of [6]. The spin polarised band calculations give the spin magnetic moment on Pr  $m_{\text{spin}}=2.33\mu_B$  and the orbital magnetic moment  $m_{\text{orb}}=-3.11\mu_B$ .

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## **O-4-01**

### **CORRELATION INDUCED SPIN CURRENT POLARIZER**

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We propose a spin polarizer device [1] composed of a quantum dot connected to the spin polarized leads. The spin control of the current flowing through the device is entirely due to the Coulomb interactions present inside the dot. We show that the initial polarization present in the source lead can be reverted or suppressed just by manipulating the gate voltage acting on the dot. The most effective spin current switching is for the gate voltages when the dot level Hubbard subbands cross the chemical potential in the leads. The effect is robust to the increase of temperature and favored by inevitably encountered experimental conditions: asymmetry of the dot-lead coupling and partial loss of the initial current polarization at the dot-lead interface. It also offers a new, correlation-based mechanism for recently experimentally observed sign change of the tunneling magnetoresistance for semiconductor quantum dots coupled to ferromagnetic leads. Moreover, the model can also be applied to the transport description through layered heterostructures with spin-polarized components, where at the interface bound states can be formed due to the spatial confinement and energy structure mismatch.

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## **O-4-03**

### **SPIN DEPENDENT ELECTRON TUNNELING IN A FERROMAGNET SUPERCONDUCTOR FERROMAGNET JUNCTION**

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We study the spin polarized charge transport through a junction consisting of two ferromagnetic metals connected to a superconductor. Using the Bogolubov- de Gennes equation with appropriate boundary conditions we calculate the current and magnetoresistance for the parallel and antiparallel configurations of the magnetic electrodes. In particular, we discuss the nonlocal processes such as the crossed Andreev reflection and elastic co-tunneling. These processes contribute to tunneling a current when the distance between the two magnetic electrodes is comparable to the superconducting coherence length. The dependences of the tunneling transport processes on the strength of the exchange field in the ferromagnetic electrodes, and on the height of the tunnel barriers are presented.

## O-4-04

### ATOMIC DISORDER IN SPUTTERED THIN FILMS OF Co<sub>2</sub>FeAl<sub>1-x</sub>Si<sub>x</sub> Heusler ALLOYS: <sup>59</sup>Co NMR STUDY

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Half metallic ferromagnets are a very important group of materials due to their potential application as electrodes in the TMR and CMR based devices. For this application, full spin polarization and Curie temperature above RT are requested. Co based Heusler alloys (Co<sub>2</sub>FeZ, Z=Al, Si) with L2<sub>1</sub> structure are characterized by the highest Curie temperature among the materials which are theoretically predicted to display a full polarization at the Fermi energy. However, disorder phenomena play an important role for this class of compounds, as some types of antisites disorder destroy the half-metallic properties. Recent theoretical electron structure calculation have shown that the substitution of Al by Si in quaternary Co<sub>2</sub>FeAl<sub>1-x</sub>Si<sub>x</sub> can be seen as an electron doping which stabilizes the Fermi energy at the middle of the minority gap and makes the half-metallic properties less sensitive to disorder effects. In this work we investigate the local structures around Co atoms in Co<sub>2</sub>FeSi<sub>1-x</sub>Al<sub>x</sub> ( $x = 0, 0.5, 1.0$ ) Heusler alloys using <sup>59</sup>Co NMR with spin echo method and discuss their effect on the tunneling magnetoresistance (TMR) for the junctions using Co<sub>2</sub>FeAl<sub>0.5</sub>Si<sub>0.5</sub> electrodes.

## O-4-06

### CHARGE TRANSPORT THROUGH SYMMETRIC AND ANTISYMMETRIC CHAINS OF IONIC BLOCKS

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A new approach to spin-polarised charge transport through short chains, consisting of different ionic blocks, in serial configuration is presented. The ionic blocks with different point symmetry consisting of central cations surrounded by anions, are natural building units of certain semiconducting magnetic oxides. The three-band Hubbard Hamiltonian is used for description of the single ionic block and, subsequently, diagonalised in an exact manner. A minimal, but sufficient set of the single-block four eigen-states, which are linear combinations of the cation and anion atomic states, serves as a good basis for further analysis. The charge transport is mediated by the overlap and resulting hybridisation of wave functions of the nn blocks [1]. A second novel feature of the model lies in working out suitable different adaptations of the non-equilibrium contour Green function technique, employed in a derivation of the electric current, for symmetric and anti-symmetric chains. Symmetric chains have the same outer ionic blocks at their both ends, whereas the outer ionic blocks of the anti-symmetric chains are different from each other [2,3].

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## O-4-07

### SPIN-ORBIT COUPLING EFFECTS IN Fe/GaAs JUNCTIONS

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The spin-orbit interaction, as a fundamental property of a particle motion and its spin, plays an important role in nowadays spintronics investigations. In particular, the spin-orbit coupling gives rise to the tunneling-magnetoresistance effect (TAMR). TAMR essentially means that the tunneling current depends on the direction of the magnetization of the ferromagnet; if strong enough, this anisotropy can give a nice spin-valve-like signal. Important, TAMR has recently been observed in a metallic system, namely, in Fe/GaAs/Au junctions. Surprisingly, while all the bulk components of the system are cubic, the observed anisotropy is twofold. This suggests that rather than coming from the bulk anisotropy of the density of states, the effect arises from the interface that indeed has a reduced symmetry. A phenomenological model reflecting this symmetry in the form of the Bychkov-Rashba and the Dresselhaus spin-orbit coupling was proposed, giving a quantitative fit to the experiment. In the talk we report on comprehensive ab initio calculations of the spin-orbit effects stemming from the interface anisotropy, providing strong support to the phenomenological theory. In particular, we have performed FPLAPW density functional calculations of an Fe/GaAs slab to extract quantitative information about the proposed model as well as to provide guidance to future experiments.

## O-4-08

### FERROMAGNETIC (Ge,Mn)Te SEMICONDUCTOR THIN LAYERS

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Magnetic properties of monocrystalline (Ge,Mn)Te epitaxial layers with varying crystal stoichiometry and carrier concentration have been studied experimentally. The 0.5-1 micron thick (Ge,Mn)Te layers were grown on insulating BaF<sub>2</sub> substrates by molecular beam epitaxy technique with crystal stoichiometry controlled during the growth by applying additional Te molecular flux. Superconducting magnetometry (SQUID) technique was used to study the temperature and magnetic field (up to 7T) dependence of the magnetization of the (Ge,Mn)Te layers with Mn content of 5-20 atomic percent. The results indicated a ferromagnetic transition with the Curie temperature in the range 10-100 K. Depending on the growth conditions, (Ge,Mn)Te layers exhibit either a standard (mean-field like) or an unusual (concave-like) temperature dependence of magnetization, with a broad paramagnet to ferromagnet transition region. In (Ge,Mn)Te layers both standard (in-plane) as well as unusual (normal to the layer plane) location of magnetization easy axis is observed. These experimental findings are discussed considering crystal lattice distortions and stress present in (Ge,Mn)Te layers as well as possible micro-scale phase separation effects of either electronic or physico-chemical origin.

## O-4-09

### TWO-DIMENSIONAL ELECTRON GAS IN A PERIODIC MAGNETIC-FIELD LATTICE

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Recent advances of nanotechnology made it possible to manufacture periodic lattices of magnetic nanocylinders, which can be used to realize a periodic magnetic-field superlattice for the two-dimensional electron gas. Using real parameters of such a field lattice, we theoretically analyzed electronic properties of the electron gas in this lattice. Due to the absence of average magnetic field, the spectrum of "magnetic-field crystal" consists of a set of electron energy bands, and the energy structure can be controlled by varying the amplitude of periodic field. At relatively large fields, the electron bands are almost flat, and the electrons are localized in the vicinity of zero field lines. We found that these lines are closed and form some circles, with the equilibrium persistent currents along the lines, so that the whole "crystal" consists of a periodic lattice of persistent currents. This is related to the chirality of electron states in the magnetic-field lattice. We also demonstrated the existence of anomalous Hall effect in the absence of average magnetic field and zero magnetization. We calculated the Chern numbers characterizing the filled electron bands and demonstrated the quantization of Hall conductivity if the chemical potential is located within the gap.

## O-4-10

### IMPURITY-ION PAIR INDUCED HIGH-TEMPERATURE FERROMAGNETISM IN Co-DOPED ZnO

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ZnO has been the focus, in recent years of intense scientific enquiry. Numerous experimental results reported in the literature supported early mean field predictions of a high critical temperature for the onset of ferromagnetism. The impetus for this research arises from the hope that ZnO may sustain its apparent magnetism above room temperature and thus become a material combining semiconducting, magnetic, optical and mechanical properties, in essence the ultimate multifunctional material. Despite the experimental claims of ferromagnetism in Co doped ZnO a definitive theoretical explanation for the magnetic interaction over long range has so far been lacking. Here we present a mechanism which describes not only the origin of this previously inexplicable magnetism but also explains the experimental findings to date and suggests a recipe for tailoring the magnetic properties of ZnCoO based spintronic devices. We demonstrate that the magnetism originates from a Co<sup>2+</sup> oxygen vacancy pair (CoV) with a partially filled level close to the ZnO conduction band minimum. The long range coupling then occurs via conduction electrons at moderate n doping. Furthermore we demonstrate how experimental findings may be explained by a combination of this proposed mechanism and superparamagnetically blocked clusters. Based upon these results we are now in a position to propose a definitive phase diagram of ZnCoO.



### **P-4-01**

## **TRANSFORMATION OF THE POLARITONIC SPECTRUM OF A ONE-DIMENSIONAL MAGNETIC PHOTONIC CRYSTAL IN EXTERNAL CROSSED DC ELECTRIC AND MAGNETIC FIELDS**

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The conditions are determined for a one-dimensional magnetic photonic crystal (*MPC*), under which square-low magneto-optical interaction leads to a number of specific features upon propagation and localization of magnetic *TE* and *TM* polaritons in external crossed dc electric  $\mathbf{E}$  and magnetic  $\mathbf{H}$  fields. Superlattice of easy-axis antiferromagnet nonmagnetic dielectric type choose as a basis for *MPC*. Easy magnetization axis of antiferromagnet  $\mathbf{l}$ , external electric  $\mathbf{E}$  and magnetic  $\mathbf{H}$  fields are mutually perpendicular ( $\mathbf{H} \perp \mathbf{E} \perp \mathbf{l}$ ).

In particular it is shown: i) The spectrum of normal and surface magnetic polaritons is nonreciprocal ( $\omega(\mathbf{k}) \neq \omega(-\mathbf{k})$ ). ii) Dispersion properties and character of localization of polaritonic excitations being dependent essentially on the ratio of electric and magnetic fields  $E/H$ , and relative orientation of vectors  $\mathbf{E}$ ,  $\mathbf{H}$  and  $\mathbf{n}$  ( $\mathbf{n}$  is unit vector of a normal line to surface of a superlattice). iii) Varying size of magnetic and electrical fields it is possible effectively and in a wide range to change character of refraction of bulk electromagnetic wave which falling from without on a surface of *MPC*.

### **P-4-02**

## **SPIN-DEPENDENT TUNNELING CURRENT IN MAGNETIC TUNNEL JUNCTIONS**

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The tunneling current through a hybrid structure where a confined nonmagnetic insulator is sandwiched between two ferromagnetic metals is calculated within the non-equilibrium Keldysh formalism. The metals are assumed to be band ferromagnets, such as Co, and are described by the single-band Hubbard model. The interaction is treated both in Mean Field (MF) and the Spectral Density Approximation (SDA) which takes into account higher correlations. It is found that the SDA gives better physical results over a broad parameter range than the simple MF approximation.

Special emphasis is made to explain the tunneling current features in terms of the quasi-particle density of states of the materials. Also the relationship between the current and the inter-layer exchange coupling is discussed. Furthermore we show how a generalization of the model presented here can be used to model current-induced switching of magnetization in a self-consistent way.

### **P-4-03**

#### **MAGNETIC, TRANSPORT AND POSITRON ANNIHILATION STUDIES OF $\text{Zn}_{1-x}(\text{Mn};\text{Co})_x\text{GeAs}_2$ SEMIMAGNETIC SEMICONDUCTOR**

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We have performed magnetic, transport, and defect studies of  $\text{Zn}_{1-x}(\text{Mn};\text{Co})_x\text{GeAs}_2$  mixed crystals with  $0.052 \leq x \leq 0.182$ . Magnetic investigations showed appearance of a ferromagnetic phase for  $x \geq 0.078$  with  $T_C > 320$  K. Transport measurements performed at  $1.3 \leq T \leq 400$  K included basic resistivity and Hall effect measurements as well as high magnetic field (up to  $B = 13$  T) studies. Our results showed p-type conductivity (semiconducting or metallic, depending on the alloy composition) with carrier concentrations  $p > 10^{19} \text{ cm}^{-3}$ . High magnetic field studies revealed negative magnetoresistance for  $T < 15$  K (up to 33%) with values strongly depending on the sample composition. We were also studying Schottky type defects using positron annihilation spectroscopy technique. Results of positron lifetime and Doppler broadening measurements showed that there are significant differences in defect parameters for samples with different compositions. Performed measurements showed that via alloying we are able to control significantly many properties of studied semimagnetic semiconductor.

### **P-4-04**

#### **SPIN-DEPENDENT TRANSPORT THROUGH A METALLIC SYSTEM WITH MAGNETIC IMPURITIES**

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The problem of spin-dependent transport of electrons through a metallic nanostructure is considered. The system consists of non-magnetic metal with two magnetic impurities and is connected to two ferromagnetic leads. The differential conductance is calculated by using the transfer matrix method.

## **P-4-05**

### **AB-INITIO STRUCTURAL, ELECTRONIC AND TRANSPORT PROPERTIES OF $\text{Fe}_{1-x}\text{Co}_x/\text{AlAs}/\text{Fe}_{1-x}\text{Co}_x$ (001) TUNNEL JUNCTION**

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The electronic structure of  $\text{Fe}_{1-x}\text{Co}_x/\text{AlAs}/\text{Fe}_{1-x}\text{Co}_x$  (001) heterostructures are calculated by means of a self-consistent Green's function technique implemented in the framework of the tight-binding linear muffin-tin orbital method (TB-LMTO) in its atomic sphere approximation (ASA) and in conjunction with the coherent potential approximation (CPA) in order to describe the interdiffusion at the FeCo/AlAs interfaces. The conductance and the tunneling magnetoresistance ratio (TMR) are estimated in the current perpendicular to-the-plane geometry (CPP) by means of the transmission matrix formulation of the Kubo-Landauer approach. The results show that at the FeCo/AlAs interfaces there is a net charge transfer from the FeCo magnetic slab to the AlAs semiconducting spacer resulting in a Schottky barrier. The magnetic behavior of interface Fe and/or Co atoms are dependent on the interface structure as well as on the semiconductor terminations. Thus, at the Fe/AlAs interface for Al termination the Fe magnetic moment increase over corresponding bulk value and for As termination it remains almost unchanged while at Co/AlAs interfaces, for both terminations, the Co magnetic moment is reduced. The TMR ratio is composition dependent and increase from 15% up to 60% with increasing Co concentration. Also, the TMR values are sensitive to the semiconducting spacer terminations.

## **P-4-06**

### **MAGNETIC AND SPIN-DEPENDENT TRANSPORT PROPERTIES OF $\text{Co}/\text{Cu}/\text{Ni}$ JUNCTION**

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The electronic structure of fcc  $\text{Co}/\text{Cu}/\text{Ni}$  (001) trilayer systems have been studied by means of a self-consistent Green's function technique based on the tight-binding linear muffin-tin method (TB-LMTO) in the atomic sphere approximation (ASA). The results show that at the Co/Cu interfaces the cobalt magnetic moment retains its bulk value while at the Ni/Cu interfaces the nickel magnetic moment is reduced. The different magnetic behavior of interface Co and Ni atoms are explained as a competition effect between the narrowing of the density of states (DOS) at the Fermi Level due to the low coordination number and respectively, the hybridization between Co(Ni) and Cu states. An oscillatory interlayer exchange coupling with respect to the Cu spacer thickness is evidenced. The conductance and the giant magnetoresistance ratio (GMR) in the current perpendicular to-the-plane geometry (CPP) are calculated by means of the transmission matrix formulation of the Kubo-Landauer formalism. In either anti- or ferromagnetic states the conductance is determined by the majority-spin electrons whose contribution to the transmission amplitude is higher due to the difference in the electronic structure at the Co(Ni)/Cu interfaces. Damped oscillations of the GMR ratio with increasing Cu spacer thickness are obtained.

## **P-4-07**

### **SPIN TORQUE IN DOUBLE PLANAR TUNNEL JUNCTIONS**

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In ferromagnetic tunnel junctions with non-collinear orientations of magnetizations of the electrodes, a spin torque is generated due to a spin transfer from conduction electrons to localized magnetic moments. This torque can lead to the switching of magnetic configuration, which may be useful for applications in magnetic memories. Two components of the torque exerted on the central electrode of the double junction are analyzed in the free-electron-like model. The in-plane component lies in the plane determined by the magnetic moments, while the normal one is perpendicular to this plane. The torque depends on the orientation of magnetization in the central layer, described by the angle  $\theta$ , and on the relative orientation of the leads' magnetizations. In junctions with a thick central layer and for small bias voltages, the magnitude of the in-plane torque is generally smaller in the parallel configuration of spins in the leads than in the antiparallel one. The opposite relation is observed for the normal torque. The spin torque depends strongly on the central layer thickness and can be essentially enhanced for special thickness of this layer. The  $\theta$  dependence of the torque appears to be more complex than in single tunnel junctions.

## **P-4-08**

### **PHONON-ASSISTED KONDO RESONANCE IN SPIN-DEPENDENT TRANSPORT THROUGH A QUANTUM DOT**

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Electron transport through a quantum dot coupled to ferromagnetic electrodes is studied in the Kondo regime and effects of local vibrational modes on transport characteristics are analyzed. The approach is based on the non-equilibrium Green function formalism using the equation of motion method. For symmetric junctions and antiparallel configuration of magnetic moments the Kondo anomaly in differential conductance appears in the zero bias limit and the two Kondo satellites due to coupling to phonon bath develop at phonon energies  $\pm\omega$ . In the parallel configuration the main resonance is split and the two components move away from the zero bias limit. The Kondo satellites move accordingly. Positions of the main peaks and their satellites depend on the leads polarization and on the electron-phonon coupling strength. In non-symmetric systems the shifting of the main components and their satellites takes place also in antiparallel configuration. As a compensating magnetic field is applied, the splitting is fully reduced and the main resonance appears at the zero bias, whereas the satellites appear at energies  $\pm\omega$ .

## **P-4-09**

### **MAGNETIC SWITCHING OF SINGLE-MOLECULE MAGNETS BY CURRENT PULSES**

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Dynamics of current-induced magnetic switching (CIMS) of a single magnetic molecule (SMM) weakly coupled to two ferromagnetic contacts with collinear magnetic moments is investigated theoretically. Electronic transport is assumed to take place *via* the lowest unoccupied orbital (LUMO) level of the molecule. In such a case, the CIMS can occur as a result of exchange coupling between the electrons in the LUMO level and the molecule's spin. The key objective of the work is to analyze the possibility of the SMM's spin manipulation with short current pulses, which is believed to be a promising method for writing a bit of information in the molecule. Furthermore, the role of physical processes influencing the molecule switching is considered with the main emphasis put on the intrinsic spin relaxation in the molecule. Time dependence of transport characteristics as well as the average value of the total spin is derived by means of the perturbative approach and relevant master equations. It is shown that despite spin relaxation a current pulse of a proper length can be used to switch the magnetic moment of the molecule. The obtained results are discussed in terms of potential applications of SMMs as elements of novel spintronics devices.

## **P-4-10**

### **AB INITIO CALCULATIONS OF MAGNETIC PROPERTIES OF WURTZITE $\text{Al}_{0.9375}\text{TM}_{0.0625}\text{N}$ , (TM=V, Cr, Mn, Fe, Co, Ni)**

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The electronic and magnetic properties of  $\text{Al}_{1-x}\text{Mn}_x\text{N}$  in zinc-blende phase were studied recently [1, 2]. In this work we have analyzed the influence of six transition metals from V to Ni on the electronic and magnetic properties of wurtzite AlN. We applied an ab initio method based on density functional theory within generalized gradient approximation (GGA) and the pseudopotential method [3]. The spin polarized self-consistent calculations were made for the supercell of 32 atoms. The transition metal was substituted in the place of Al.

In case of Co, Cr and Mn the electronic states at the Fermi level are 100% spin polarized. In other cases we obtain zero density of states at Fermi level.

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## **P-4-11**

### **CURRENT-PULSE-INDUCED SWITCHING OF SYMMETRIC AND ASYMMETRIC SPIN VALVES**

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Spin-polarized current can transfer spin angular momentum from conduction electrons to localized magnetic moments and generate magnetic switching and magnetic excitations. This phenomenon is important for its wide range of technological applications, including magnetic memory and magnetic sensors. By this reason designing of new bistable devices able to be fast switched by electric current as well as thorough understanding of the current-induced spin dynamics are needed. Therefore, we have performed relevant dynamical study of the standard spin valve Py/Cu/Py and the asymmetric one Co/Cu/Py, both connected to Cu electrodes. The dynamics has been described in terms of the macrospin model, using the generalized Landau-Lifshitz-Gilbert equation. The thermal effects have been considered and modelled by an additional stochastic magnetic field. The spin transfer torque has been calculated in the diffusion transport limit. Detailed dependence of switching properties of examined pillars on the relevant current-pulse parameters has been obtained.

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## **P-4-12**

### **FIRST PRINCIPLES STUDIES OF MAGNETIC PROPERTIES OF WURTZITE Ga<sub>0.9375</sub>TM<sub>0.0625</sub>N, (TM=V, Cr, Mn, Fe, Co, Ni)**

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The aim of this work is study of the influence of V,Cr,Mn,Fe,Co and Ni on the electronic and magnetic properties of Ga<sub>1-x</sub>TM<sub>x</sub>N in wurtzite structure. The electronic structure of zinc-blende phase were studied recently [1,2]. In this work we present the results obtained by ab initio method based on the density functional theory within generalized gradient approximation (GGA) and the pseudopotential method [3]. The calculations were performed for 32-atoms supercell model. The transition metal was substitute in the place of Ga. For Cr, Fe, Ni and Mn the electronic states at the Fermi level are 100% spin polarized, however for V and Co atoms the densities of states at the Fermi level are partially polarized.

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### **P-4-14**

## **EFFECT OF SPIN-FLIP PROCESSES ON ELECTRONIC TRANSPORT THROUGH A QUANTUM COUPLED TO FERROMAGNETIC ELECTRODES**

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Using nonequilibrium Green function formalism the spin-polarized electronic transport through a quantum dot coupled to ferromagnetic electrodes is studied. Arbitrary Coulomb correlations and spin-flip processes are considered within the dot, for both parallel (P) and antiparallel (AP) magnetic configurations of the junction. It is found that spin-flip processes suppress the magnetoresistance between each pair of the threshold bias voltages, thus giving rise to sharp TMR maxima at the thresholds. Spin-flips reduce also the magnetically induced asymmetry in the current-voltage characteristics with respect to the bias reversal. The spin relaxation on the dot may lead to accumulation of the spin transverse components on the dot, to a negative differential conductance, to splitting of the resonance peaks in the differential conductance as well as to widening of the corresponding TMR maxima at threshold bias voltages. It is also found that in the linear response limit TMR may be inverted and significantly enhanced due to spin-flip processes on the dot. Interestingly, a similar behavior of TMR in the linear response regime was observed recently in experiments on tunneling through semiconducting quantum dots coupled to nickel or cobalt electrodes.

### **P-4-15**

## **MAGNETIC AND MAGNETOTRANSPORT PROPERTIES OF MAGNETITE/Co-FERRITE TRILAYERS**

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The aim of this work was the investigation of the magnetic and magnetotransport properties of  $\text{Fe}_3\text{O}_4/\text{CoFe}_2\text{O}_4/\text{Fe}_3\text{O}_4$  tunnelling junctions. The trilayers were fabricated by pulsed laser deposition from stoichiometric  $\text{Fe}_3\text{O}_4$  and  $\text{CoFe}_2\text{O}_4$  targets onto MgO (001) substrates at  $450^\circ\text{C}$  in an oxygen partial pressure of  $10^{-5}$  mbar. Magnetization measurements indicate significant Co diffusion into the bottom magnetite layer. Vertical magnetotransport measurements were performed with the current flowing between the magnetite electrodes. The magnetoresistance was comparatively small and did not exceed 3% in a magnetic field of 0.5 T. At lower temperatures the magnetoresistance measurements showed two clearly separated maxima. Since the current-voltage characteristics were linear, spin dependent tunnelling is excluded as origin of this magnetoresistance. It is rather attributed to anisotropic and grain-boundary magnetoresistance in the magnetically hard and soft layers. Comparison of full and minor resistance hysteresis loops did not reveal any significant exchange coupling between the layers, presumably due to diffuse interfaces.

## **P-4-16**

### **MAGNETIC MICROSTRUCTURE AND ELECTRICAL PROPERTIES OF EUROPIUM FERROMANGANITES**

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Crystalline structure, magnetic microstructure, electrical properties; conductivity, thermopower and magnetoresistance of perovskite-like europium ferromanganites were investigated. The  $Eu_{0,65}Sr_{0,35}Mn_{1-x}Fe_xO_3$  ( $x=0.2; 0.25; 0.3; 0.35; 0.4$ ) samples were prepared using the ceramic method from mixture of oxides. Fe-57 isotope was added to the concentration 20-25 % during synthesis. The single-phase nature of samples was controlled by X-ray diffraction. All ferromanganites were studied by Fe-57 and Eu-151 Mossbauer spectroscopy. The spectra of samples with low Fe concentration contain only paramagnetic doublet. The spectra of samples with  $x=0,35$  and  $x=0,4$  contain, beside quadrupole doublet, two Zeeman sextets with  $H = 450$  kOe and relatively intensity of 50-60 %. All samples under investigations were n-type semiconductors. The activation energy of conductivity is 0,1 eV for all samples. This value is approximately 1/2 of energy gap, calculated for the rare-earth ferromanganites. In the  $Eu_{0,65}Sr_{0,35}Fe_{0,4}Mn_{0,6}O_3$  we observed "bipolar" magnetoresistense: negative at the temperatures below 316 K, and positive at higher temperatures. Positive MR have value 12 % at relatively small field ( $B \approx 0,6$  ).

## **P-4-17**

### **ANOMALOUS HALL EFFECT IN IV-VI SEMICONDUCTORS**

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In ferromagnetic metals and magnetic semiconductors, the off-diagonal conductivity is proportional to the external magnetic field, which is connected with ordinary Hall effect, and an additional term which is proportional to the magnetization of the sample and does not disappear at zero magnetic field. This extraordinary term is known as the anomalous Hall effect (AHE). The origin of the AHE is the spin-orbit interaction in the presence of spin polarization. There are two groups of mechanisms that are responsible for AHE: so called extrinsic mechanisms (skew scattering and side jump) and intrinsic mechanisms which are related to the topology of electron energy bands.

We consider narrow-gap IV-VI magnetic semiconductors where the relativistic terms are not small and determine both the non-parabolicity of the energy spectrum and strong spin-orbit interaction. We use the relativistic Dirac model and the theory of linear response to calculate the topological contribution to the off-diagonal anomalous Hall conductivity. We also present some experimental data and make the comparison of numerical and experimental results. Owing to this, we can estimate the magnitude of intrinsic contribution to AHE in IV-VI magnetic semiconductors.



## **P-4-18**

### **CURRENT-INDUCED MAGNETIC DYNAMICS IN FERROMAGNETIC SINGLE-ELECTRON DEVICES**

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Current-induced dynamics of a magnetic moment of the central electrode in a ferromagnetic single-electron transistor is considered theoretically. The spin-transfer torque due to spin current absorbed by the central electrode is calculated numerically in the sequential tunneling regime. Spin accumulation in the central electrode has been taken into consideration. Such spin relaxation appears in the limit of slow spin relaxation. The description and numerical calculations are limited to the in-plane component of the spin torque, assuming that the out-of-plane component of the spin torque is small and therefore can be omitted. Dynamics of the magnetic moment of central electrode is described by the Landau-Lifshitz-Gilbert equation, which includes the torques due to magnetic field (external and internal), damping processes, and spin current. The time evolution of the magnetic moment has been obtained by integrating numerically the Landau-Lifshitz-Gilbert equation. The conditions which are necessary for switching the magnetic moment are also discussed.

## **P-4-19**

### **MAGNETIZATION PROCESS AND MAGNETIC ANISOTROPY OF Ga<sub>1-x</sub>Mn<sub>x</sub>As ON GaAs (311)A SUBSTRATE**

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We have studied magnetization processes and magnetic anisotropy of Ga<sub>0.94</sub>Mn<sub>0.06</sub>As thin film grown by low-temperature molecular beam epitaxy on GaAs (311)A substrates by means of superconducting quantum interference device (SQUID) and magneto-optic microscopy. The magnetization curve obtained by SQUID are explained phenomenologically using two main contributions to the magnetic anisotropy: a cubic magnetocrystalline anisotropy with easy <001> axes, and an effective uniaxial magnetic anisotropy with hard axis along [311] caused by the epitaxial compressive strain from the substrate. We find the uniaxial anisotropy constant to depend linearly on  $M_S^2$  and the cubic anisotropy constant to follow  $M_S^4$  (here  $M_S$  is saturation magnetisation), confirming the validity of the single domain model used to describe magnetization rotations in this material. Our results are in agreement with ferromagnetic resonance data<sup>1</sup> and expectation of the p-d Zener model of the carrier mediated ferromagnetism<sup>2</sup>.

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### **P-4-20**

## **TRANSPORT THROUGH INHOMOGENEOUS MAGNETIZATION TEXTURES - DOMAIN-WALL RESISTANCE**

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We use the Keldysh Greens function formalism to derive transport equations for conducting magnetic materials with a ferromagnetic order parameter that can be inhomogeneous in space and time. Spin-flip scattering at magnetic impurities is also included. We consider a contact with a quasi one-dimensional geometry, in which the current flows in the same direction as the magnetization gradient of a single domain wall. In the diffusive regime and in the limit of walls much longer than the spin-diffusion length, it is possible to obtain analytical results for the domain-wall resistance which can also become negative. Our results differ from previous works, which used different theoretical frameworks like Kubo formula.

### **P-4-21**

## **KONDO EFFECT IN CARBON NANOTUBE QUANTUM DOT IN A MAGNETIC FIELD**

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The out-of-equilibrium electron transport of carbon nanotube semiconducting quantum dot placed in a magnetic field is studied in the Kondo regime. The mean field finite U slave boson approach of Kotliar Ruckenstein and the equation of motion method are used. For parallel magnetic field the Kondo peak splits in four peaks, following the simultaneous splitting of the orbital and spin states. As a consequence the high conductance lines on bias voltage-field plane are observed. For orbitally nondegenerate states the field can recover orbital degeneracy and high spin polarization of conductance results. Finite direct or tunneling interorbital mixing prevents the full recovery of degeneracy and nonmonotonic field dependence of conductance is observed.

## **P-4-22**

### **TRANSPORT PROPERTIES OF SINGLE-WALL METALLIC CARBON NANOTUBES WEAKLY COUPLED TO FERROMAGNETIC LEADS**

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Using the real-time diagrammatic technique and taking into account both the sequential and cotunneling processes, we analyze the transport properties of single-wall metallic carbon nanotubes coupled to ferromagnetic leads in the full range of parameters. In particular, considering the two different shell filling schemes of the nanotubes, we discuss the behavior of the differential conductance, tunnel magnetoresistance and the shot noise. We show that in the Coulomb diamonds corresponding to even occupations, the shot noise becomes super-Poissonian due to bunching of fast tunneling processes resulting from the dynamical channel blockade, whereas in the other diamonds the noise is roughly Poissonian, in agreement with recent experiments. The tunnel magnetoresistance is very sensitive to the number of electrons in the nanotube and exhibits a distinctively different behavior depending on the shell filling sequence of the nanotube. Furthermore, the TMR also strongly depends on the spin state of the nanotube. When the ground state of the nanotube is a triplet, the TMR becomes much enhanced as compared to the situation where the ground state is a singlet.

## **P-4-23**

### **IMPLEMENTATION OF A SPINTRONICS FULL ADDER**

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In this paper a novel technique has been proposed for the implementation of the spintronics FULL ADDER using the concept of magnetic resonant tunneling diode. Both the quantum well (QW) and the injector are made of dilute magnetic semiconductor which exhibit giant Zeeman splitting (GZS) on application of magnetic field. The field in the injector region is to be kept ON always at a fixed value to give a constant desired GZS. The field in the QW is switched on and off and it acts as one of the input bits. A gate is provided around the QW region so that shifting of the energy levels in the well is possible by application of gate bias which acts as the second input bit. The spin of the electron is taken to be the 3<sup>rd</sup> input bit while the current is the output. In the paper the principle for realization of the sum and carry has been elaborated. It has also been proved that any logic function with three bit input can be realized with the help of magnetic RTD by proper control of the device structure parameters.

## **P-4-24**

### **EXCHANGE COUPLING IN WEDGED Fe/Ti/Fe TRILAYERS**

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Fe/Ti/Fe trilayers with wedge-shaped Ti interlayer were prepared using UHV magnetron sputtering. The planar growth and interface alloying of the Fe and Ti layers was confirmed in-situ by X-ray photoelectron spectroscopy. Furthermore, structural and magnetisation studies revealed spontaneous formation of a quasi-amorphous Fe-Ti alloy layer at the interfaces during the deposition process. The hysteresis measurements showed that the Fe layers are weakly ferromagnetically (FM) coupled for  $\sim 3.5 \text{ nm} > d_{\text{Ti}} > \sim 2 \text{ nm}$ . The above behaviour was also revealed by systematical domains observation during the magnetisation reversal process in a magnetic field equal to  $H_c$ . Above  $d_{\text{Ti}} > 3.5 \text{ nm}$  a progressive transition to large independent domains takes place. The rapid decrease of the interlayer exchange coupling could be explained by its strong damping due to formation of a non-magnetic quasi-amorphous Ti-Fe alloy layer at the interfaces.

## **P-4-25**

### **INFLUENCE OF ANNEALING ON CRYSTALLIZATION AND MAGNETIC PROPERTIES OF SPIN VALVE MgO BASED TUNNEL MAGNETORESISTANCE JUNCTIONS**

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Exchange bias spin valves (EB - SV) with different thicknesses  $t$  of the amorphous  $(\text{Co}_{52}\text{Fe}_{48})_{75}\text{B}_{25}$  electrodes: glass/Ta5/Ru18/Ta3/Pt<sub>46</sub>Mn<sub>54</sub>20/Co<sub>82</sub>Fe<sub>18</sub>20/Ru0.9/ $(\text{Co}_{52}\text{Fe}_{48})_{75}\text{B}_{25}(t)/\text{MgO}1.35/(\text{Co}_{52}\text{Fe}_{48})_{75}\text{B}_{25}(t)/\text{Ru}5/\text{Ta}5$  ( $t = 3, 7, 15 \text{ nm}$ ) were prepared by sputtering deposition and annealed from 340 °C to 375 °C. X-ray diffraction analysis (XRD), vibration sample magnetometer (VSM), magneto-optical Kerr effect (MOKE) hysteresis and domain structure imaging were performed. XRD showed that CoFeB electrodes are amorphous in as-deposited state and crystallize to bcc(200) CoFe phase after annealing. The bottom CoFeB electrode deposited on thin Ru exhibited weaker crystallization than the top electrode on (100) oriented MgO. MOKE and VSM measurements showed that annealing above phase transition temperature led to increase of coercivity of the top CoFeB due to higher anisotropy of crystalline CoFe than amorphous CoFeB. This correlates with domain imaging: for as-deposited samples large domains were observed, after annealing their size significantly decreased. Tunneling magnetoresistance of the samples with  $t = 3 \text{ nm}$  increased with temperature and reached 138 %. This work was supported by the EU MRTN-CT-2006-035327 SPINSWITCH.

## **P-4-26**

### **INELASTIC COTUNNELLING MEDIATED SINGLET-TRIPLET TRANSITION IN CARBON NANOTUBES**

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Cotunnelling transport through a quantum dot (QD) is one of the simplest quantum many-body effects. In the Coulomb-blockade regime, when sequential tunnelling of single electrons in a dot is suppressed, only two (or more) electrons may tunnel in the correlated manner: into and simultaneously out of the dot leaving dot's charge unchanged. We study experimentally as well as theoretically the cotunneling transport in a carbon nanotube quantum dot for even and odd occupancy regimes. In both regimes characteristic cotunneling resonances were observed in the transport current  $I$  as a function of magnetic field  $B$  centered at  $B = 0$  ( $B > 0$ ) for odd (even) dot's occupancy. While for odd occupancy the signal is associated with the Kramers doublet, for the odd occupancy it is related to the singlet-triplet transition (STT). This experimental setup ( $I$  vs.  $B$ ) provides clear separation between elastic and inelastic cotunneling components. Different coupling strengths of the QD's levels allow mapping of the STT model into the model of a QD attached to ferromagnetic leads, where the non-equilibrium spin accumulation and spin-dependent transport are expected. The theoretical study of the second order perturbation theory agrees well with the experiment, which allows precise fit of the cotunneling line shape and extraction of the information about effective spin asymmetry, spin accumulation, and spin-flip relaxation in the dot.

## **P-4-27**

### **SPIN-POLARIZED SEQUENTIAL TUNNELING THROUGH QUANTUM DOTS COUPLED TO MAGNETIC LEADS: A REAL-TIME DIAGRAMMATIC APPROACH.**

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Spin-dependent transport through two coupled single-level quantum dots attached to ferromagnetic leads with collinear (parallel and antiparallel) magnetizations is considered theoretically. Transport characteristics, including current, linear and nonlinear conductances, and tunnel magnetoresistance associated with the magnetization rotation from the antiparallel to parallel configurations, are calculated using the real-time diagrammatic technique. The real-time diagrammatic technique is based on the perturbation expansion of the reduced density matrix. In this approach each class of tunneling processes can be represented by a relevant diagram. Some limiting situations, like for instance quantum dots connected in series and in parallel, in the limit of weak dot-lead coupling is discussed.

### **P-4-28**

## **ANALYSIS OF THE KONDO RESONANCE IN A SINGLE QUANTUM DOT ASYMMETRICALLY COUPLED TO FERROMAGNETIC ELECTRODES WITH NON-COLLINEAR MAGNETIZATIONS**

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The Kondo effect is studied theoretically in the framework of the non-equilibrium Green function formalism. The system under consideration consists of a single quantum dot asymmetrically coupled to ferromagnetic electrodes, whose magnetic moments are non-collinear. The spin-dependent density of states, as well as the transport characteristics like differential conductance and tunneling magnetoresistance through the system are obtained using the equation of motion method. Numerical illustration of the mentioned quantities for a few magnetic configurations and coupling strengths is presented and discussed.

### **P-4-29**

## **SPIN-VALVE EFFECT IN A SINGLE FERROMAGNETIC LAYER**

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In the present paper we propose a theoretical model of the recently observed (Yanson et al., 2007) surface spin-valve effect in a single ferromagnetic (FM) layer. We consider the surface of FM layer as a separate phase and assume that due to a lower (compared to bulk) coordination number and possible presence of the defects the exchange coupling between the surface spins is too weak to establish FM order. On the other hand, surface layer can be polarized by external magnetic field or by the biased electric current. Flowing through the interface with FM layer the free electron gas became polarized due to the difference in reflection/transmission coefficients of spin-up and spin-down electrons. Due to the strong exchange interaction between the collective and localized electrons, the formers impose a FM ordering of the localized spins. In the case when the electrons flow from normal to FM metal, polarization is governed mainly by the reflection processes. As a result, the surface layer is magnetized in the direction opposite to the bulk magnetization, resistance of the contact increases. When the electrons flow from FM to normal metal, both surface and bulk magnetizations are parallel and contact resistance is low. Thus, current-induced nonequilibrium excess of spin up (spin-down) conductivity electrons acts as external magnetic field and thus is responsible for the magnetic switching in a single FM film.

## **P-4-30**

### **ANGULAR DEPENDENCE OF MAGNETORESISTANCE IN CPP-GMR SPIN VALVES: A DIFFUSIVE APPROACH**

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Electrical current flowing through a spin-valve structure can lead to magnetic switching when the current exceeds a certain critical value. In typical spin valves current of a certain orientation leads to switching from the parallel to antiparallel configuration, while the opposite current restores the parallel configuration. In systems showing normal GMR effect, resistance of the system in parallel configuration is lower than in the antiparallel one, and the angular dependence of the magnetoresistance is a monotonous function of the angle between the leads' magnetic moments. In contrast, in asymmetric spin valves both the parallel and antiparallel configurations could be stable for one bias polarization and unstable for the opposite current direction. This leads to the non-standard angular dependence of the spin-transfer torque. We have found that the angular dependence of magnetoresistance in asymmetric valves can reveal a minimum at a non-collinear configuration. Here we report on the correlation between the non-standard spin-transfer torque and non-standard angular dependence of the magnetoresistance.





## O-5-01

### HIGH WAVE VECTOR MAGNONS AT THE Fe(110) SURFACE

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Spin polarized electron energy loss spectroscopy (SPEELS) is a unique and novel technique enabling the studies of the high wave vector spin waves (SW) in thin films and surfaces [1,2]. For the first time the full spin wave dispersion has been recently measured for 2 monolayers (ML) Fe/W(110) film with this technique [3]. Here, we present the results of the SPEELS studies of the SW excitations in the Fe(110) surface. The surface mode dispersion has been measured for the 24 ML Fe/W(110) film along the [001] direction. The iron film is deposited using molecular beam epitaxy in ultra high vacuum at room temperature, and subsequently annealed, in order to obtain an atomically flat and clean Fe(110) surface. We find that the surface SW energies are lower than that in the bulk Fe, and even lower than the SW energies for the 2 ML Fe/W(110) film. However, for the states above  $1.0 \text{ \AA}^{-1}$ , an energy difference of the excitations in the 2 ML and 24 ML films diminishes with an increase of the wave vector. In contrary to the 2 ML Fe case, the spin wave peaks reveal characteristic broadening at higher energy losses related to the Stoner excitations, or to the excitations of the higher modes.

[1] M. Plihal, D. L. Mills, and J. Kirschner, Phys. Rev. Lett. **82**, 2579 (1999).

[2] R. Vollmer et al., Phys. Rev. Lett. **91**, 147201 (2003).

[3] W.X. Tang et al., Phys. Rev. Lett. **99**, 087202 (2007).

## O-5-02

### BUFFER INDUCED MAGNETIC PATTERNING OF ULTRATHIN Co LAYER

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Magnetic anisotropy of ultrathin Co layer is substantially influenced by its thickness as well as by the type of buffer and overlayer material. In the case of Au/Co/Au sandwiches the spin reorientation transition from the out-of-plane to the in-plane configuration with increasing Co layer thickness is observed for 1.9 nm. The application of materials different than Au as the buffer and/or overlayer usually suppresses the Co thickness range, for which the perpendicular magnetization is stable. Thus the spatially patterned buffer is expected to modify accordingly the magnetic anisotropy of Co ultrathin film. The unique growth of Au on Mo in the form of islands ca. 100 nm in diameter offers the possibility to obtain such patterned buffer. Magneto-optical measurements (P-MOKE) reveal the existence of two different magnetic phases in the wide range of Co thickness. For particular Co thickness between 1.1 and 1.9 nm the magnetization of Co layer grown on Au islands is oriented in perpendicular whereas between islands in parallel direction to the film plane, giving rise to the array of spatially stable dots several dozen nanometers in lateral size with perpendicular magnetization.

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### **O-5-03**

#### **MAGNETIC PROPERTIES OF $\text{CaMnO}_{3-\delta}$ AND $\text{La}_{1-x}\text{MnO}_{3+\delta}$ NANOPARTICLES**

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Magnetic properties of  $\text{CaMnO}_{3-\delta}$  nanoparticles with particles size of 50 nm and of  $\text{La}_{1-x}\text{MnO}_{3+\delta}$  nanoparticles with size of 20, 25 and 30 nm will be presented and compared. Especially interesting effect was noticed for 50 nm  $\text{CaMnO}_{3-\delta}$  nanoparticles. They consist of antiferromagnetic (AFM) core and ferromagnetic (FM) shell. Observed asymmetric magnetization hysteresis loops were attributed to exchange-bias effect. This is the first observation of exchange bias effect in manganite nanoparticles with inverted AFM-core-FM-shell structure, as compared to the typical FM-core-AFM-shell structure. The effects of surface and exchange anisotropy will be discussed. For 20 nm  $\text{La}_{1-x}\text{MnO}_{3+\delta}$  particles, the smallest nanoparticles studied, different metastable states with highly reduced FM phase and "negative ferromagnetism" developed after a series of quick coolings were observed. Peculiar magnetic memory effects will be presented.

### **O-5-04**

#### **MAGNETIC ANISOTROPY AND DZYALOSHINSKI-MORIYA TYPE COUPLING IN SMALL MAGNETIC CLUSTERS**

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The results of a theoretical study of relativistic influences on the exchange coupling of small magnetic clusters will be presented. The use of the torque method allowed to investigate the magnetic anisotropy and angular dependence of the exchange coupling in detail and to determine the contribution of the Dzyaloshinski-Moriya-type coupling. Results will be presented for Fe, Co and Ni clusters deposited on Pt(111) surface, that have been investigated by means of the fully relativistic TB-KKR Green's function method within the framework of spin-density functional theory. The data are compared with the results of direct calculations of Dzyaloshinski-Moriya coupling in clusters and are analysed concerning their relation to the electronic structure and symmetry of the clusters. The influence of the substrate will be discussed as well. Also a non-collinear magnetism caused by Dzyaloshinski-Moriya couplings in FePt cluster deposited on Pt(111) surface will be discussed.

## O-5-05

### INVESTIGATIONS OF THE Co<sub>2</sub>MnSi/MgO(001) INTERFACE - LOOKING FOR HALF-METALLICITY

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Magnetic memory devices that exploit the tunneling magneto-resistance (TMR) effect depend crucially on the spin polarization of the electrode materials. Ferromagnetic half-metals make perfect electrodes leading to a (theoretically) infinite TMR ratio. The full Heusler alloy Co<sub>2</sub>MnSi is predicted to be half-metallic and has recently been integrated in a magnetic tunnel junction[1] where a high TMR value and huge spin polarization have been measured.

Here, we use density functional theory (DFT) calculations to model an epitaxially grown Co<sub>2</sub>MnSi/MgO(001) interface as potential TMR device. The stability and electronic and magnetic properties of different terminations of Co<sub>2</sub>MnSi (stoichiometric Co- and MnSi- and non-stoichiometric Mn- and Si- planes) and different registry with respect to the insulating barrier (Mg-top, O-top, bridge and hollow site) are investigated. We find that the electronic and magnetic properties (including the existence of the spin gap) depend strongly on the termination. The largest parts of the phase diagram consist of the interface Co/O (Co at O top site) which still has a high spin polarization ( $P = 70\%$ ) and the interface MnSi/O with only small  $P$ . The MnMn/O interface that preserves the half-metallicity lies outside the region accessible in thermodynamic equilibrium.

[1] M. Oogane *et al.*, J. Phys. D: Appl. Phys. **39**, 834 (2006)

## O-5-06

### DEPTH-RESOLVED XMCD AND XPS STUDY OF ULTRATHIN Mo/Co/Au FILMS

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Ultrathin Mo/Co/Au shows a rich variety of magnetic anisotropy, including in-plane/out-of-plane spin reorientation transition (SRT) and change in the in-plane anisotropy depending on the thickness of Co film and Mo overlayer, as confirmed by MOKE measurements[1]. In this paper we study the effect of Mo overlayer on the magnetism of Co layers by means of soft x-ray magnetic circular dichroism (XMCD). In particular, we report on the structure and magnetism at the Mo/Co interface studied by depth resolved XMCD[2] and x-ray photoemission spectroscopy (XPS). Depth-resolved XMCD shows that the magnetic moment of Co near Mo/Co interface is reduced compared to the inside of the film for the samples which have in-plane anisotropy. Moreover this effect is more prominent in the case of rougher Mo overlayer. Angular dependence of Co 2*p* and Mo 3*d* XPS shows systematic change which reflects the Mo/Co interface structure.

[1] Z. Kurant *et al.*, J. Magn. Magn. Mater. **316** (2007) e511

[2] K. Amemiya *et al.*, Phys. Rev. B **70** (2004) 190554

## O-5-07

### STUDY OF DEFECT MODES IN PHOTONIC BAND STRUCTURE OF MAGNETIC PHOTONIC CRYSTALS BY MEANS OF GREEN'S FUNCTION

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In this paper, we create an analytical model to investigate the localized defect modes associated with a defect cell inserted into a one dimensional magnetic photonic crystal (MPC). The structure is a magnetic superlattice with alternative layers of two different magnetic permeability containing a defect cell which is a layer of different nature (material or/and size) from the other layers. This leads to appearance of several localized defect modes within the photonic band gap. By inserting a defect into an MPC, it is possible to create highly localized defect modes within the photonic band gap (PBG). The design of controllable defect modes in MPCs requires predictive formulas for the frequency dependence of the defect modes on physical parameters of MPCs. Here, we develop an analytical approach based on the transfer matrix and Green's function methods to calculate the frequency and number of the defect modes which can be controlled easily by varying parameter values of the constituent layers of the MPC. An exact formula for the frequency of the defect modes is derived for both TE and TM polarizations at arbitrary angle of incidence.

## O-5-09

### ANISOTROPY DISTRIBUTION IN Ni-Fe/Au/Co/Au MULTILAYERS

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Multilayers comprising thin exchange decoupled Ni-Fe (2 nm) and Co (0.4, 0.6, 0.8, and 1.2 nm) layers in contact with Au (2 nm) are known to possess alternating in-plane (Ni-Fe) and out-of plane anisotropies (Co). However, little is known how the anisotropy is distributed across these multilayers. In this contribution we investigated anisotropy distribution in [Ni-Fe/Au/Co/Au]<sub>10</sub> multilayers grown by sputtering on Si (100) substrates. The samples were studied by means of ferromagnetic resonance at X- and Q-bands. The angular dependent energy density observed can be explained by two main contributions to the magnetic anisotropy: the uniaxial shape anisotropy,  $K_{sh}$ , and an effective second order anisotropy,  $K_{eff}^U$ . Due to negligible exchange interlayer coupling, the Ni-Fe and Co layers can be regarded as independent. It is concluded that for Ni-Fe layers the uniaxial anisotropy negligible except the first layer(s) next to the substrate. The uniaxial perpendicular anisotropy of Co layers depends on Co thickness in a standard way,  $K_{eff}^U \times t \propto t$ , and varies as a function of the position from the substrate in a range of  $\sim 10\%$  of  $K_{eff}^U$  (i.e.,  $\sim 1.5 \times 10^6$  erg/cm<sup>3</sup>). Detailed information on the internal magnetic structure of the multilayers can be inferred from our investigations.

## O-5-10

### COMPARATIVE STUDIES ON GIANT MAGNETORESISTANCE IN CARBON NANOTUBES AND GRAPHENE NANORIBBONS WITH FERROMAGNETIC CONTACTS

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Carbon-based structures evoke enormous interest in search for new materials for future nanoelectronics, expected to replace the conventional electronics soon. Along with carbon nanotubes, also graphene has recently given an additional impetus to this type of studies, after it was demonstrated that individual monolayers of graphite can be successfully synthesized and electrically contacted. Although it has already been realized for several years that ferromagnetically contacted carbon nanotubes reveal quite a noticeable giant magnetoresistance (GMR) effect, in the case of graphene this problem still remains to be explored. This contribution reports on comparative studies on GMR in CNTs and graphene nanoribbons of similar aspect ratios (i.e. perimeter/length and width/length ratios, for the former and the latter, respectively). The problem is solved at zero temperature in the ballistic transport regime, by means of the Green function technique within the tight-binding model with the so-called wide band approximation for electrodes. It turns out that graphene, analogously to CNTs may be quite an interesting material for spintronic applications.

## O-5-11

### COUPLED MAGNETIC AND STRUCTURAL TRANSITIONS IN THE $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3$ SYSTEM

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$\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO) films and LSMO/ $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  (PZT) multilayers were grown on vicinal (miscut angle  $0.1^\circ - 0.2^\circ$ )  $\text{SrTiO}_3$  (100) substrates by pulsed laser deposition at an oxygen partial pressure of 300 mbar and a substrate temperature of  $600^\circ\text{C}$ . XRD and TEM cross-sectional investigations showed heteroepitaxial growth with excellent structural quality of the LSMO and PZT layers. The focus of this contribution will be on the magnetic properties of bare LSMO films at the structural transition of the  $\text{SrTiO}_3$  substrates at about 105 K. For this three LSMO films with thickness of 40, 15 and 5 nm, respectively, were selected for further magnetic characterization by SQUID magnetometry and ac-susceptometry. In agreement with the high structural quality the films were found to be magnetically soft with coercive fields below 1 mT near 100 K. Below 105 K the development of a multiple-step transition in the magnetization reversal characteristics is clearly observed. The coercive field versus temperature curve splits into three branches below the structural transition. This is attributed to the formation of three different types of structural domains in the LSMO films as a response to twinning in the  $\text{SrTiO}_3$  substrate. The influence of strain at the LSMO/ $\text{SrTiO}_3$  interface as well as the modification of this transition in the LSMO/PZT multilayers is analyzed and discussed.

## O-5-12

### ION IRRADIATION INDUCED SUB-100 NM FERROMAGNETIC PATTERNS

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Focus ion beam (FIB) patterning of Fe<sub>60</sub>Al<sub>40</sub> provides the potential to create arrays of microscopic ferromagnetic regions embedded in a paramagnetic matrix. As the consequence of low fluence irradiation such a method does not affect the surface roughness. Due to the ion damage distribution the phase transition from the chemically ordered B2-phase to the chemically disordered, ferromagnetic A2-phase is setup. The magnetic phase transformation is studied as a function of noble gases mass and is directly related to the number of displacements per atom (dpa) during ion irradiation. In case of heavy ions (Ar<sup>+</sup>, Kr<sup>+</sup> or Xe<sup>+</sup>) the phase transformation originates purely from ballistic nature of the disordering process. For light ions (He<sup>+</sup>, Ne<sup>+</sup>) the disordering conditions deviates from the former case. The bulk vacancy diffusion from dilute collision cascades, that leads to a partial recovery of the thermodynamically favored B2-phase, plays a major role. Furthermore, by means of moderately high temperature annealing (about 900 K) the paramagnetic phase is completely recovered due to the annealing-induced atomic reordering. Therefore, local ion irradiation may lead to a novel type of patterned recording media free from tribological and exchange coupling effects.

## O-5-13

### GRAPHENE NANORIBBONS: A KEY INGREDIENT FOR SOLID-STATE QUANTUM INFORMATION PROCESSING?

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Graphene, an atomically-thin carbon monolayer, is a unique condensed-matter system which shows the features predicted by relativistic quantum mechanics [1]. Apart from merging the two rather distant fields of physics together, the world of graphene is also considered as a promising environment for solid-state quantum computing. We review the existing theoretical proposals for physical realization of a qubit in graphene nanostructures [2,3,4] which were recently followed by a remarkable progress in nanoribbon fabrication [5]. The role of spontaneous magnetic order predicted for zigzag-edge ribbons [4] is stressed. Finally, we present the original proposal for building graphene quantum dots by trapping electrons with the help of sublattice-mismatch.

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[3] A. Rycerz, J. Tworzydło, and C.W.J. Beenakker, *Nature Physics* **3**, 172 (2007).

[4] M.Wimmer *et al.*, [arxiv:0709.3244](https://arxiv.org/abs/0709.3244); S.Dutta *et al.*, *Phys. Rev. B* **77**, 073412 (2008).

[5] X. Li *et al.*, *Science* **319**, 1229 (2008).

## **P-5-01**

### **GRAIN SIZE EFFECT ON ELECTRIC AND MAGNETIC PROPERTIES OF R{R=Sc,Y,La}-Fe-Ge THIN FILMS**

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The data on the crystal structure, electric and magnetic properties of R-Fe-Ge {R=Sc,Y,La} thin films composition are presented depending on the preparation conditions {annealing temperatures and the effects of the applied electric field on a molecular vapour}, thickness, and sizes of crystalline formations in amorphous matrixes. In most cases the binary Fe-Ge nanostructures at a certain temperature are double phased, i.e. in the germanium amorphous matrix the clusters of a metallic constituent may be segregated. An excess of approximately 20 wt. % of the rare earth metal in the deposited condensate stabilizes an amorphous phase at a certain temperature interval. The film condensates, in which the cluster sizes are commensurate with the distances between them, are very attractive. In these films a conductivity mechanism is predetermined by a tunneling of electrons through small gaps between nanoparticles and so the resistivity depends on these particles sizes, width and configuration of the tunnel barriers, temperature and origin of the substrate materials. Exchange interaction between iron and rare earth atoms in the films of the ternary R-Fe-Ge {R=Sc,Y,La} systems is a main factor which determines the low temperature electric and magnetic properties. The equilibrium radius of clusters was calculated at vapor supersaturation during the process of condensation taking into account the influence of the electric field using the Gibbs energy change.

The experimental dependencies of the resistivity and coercivity in the 77-500 K temperature range enable us to predict the evolution of the films properties for application them as the soft magnetic materials.

## **P-5-02**

### **SELECTIVE MODIFICATION OF MAGNETIC PROPERTIES OF Co<sub>1</sub>/Au/Co<sub>2</sub>/Au MULTILAYERS BY He ION BOMBARDMENT**

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The possibility to locally change the properties of magnetic thin film materials is becoming increasingly important in view of their applications in magnetic storage elements. Particularly interesting, promising higher storage densities, are systems displaying perpendicular magnetic anisotropy. We show that in [Co<sub>1</sub>/Au/Co<sub>2</sub>/Au]<sub>N</sub> (N = 2÷4) multilayers (MLs), where Co<sub>1(2)</sub> denote the Co layers of different thickness, the 10 keV He-ion bombardment (IB) leads to changes of the easy direction from out-of-plane to in-plane in thicker Co layers (t<sub>Co1</sub> = 1 nm) while the perpendicular anisotropy of thinner Co layers (t<sub>Co1</sub> = 0.6 nm) is preserved. The investigated MLs were obtained by sputtering and the thickness of Au layers (t<sub>Au</sub> = 4÷6 nm) ensured that the influence of direct coupling between Co layers (through pinholes) and RKKY-like interactions were negligible. It is shown that IB with ion doses ranging from 6 to 8×10<sup>14</sup> ions cm<sup>-2</sup> leads to changes of magnetoresistance dependencies which correlate well with the magnetization changes observed by magnetometry. The X-ray diffraction measurements show no significant changes of MLs microstructure related to IB.

### **P-5-03**

#### **THE ORIGIN OF TEMPERATURE DEPENDENCE OF MAGNETIC ANISOTROPY IN Co/Cu(111) SUPERLATTICES**

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The temperature dependence of FMR spectra of superlattices *Co/Cu* was studied for determination of magnetic anisotropy mechanism. We have investigated the series of samples  $[Co(8\text{\AA})/Cu(d_{Cu})(111)]_{20}$  with thicknesses of nonmagnetic copper layers  $d_{Cu} = 7-22 \text{ \AA}$ . The measurements of FMR spectra were made in 3-cm wavelength range in temperature interval from 300 to 360 K. The temperature dependence of anisotropy constant  $K_1$  is close to linear behavior for all samples of series. Such temperature dependence  $K_1$  can be considered with magnetoelastic mechanism and the contribution of crystal anisotropy. In this work the calculation estimations of both contributions are made. For given temperature interval the variations of magnetoelastic contribution to the anisotropy constant are about  $4 \cdot 10^3 \text{ erg/cm}^3$ , while in experiment the value  $\Delta K_1 \approx 0,9 \cdot 10^6 \text{ erg/cm}^3$  is observed. Whereas the axial part of the crystal anisotropy makes about  $\approx 10^6 \text{ erg/cm}^3$ . So, the magnetoelastic contribution is not an appreciable source of temperature dependence of anisotropy in multilayered system under consideration. The main contribution to this dependence is given by the axial component of crystal anisotropy.

### **P-5-04**

#### **RKKY-REMINISCENT INTERACTION IN A "NET FRACTAL SYSTEMS"**

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Within the RKKY model the effective, magnetic interaction arises due scattering of the uniformly distributed electrons on the magnetic moments of the impurity ions. This picture is valid provided that the dopant ions are randomly distributed within a metallic-like matrix. However, in many cases the dopant magnetic ions show tendency towards clustering. These spontaneously patterned structures can be assembled in various geometries. The resulting clusters immersed within the matrix often show fractal symmetry. In this case the restrictive assumption of an isotropic surrounding that validates the RKKY model doesn't hold. That's why different concepts that account the effect of reduced geometry on magnetic interactions are still under debate. In our contribution, with the use of logarithmic coordinates, we show that in "net fractals", a specific class of fractals [1], the indirect exchange mediated by itinerant electrons can be presented in the form that is reminiscent of the RKKY interaction in a system of fractional spectral dimensionality [2]. Finally, we prove that in spite of reduced geometry the long range magnetic order is possible.

[1] Z. Bak, Phase Transitions **80**, 79 (2007).

[2] Z. Bak, R. Jaroszewicz, W. Gruhn: J. Mag. Mag. Mater. **213**, 340 (2000).



## **P-5-05**

### **MAGNETIC CHARACTERISTICS OF MAGNETIC BILAYERS WITH DISORDERED INTERFACES**

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A great number of studies have been performed on the properties of magnetic multilayers exchange coupled via metallic nonmagnetic spacer. Usually the interfaces in such nanostructures have been treated as the perfect ones. In order to describe properties of multilayers in agreement with experimental indications the atomic scale disorder in the region of interface should be taken into account. In presented work the Green function method is applied to study magnetic properties of bilayer system with disorder at interface layers caused by an alloying process. Magnetisation distribution in constituent magnetic layers, the phase transition temperature and the spin wave parameter are obtained as a function of spacer thickness for different parameters describing diffuse and non-diffuse scattering of electrons at interface. The results are compared with those obtained taking into account roughness in interface region. The parameters describing the interlayer exchange coupling between layers with disordered interface are estimated for Fe and Co layers with Au and Cu spacers. The substrate is characterised by parameters corresponding to GaAs.

## **P-5-06**

### **SOME MAGNETIC PROPERTIES OF ULTRATHIN MAGNETIC DOT ARRAYS**

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Modern experimental techniques make it possible to fabricate arrays of small magnetic particles of nanometer size and well-defined shape. These structures are interesting not only because of possible applications in magnetoelectronic devices but also from a point of view of their basic properties. In presented work we consider array of magnetic dots of thickness of several monatomic layers. The distance between dots is chosen in such a way that dipolar coupling between them can be neglected. The Heisenberg Hamiltonian consisting of the exchange, single ion anisotropy and Zeeman terms, respectively, is employed to calculate low temperature characteristics of the system. Spin wave profiles and temperature dependence of spontaneous magnetisation is investigated as a function of the dot diameter. In calculation the anisotropy parameters at the edges of the dots have been estimated for the system of Fe dots. It is shown that the spin wave parameter  $B$  describing Bloch's law increases in non-linear way with decreasing of the size of the dot. The results obtained are compared with results for continuous layer of the same thickness.

### **P-5-07**

#### **MAGNETIC AND TRANSPORT PROPERTIES OF NANOPOWDER $(La_{0.7}Sr_{0.3})_{0.9}Mn_{1.1}O_3$ MANGANITES.**

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We report on the X-ray diffraction, magnetic, transport and NMR measurements of nanosize  $(La_{0.7}Sr_{0.3})_{0.9}Mn_{1.1}O_3$  manganites. The nanoparticles were synthesized with use of co-precipitation method at different temperatures. The average size of nanoparticles (40 - 100 nm) was estimated by both BET's method and X-ray diffraction measurements. All the nanosize samples show ferromagnetic-like ordering and have close phase transition temperatures. The magnetization decrease with decreasing particle is due to increasing ratio of the surface to volume of the grains. Comparison of experimental and calculated temperature dependences of the magnetic moment shows that the spontaneous magnetization is well described in the frame of the double exchange model. The resistivity becomes higher with reducing the particles size at any temperatures. The magnetocaloric effect calculated from initial magnetization curves is larger for the larger particles.

### **P-5-08**

#### **FABRICATION AND CHARACTERIZATION OF HYBRID TUNNEL MAGNETORESISTANCE STRUCTURES WITH EMBEDDED SELF-ASSEMBLED NANOPARTICLE TEMPLATES**

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We report on an incorporation of self-assembled templates of superparamagnetic Fe-O nanoparticles into tunnel magnetoresistance (TMR) devices. We fabricated a multi-layer stack composed of the following layer sequence: Cr/Au/Co/NP/Co/Cu on Si(100) substrate where NP stands for a self-assembled layer of nanoparticles deposited by Langmuir-Blodgett technique. The X-ray reflectivity (XRR) and grazing-incidence small angle X-ray scattering (GISAXS) were employed to study the layers thicknesses and interface morphology in each preparation step. In particular, the XRR and GISAXS were measured before and after the nanoparticle incorporation as well as on the complete TMR stack. In this way, in-depth morphology profile during subsequent preparation steps was obtained. We demonstrate that X-ray analysis of the deposited TMR stack is essential for successful fabrication of novel hybrid devices consisting of self-assembled nanoparticles.

## **P-5-09**

### **PECULIARITIES OF MAGNETIC AND MAGNETO-OPTICAL PROPERTIES OF MULTILAYERED Co/Cu FILMS**

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The results of magneto-optical Kerr effect measurements for the series of the multilayered [Co/Cu]<sub>20</sub> ultra-thin films are presented. The Cu-layer thicknesses ( $d_{\text{Cu}}$ ) (from 6 to 20 Å) were different in various films, but they were identical within one film. The Co-layer thickness in all films was 8 Å. The multilayers were deposited by the magnetron sputtering.

The decreasing Cu-thickness dependence of the spontaneous Kerr rotation  $\theta_{\text{S}}(d)$  had the peculiarities at  $d_{\text{Cu}} = 9, 13.5$  and  $18$  Å – two significant peaks and the minimum of  $\theta_{\text{S}}$ , respectively. In these three films the strong linear enhancement of the Kerr rotation at magnetic field strengths  $H > 6$  kOe was revealed. Such magneto-optical properties point out periodicity in changing of electronic energy spectrum and magnetic properties of the Cu/Co interfaces as a function of  $d_{\text{Cu}}$ . The most probable reason of these changes can be a quantum size effect for spin-polarized electrons, having Fermi energy, in the Cu-layers and its influence on hybridization of d(Co)- and sp(Cu)-electrons at the Cu/Co interfaces. The quantum size effect also is supposed to influence the formation of Co-layer and Co/Cu interface structures (ferromagnetic jumper between Co-layers). It is confirmed by the periodical with the Cu-layer thickness changes of the magnetic characteristics of these films – the normalized remanent Kerr rotation and the coercive field.

## **P-5-10**

### **ELECTRON TRANSPORT MODELING IN TWO COUPLED QUANTUM WIRES**

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This work presents transport modeling through the two coupled quantum wires in incoherent and coherent regime. We try to explain electron switching effect caused by asymmetry of voltage biased to the gates [1]. Using circuit theory we can model switching characteristics in incoherent regime. Using the Green function method and multi probe Landauer - Büttiker formula and combining external conducting elements we are able to calculate transport in the coherent regime. We found  $I - V$  characteristics and the switching effect. The influence of quantum interference on  $I - V$  characteristics and switching effect is presented as well. The electronic waves penetrating the floating electrodes changes the interference patterns and modify  $I - V$  characteristics. The theoretical studies are related to the recent experiments [1] in such the systems.

[1] A. Ramamoorthy, J. P. Bird and J. L. Reno *J. Phys.: Condens. Matter* **19** 276205 (2007).

## **P-5-11**

### **THE STRUCTURAL PHASE TRANSITIONS IN 6CB-BASED FERRONEMATICS**

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Ferronematics are magnetic colloids based on a liquid crystal matrix and were first suggested on theoretical grounds in 1970 by Brochard and de Gennes. The surface anchoring in the magnetic particles couples the magnetic and nematic order and dramatically increases the weak magnetic interaction. The structural transitions in ferronematics based on the thermotropic nematic liquid crystal 6CB (p-hexyl-p'-cyanobiphenyl) were studied. The ferronematic samples were prepared by doping with magnetic suspension consisting of Fe<sub>3</sub>O<sub>4</sub> particles (10 nm in diameter) coated with oleic acid as a surfactant, with volume concentration of magnetic particles  $\phi_1 = 10^{-4}$ ,  $\phi_2 = 2 \times 10^{-4}$  and  $\phi_3 = 10^{-3}$ . Freedericksz transitions were studied in combined electric and magnetic fields. The obtained results show the decrease of the critical magnetic field with increasing volume concentration of magnetic particles.

## **P-5-12**

### **INFLUENCE OF THE STRUCTURE ON THE MAGNETIC AND MAGNETO-OPTICAL PROPERTIES OF Co ON Pd(100) OVERLAYERS**

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The electronic, magnetic and magneto-optical properties of Co on Pd(111) overlayers have been studied using relativistic linear muffin tin orbital band structure calculations within density functional theory. The models of 1- and 2- monolayer thick Co with ordered and disordered structures corresponding to experimentally studied ones [1] have been studied using supercell approach. The calculated dependences of the magneto-optical Kerr effect on the structural disorder are compared with the observed in the experiment, and their correlation with the electronic, magnetic and anisotropic properties of the systems is discussed.

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## **P-5-13**

### **MAGNETIC PROPERTIES OF SPUTTERED Fe/Au MULTILAYERS**

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The Fe/Au multilayered structures (MLS) exhibit many interesting physical properties depending on Fe, Au sublayer thicknesses, crystal structure and level of structure imperfections. We report studies on the temperature dependence of magnetic and magneto-optical properties for the series of Fe/Au (111) prepared by dc-sputtering on GaAs(001) substrates with the Fe sublayer thicknesses < 0.4 nm. The magnetization processes were measured by magneto-optical technique in polar and longitudinal geometry in the temperature range 8 - 315 K. The temperature evolution of the experimental Kerr hysteresis loops for the Fe/Au (111) MLS studied shows that the systems are composed of different magnetic phases. The observed in-plane and out of plane field dependences of Kerr angle exhibit superparamagnetic and ferromagnetic character depending on MLS sublayer thickness. To interpret quantitatively the experimental data we adopted the models developed by M. Rubinstein [1] and P. Allia [2]. In the frame of the models the developed fitting procedure was used in different temperature ranges to separate the superparamagnetic and ferromagnetic phases in the Fe/Au MLS. The analysis of the temperature dependences of the coercivity performed strongly supports the conclusion on increasing role of the superparamagnetic phase in the Fe/Au MLS with decreasing layers thickness ratio  $t_{Fe}/t_{Au}$  below 0.3. The role of interacting superparamagnetic phase related to the dipolar interacting uniaxial and randomly oriented nanoparticles is discussed.

## **P-5-14**

### **INFLUENCE OF FE LAYER THICKNESS ON MAGNETIC AND MAGNETO-OPTICAL PROPERTIES OF Fe/Si MULTILAYERS**

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Structures containing magnetic metallic layers separated by semiconducting spacer layers attract a lot of interests because of their possible applications in the field of spintronics. In this work results of the experimental study of the Fe/Si multilayer films (MLS), prepared by magnetron-sputtering method onto (001) Si substrate, obtained by the optical and magneto-optical technique are presented. The Fe/Si MLS have been prepared with fixed Si spacer layer thickness ( $d_{Si}=1.1$  nm) and varied Fe layer thicknesses within the range  $d_{Fe}=0.5-4.0$  nm. The temperature dependences of the polar and longitudinal Kerr hysteresis loops for the films under study were measured in the range 10-300 K and show character typical for the antiferromagnetically coupled sublayers. The interlayer coupling depends on Fe thickness and is influenced by interfacial mixing between Fe and Si layers as it was derived from temperature dependence of magnetization processes. For thin Fe layer ( $d_{Fe}=0.5$  nm) superparamagnetic behaviour at room temperature has been observed and ferromagnetic one at low temperature. Nonuniform nonmagnetic Fe-Si interface mixture formed during deposition plays a crucial role for the interlayer coupling observed in the systems studied.

**P-5-15**  
**SLOW RELAXATION OF RESISTIVITY IN MANGANITE  
PEROVSKITE NANOCONSTRICTIONS**

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We have investigated a significant time resistivity relaxation in the perovskite nanoconstrictions (PNC) obtained by break technique at LN. The time  $t$  dependence the resistivity  $R$  of the PNC has been measured by computer devices at several temperatures, between LN and 370 K. The relaxation effects of  $R$  vs.  $t$  can be described by two-term formula: stretched exponential function + logarithmic one can describe a slower relaxation processes - the relaxation times values are about few seconds. The appearance of both contributions evidences the existence of two sources of relaxation, which can be assigned to inhomogeneous changes of the angle between the magnetic moments of the neighbouring Mn ions at different "spin blocks" of PNC. Due to the close relation between resistivity and the magnetization in manganese compounds, according to Zener model, the  $R(t)$  measurements provide an excellent indirect method to characterize the magnetic relaxation. The magnetic relaxations are dependent of the basis current flowing through the PNC. The magnetic viscosity coefficient  $S$  of the PNC displayed characteristic like bell-shaped curves vs. basis current. These results point out the important role of structural arrangements of the Mn-ions clusters on the surfaces of the tip and target, respectively. In conclusion, the measurements time decay of the resistance, these relaxations are due to change of the magnetic correlation between  $Mn^{3+}$  and  $Mn^{4+}$  ions, are excellent indirect method for characterizing the magnetic relaxation in perovskite atomic scale constrictions.

**P-5-16**  
**RKKY INTERACTION IN COUPLED QUANTUM DOTS**

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In electronic devices based on quantum dots the control of single, localized spins is of technological importance. From the physical point of view quantum dot can be assumed as an artificial magnetic impurity. Localized moment of quantum dot can interact with the adjacent one by exchanging electrons that are transmitted either by the metallic substrate or by metallic lead. As the result of that there arises effective magnetic interaction between spins of quantum dots that displays RKKY features [1]. We show that due boundary conditions imposed onto electron mobility their spectrum changes and the density of electron states shows fractional spectral dimension. In our contribution we study specific features of the RKKY interaction between quantum dots basing on the idea of fractional spectral dimensionality [2]. We prove that RKKY range function of interacting quantum dots interpolates between the 2D and 3D cases in the case of substrate mediated interaction. Furthermore, we show that in the chain geometry, when interaction is mediated *via* electrons of a quantum wire that joins quantum dots the the spectral dimension that determines RKKY interaction can exceed 3.

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## **P-5-17**

### **DOMAINS STIMULATED MAGNETOSTATIC COUPLING IN NiFe/Au/Co/Au MULTILAYERS INVESTIGATED BY COMPLEMENTARY METHODS**

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We report on magnetization reversal of NiFe/Au/Co/Au multilayers characterized by in-plane and out-of-plane anisotropy of NiFe and Co layers respectively. For such films the transition from a weak to a strong ferromagnetic coupling correlated with creation of stripe domains in Co layers is observed. The strengths of this magnetostatic coupling and the magnetic field range in which this coupling exists can be regulated by a proper choice of the ferromagnetic and/or spacer layers thickness. The manifestation of the coupling in magnetization reversal, magnetoresistance, Mössbauer spectroscopy, and soft x-ray resonant magnetic scattering measurements performed for different samples will be discussed. On the basis of these complementary measurements the evolution of the magnetic structure with magnetic field will be described.

## **P-5-18**

### **MAGNETIC STRUCTURE MODIFICATION OF NiFe/Au/Co/Au MULTILAYERS BY He<sup>+</sup> ION BOMBARDMENT THROUGH NANOSPHERES**

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Magnetic patterning, i.e., local changes of magnetic properties without topographical changes is of particular interest due to possible applications in new generation of magnetic storage media. This effect, originating from the structure modification, can be induced by ion bombardment. Because of special requirements for magnetic hard discs technology the attention is focused on magnetic layered films with perpendicular anisotropy (e.g., Co/Pt, Co/Au). As a result of intermixing at the interfaces the perpendicular anisotropy decreases with increasing ion dose. Magnetic patterning in nanoscale was realized by focused ion beams or bombardment through mechanical or lithographic masks. In our contribution we demonstrate that large area magnetic patterning in nanoscale can be realized by ion bombardment of NiFe/Au/Co/Au multilayers through a single layer of latex nanospheres arranged in regular structure.

## **P-5-19**

### **THE INFLUENCE OF He<sup>+</sup> ION BOMBARDMENT ON MAGNETIC PROPERTIES OF NiFe/Au/Co/Au MULTILAYERS**

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The influence of helium ion bombardment on magnetoresistance (MR), magnetization reversal and domain structure of sputtered (Ni<sub>20</sub>Fe<sub>80</sub>-2nm/Au-2nm/Co-0.6nm/Au-2nm)<sub>10</sub> multilayers (MLs) was investigated. The MLs consist of ferromagnetic layers with alternating in-plane (NiFe) and out-of-plane (Co) magnetic anisotropy. The samples were bombarded by He<sup>+</sup> (30 keV) ions with fluences varied in the range  $10^{13} \leq D \leq 3 \times 10^{16}$  He<sup>+</sup>/cm<sup>2</sup>. With increasing fluences of helium ions the following changes in magnetic properties were observed: (i) the saturation field of Co layers exponentially decays what is caused by a transition from the out-of-plane to the in-plane anisotropy of Co layers, (ii) the MR decreases progressively whereas the resistance remains almost constant (up to  $4 \times 10^{15}$  He<sup>+</sup>/cm<sup>2</sup>), only for higher fluences it strongly increases, (iii) the period of maze stripe domain linearly decreases with  $\log(D)$ . However, domain structure for  $D=3 \times 10^{16}$  He<sup>+</sup>/cm<sup>2</sup> is hardly visible.

## **P-5-20**

### **EVOLUTION OF Fe LAYER COMPOSITION IN Fe/Si MULTILAYERS OBSERVED BY IN-SITU CONDUCTANCE MEASUREMENTS**

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The Fe/Si multilayers exhibit a strong antiferromagnetic (AF) coupling [1,2]. The crucial role in the appearance of AF interlayer coupling play nonmagnetic Fe-Si mixtures at interfaces. In present work the analysis of the in-situ thickness dependent conductance  $G(d)$  is given. During Fe deposition two  $G(d)$  ranges with different slopes can be distinguished with an abrupt change between them. Such a behaviour suggests a modification of iron growth mode or structural transition. Correlations between the Fe thickness corresponding to the growth mode transition, the height of the abrupt change, surface roughness and the number of deposited bilayers have been noticed. During Si deposition onto Fe layer, the conductance initially decreases and then saturates. It may be explained as a result of Si diffusion into Fe and formation of low-conductive Fe-Si mixture. Subsequent Si deposition on the Fe-Si mixture leads to growth of nonconductive silicon, thus  $G(d)$  plateau appears. Such a plateau was observed only in Fe/Si MLs which show no AF coupling, i.e., for  $d_{Si} > 1.3$  nm.

[1] T. Luciński et al., J. Magn. Magn. Mater. (2004) **282**, 248

[2] T. Luciński et al., phys. stat. sol. (c) (2006) **3**, 93



## **P-5-21**

### **EXCHANGE BIASED IRON-OXIDE MAGNETIC NANOCOMPOSITE**

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In recent years the exchange bias phenomenon (EB) has a great deal of attention because of its potential for use in controlling magnetization in devices, such as spin valves in magnetic reading heads and magnetic random access memories. The mechanism of exchange bias is explained on layered or core/shell systems with ferromagnetic/antiferromagnetic interfaces due to the existence of a unidirectional anisotropy induced at exchange coupling of FM/AFM system. The Fe<sub>2</sub>O<sub>3</sub> material, due to their high Néel temperature, was supposed to be a good candidate of the biasing material. In our work, the iron oxide nanoparticles were incorporated into self-assembled periodic nanoporous silica, which exhibits 2D, hexagonally arranged channel system, with mean diameter of the channels about 7 nm. Magnetic properties measured on a SQUID-based magnetometer at 2-300 K and in the field up to 5 T, experimentally confirm the existence of exchange bias effect in our system. The zero-field cooled (ZFC) loop, measured at 10 K, was symmetric around the origin whereas the 10 kOe, field-cooled (FC) magnetization curve was strongly displaced from the origin and broadened. The value of displacement defines the exchange bias field 509 Oe. The coercivity enhancement defined as  $\Delta H_c = H_c(FC) - H_c(ZFC) = 143$  Oe was obtained from the measured loops.

## **P-5-22**

### **ELECTRIC AND MAGNETIC SIGNATURES OF STRUCTURAL AND CHEMICAL ORDERING OF HEUSLER ALLOY FILMS**

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Heusler alloys have recently attracted a great attention due to martensitic transformations and half-metallic properties, respectively. Their properties heavily depend on chemical and structural ordering. Thin Heusler alloy films are ideal objects to trace various stages of ordering since they can be easily prepared in a highly disordered state (e.g., amorphous) and then they can be gradually ordered at elevated temperatures. The films were prepared by rf-sputtering or by flash-evaporation on substrates kept at ambient or at low temperature. Since the resistivity is affected by local disorder, the resistivity measurements were applied for indirect characterization of the order-disorder relations. We report the results on the temperature dependencies of resistivity and magnetization for some Heusler alloy films: Co<sub>2</sub>CrAl, Co<sub>2</sub>MnSi and off-stoichiometric Ni<sub>2</sub>Mn<sub>1+x</sub>Sn<sub>x</sub>, Ni<sub>2</sub>Mn<sub>1-x</sub>Ga<sub>x</sub> that are known to exhibit half-metallic properties and martensitic transformations in bulk, respectively. From  $\rho$  vs.  $T$  characteristics we distinguish various stages of chemical/structural ordering in the films. They appear to be quite distinct in both systems investigated. The resistivity results are compared with magnetic characteristics for some films with high  $T_C$ .

## **P-5-23**

### **INFLUENCE OF THE DEPOSITION TEMPERATURE ON MAGNETOTRANSPORT PROPERTIES OF Ni-Fe/Au/Co/Au MULTILAYERS**

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Multilayers composed of  $[\text{Ni}_{80}\text{Fe}_{20}(2\text{ nm})/\text{Au}(2\text{ nm})/\text{Co}(0.8\text{ nm})/\text{Au}(2\text{ nm})]_N$ , where  $N$  denotes the number of repetitions, have been prepared with magnetron sputtering at different deposition temperatures. In such multilayers Co layers may have the perpendicular anisotropy if its thickness ranges from 0.4 nm to 1.2 nm [1]. A correlation between the growth process and electrical properties of  $[\text{Ni}_{80}\text{Fe}_{20}(2\text{ nm})/\text{Au}(2\text{ nm})/\text{Co}(0.8\text{ nm})/\text{Au}(2\text{ nm})]_N$  was investigated. The changes in giant magnetoresistance amplitude and shape have been correlated with the changes in Co layers growth process that occur in different temperatures, what was additionally confirmed by the Hall effect measurements. The time-dependent *in-situ* conductance measurements lead to the growth mechanism identification in high temperatures as intensified formation of Co islands.

[1] F. Stobiecki, B. Szymański, T. Luciński, J. Dubowik, M. Urbaniak, K. Roell, *J. Magn. Magn. Mater.* **282**, 32 (2004)

## **P-5-24**

### **HARD AND SOFT X-RAY REFLECTIVITY STUDIES OF (NiFe/Au/Co/Au)<sub>10</sub> MAGNETIC MULTILAYERS**

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Sputter deposited  $(\text{Ni}_{80}\text{Fe}_{20}\ 2\text{nm}/\text{Au}\ 2.2\text{nm}/\text{Co}\ t_{\text{Co}}/\text{Au}\ 2.2\text{nm})_{10}$  multilayers (MLs) with  $t_{\text{Co}}$  in the  $0.4 \div 1.2$  nm thickness range were investigated using hard x-ray diffraction and soft x-ray resonant magnetic scattering (SXRMS). SXRMS combines the element specificity of magnetic circular dichroism with conventional specular reflectivity. Specular reflectivity curves were measured with standard, unpolarized Cu  $K_{\alpha}$  radiation (photon energy 8040 eV) and circularly polarized synchrotron radiation tuned to Co  $L_3$  (778.4 eV) and Ni  $L_3$  (853 eV) absorption edges. Structural properties (chemical periodicity and roughness) of the MLs were determined from reflectivity curve of the hard x-ray. Comparison of reflectivity dependence versus scattering vector  $q$  measured at different photon energies have shown: (i) different shapes of satellite Bragg peaks, (ii) small difference in their position, (iii) different ranges of  $q$  for appearance of Kiessig fringes. Analysis of soft x-ray reflectivity measured as a function of magnetic field allowed us to determine magnetization reversal of Co and NiFe layers separately.

### **P-5-25**

#### **MAGNETO-OPTICAL STUDY OF NiFe/Au/Co/Au LAYERED FILMS**

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Sputtered NiFe/Au/Co/Au layered films with noncollinear magnetizations are of scientific interest for unusual magnetization behavior and their potential applications in spintronics. Magneto-optic ellipsometry is applied to separate magnetization contributions from Co and NiFe layers. Hysteresis loops measured by polar Kerr rotation and ellipticity show strong differences in shape, which originate from different material sensitivity of the complex magneto-optic effect to the Co and NiFe layers. Polar Kerr rotation and ellipticity from the sample Si/Au(buffer)/NiFe(0–2 nm)/Au(2 nm)/Co(0–1.7 nm)/Au(2 nm) with mutually perpendicular wedges of Co and NiFe were measured. Experimental study is combined with modeling of magneto-optic response from the system using Yeh's  $4 \times 4$  matrix algebra. Effects of ferromagnetic layer thickness on magnetostatic coupling is demonstrated from analysis of magneto-optical data.

### **P-5-26**

#### **SURFACE STATES IN A SQUARE LATTICE UNDER MAGNETIC FIELD APPLIED IN THE SURFACE REGION**

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Electronic surface states localized on the edge of a semi-infinite square lattice are studied in the tight binding approximation (TBA). We have examined the existence of surface states in the presence of magnetic field applied in the surface region of a 2D lattice. The applied field is perpendicular to the lattice and confined to a stripe near the surface. We have also included a surface site perturbation caused by the presence of the surface. The magnetic field is introduced into the model by the Peierls substitution. The method is used for investigating surface states with commensurate ratio of the magnetic flux per unit cell to the flux quantum.

## **P-5-27**

### **SIMULATION OF DEFECTS AND COMPOSITION AFTER IRRADIATION OF ULTRATHIN Pt/Co/Pt FILM Ga<sup>+</sup>**

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Spin reorientation transition from in-plane to out-of-plane state in Pt/ $t_{Co}$ /Pt film ( $t_{Co} = 3\text{nm}$ ) after 30 keV Ga<sup>+</sup> ion irradiation was observed [1]. Theoretical studies of the collision intermixing and defects creation processes of irradiated are presented. By means of TRIDYN simulations the dependence of composition and sputtering yield on ion fluence in the range of  $10^{14}$  to  $5 \cdot 10^{16}$  ions/cm<sup>2</sup> is elucidated. Simulations show that ion fluence plays non-neglectable role in case of erosion and intermixing of the interface (which likely gives a certain strain to the system), which give rise to the new phenomena, the so-called swelling effect. On the other hand the swelling effect can relax the strain in the film and give rise to an increase of the magnetic anisotropy. However, the strain relaxation can be strongly non-uniform on the full square area providing a mixture of patches with in-plane or out-of-plane anisotropy. The presence of relatively large and quasi-uniform perpendicular anisotropy partially comes from peculiar strain states at the interface. Simulated compositions are compared with experimentally observed irradiation induced phenomena.

[1] J.Jaworowicz et al., Ga<sup>+</sup> ion irradiation-induced out-of-plane magnetization in Pt/Co(3nm)/Pt films, work accepted for presentation in INTERMAG 2008.

## **P-5-28**

### **SPATIAL DISTRIBUTION OF GAUSSIAN FLUCTUATIONS OF THE MOLECULAR FIELD AND MAGNETIZATION IN THE PYRAMID-LIKE ISING NANOSCOPIC SYSTEM INTERACTING WITH THE SUBSTRATE**

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We study thermodynamic properties of an Ising model of a ferromagnetic nanoscopic pyramid deposited onto a ferromagnetic bulk substrate. The influence of the interaction between the pyramid and the substrate is calculated in terms of the reduced-state (density) operator used for description of thermodynamic properties of nanoscopic systems. The spatial distribution of the magnetization in the nanoscopic pyramid is obtained in the Gaussian fluctuations approximation.

## **P-5-29**

### **INVESTIGATION OF PHOTONIC BAND GAP OF ONE-DIMENSIONAL HETEROSTRUCTURE MAGNETIC PHOTONIC CRYSTALS**

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Multiple structures in one-dimensional (1D) photonic crystals (PCs) have great potentials for ultrawide omnireflectors and controllable switches. Here, we study the propagation of electromagnetic waves in a magnetic superlattice heterostructure as a 1D heterostructure magnetic photonic crystal (HMPC). These structures consist of alternating layers with magnetic permeabilities  $\mu_1$  and  $\mu_2$  with double periods ( $\Lambda_1$  and  $\Lambda_2$ ). Photonic band gap (PBG) for both TE and TM polarizations of electromagnetic waves propagation through the HMPC has been studied by means of the transfer matrix method. Regarding the calculated PBG of the system, ideas for switching and filtering applications are discussed in the paper. Controllable magnetophotonic devices can be designed with respect to the PBG of the HMPC.

## **P-5-30**

### **MAGNETIC PROPERTIES OF BACTERIAL NANOPARTICLES**

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Magnetic nanoparticles in diluted aqueous suspensions are an important tool in medical diagnostics as contrast agent for magnetic resonance imaging and in therapy for magnetic drug targeting and hyperthermia. For these applications, special nanoparticles (magnetosomes) were isolated, which consisted of a magnetite core covered by a protein-containing lipid membrane. In our experiments bacterial magnetosomes were synthesized by magnetotactic bacteria *Magnetospirillum sp. strain* AMB-1. This bacteria is a Gram-negative  $\alpha$ -proteobacterium that is more oxygen-tolerant and easier to grow on a large scale. The morphology was studied by Transmission Electron Microscopy (TEM) and magnetic properties by SQUID magnetometer. The XRD powder diffraction peaks fit very well with standard  $\text{Fe}_3\text{O}_4$  reflections for used sample. The average particle size calculated by the Debye-Scherrer formula from XRD line width of the (311) peak was estimated to be 37 nm what corresponds with TEM measurements. The temperature dependence of magnetization measurements in zero field (ZFC) and field cooling (FC) measurement mode presents the sharp magnetic transition (Verwey transition) at 105 K what is attributed to the fact that magnetosomes organized in chains act as long dipoles with enhanced magnetic anisotropy.

### **P-5-31**

#### **TIME AND CROSS-CORRELATION HISTOGRAMS IN CONDUCTANCE MEASUREMENTS OF NANOWIRES FORMED AT SEMICONDUCTOR INTERFACES**

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We demonstrate experimentally that conductance steps can occur in nanowires formed at metal-semiconductor junction due to quantum effects such as conductance quantization and a single-atom contact formation. Electronic properties of the interface result from the band structures of the materials that form the contact leading to a Schottky barrier rising at the metal-semiconductor interface. Conductance traces obtained from measurements in nanowires formed between a cobalt tip and a germanium surface reveal long-duration plateaus at reproducible levels. We detect strongly nonlinear current-voltage characteristics typical for systems with a Schottky barrier. The high reproducibility of the conductance traces obtained from short series of measurements leads to very sharp peaks in the classical conductance histogram suggesting formation of stable atomic configurations. To analyze these highly reproducible data we develop a new type of time- and cross-correlation analysis of the preferred conductance values depicted in the form of the 2D density plots that provide new type of information on a few-atomic-nanocontact formation dynamics.

### **P-5-32**

#### **AB INITIO ANALYSIS OF A QUANTUM DOT INDUCED BY A LOCAL EXTERNAL POTENTIAL IN A SEMICONDUCTING CARBON NANOTUBE**

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Using the density functional theory [1] we study the influence of external charge probes on the electronic structure of semiconducting carbon nanotubes in vicinity of the Fermi level. We show that the spatially limited potential due to the probe can create localized electronic states in the energy gap and at the edges of the conduction band. By filling these localized states with additional electrons one obtains a quantum dot, which can be tuned by modifying the properties of the external charge probe. We analyze dependence of the electronic structure of the dot on the spatial extension of the potential as well as on the nanotube radius.

[1] J.M. Soler, E. Artacho, J.D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal J. Phys. Condens. Matter 14, 2745 (2002).

## O-6-01

### FMR SPECTRA OF EXCHANGE-BIASED FM/AFM BILAYER SIMULATED WITH INTERVAL METHODS

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The bilayer of ferromagnetic (FM) and antiferromagnetic (AFM) material, FeNi/FeMn, both 50 Å thick, exhibits an exchange bias effect as high as 420 Oe at 6 K and 7 Oe at 50 K, when first cooled down in presence of an in-plane field of 100 Oe. Similar effect, that is different values of the resonance fields when an external field is oriented in opposite directions, can be seen in FMR experiments performed at 9.248 GHz (X-band). Using the expression for the free energy density proposed by Hu *et al.* (JMMM **301**:238, 2006), it was possible to simulate this behavior with high precision, without any simplifications and for arbitrary orientation. The following terms, besides the Zeeman term and shape anisotropy, were taken into account: two kinds of uniaxial anisotropy (in-plane and out-of-plane) of the FM layer, bilinear (Heisenberg) and biquadratic exchange couplings between FM and AFM layer, as well as the energy of the domain walls located at the interface. The FM saturation magnetization was the sixth parameter to be estimated from available experimental data.

Interval simulations have revealed 1, 2 and sometimes even 4 nearby equilibrium orientations of FM magnetization vector (at resonance) when the field has a component antiparallel to that of cooling field, while only 1 such position when field points in the opposite direction. In both cases only a single resonance line is observed.

## P-6-01

### MFV STUDY OF Nd-Fe-B-BASED PERMANENT MAGNETS

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Magnetic force microscopy (MFM) was used to observe the domain structures of anisotropic sintered Nd-Fe-B-based magnets and isotropic nanocomposite Nd<sub>2</sub>Fe<sub>14</sub>B/Fe<sub>3</sub>B magnets. The former magnets were in bulk form and consisted of grains with an average size of about 10 μm, while the latter magnets were in the form of ribbons about 40–50 μm thick and consisted of grains with an average size of about 30 nm. The magnets were studied in the thermally demagnetized state. In the case of the anisotropic sintered Nd-Fe-B-based magnets, studies made on the surface perpendicular to the alignment axis showed that the magnetic domain structure is composed of the main domains typically 1–2 μm wide, surface reverse spikes typically 0.5–1 μm in diameter and fine surface domains typically 50–200 nm wide. The presence of the surface domain structure reduces the magnetostatic energy near the specimen surface. In the case of the isotropic nanocomposite Nd<sub>2</sub>Fe<sub>14</sub>B/Fe<sub>3</sub>B magnets, the so-called interaction domains a few hundred nanometers in size were observed. These domains are found to be clusters composed of many grains with exchange interaction between the grains. Within the interaction domains a fine scale image contrast could be seen, indicating that the magnetization directions of individual grains are not precisely the same but differ slightly.

## **P-6-02**

### **STRUCTURAL CHANGES IN DEFORMED SOFT MAGNETIC Ni-BASED METALLIC GLASS**

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Amorphous alloys exhibit excellent soft magnetic and good mechanical properties. Thus the understanding of structural relaxation is quite important not only for technical applications of metallic glasses but also for knowing the nature of their structure. Structural relaxation is associated to changes in the short-range order within the amorphous structure and it manifests itself by decrease in enthalpy and by changes in many structural sensitive physical properties upon thermal treatment, e.g. the Curie temperature. The changes in enthalpy associated with structural relaxation in Ni–Si–B amorphous metallic glass were measured using differential scanning calorimetry. Plasticity in metallic glasses is accommodated through the formation of shear bands, facilitated by the creation of free volume during the deformation. The shear bands creating during inhomogeneous plastic deformation influence the structural relaxation process in the amorphous ribbon.

## **P-6-03**

### **APPLICATION OF THE COUPLING MODEL TO MAGNETIC AFTER EFFECTS IN THE Fe<sub>72</sub>Co<sub>10</sub>Nb<sub>6</sub>B<sub>12</sub> AMORPHOUS ALLOY**

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The aim of the present paper is to study free volume diffusion in the Fe<sub>72</sub>Co<sub>10</sub>Nb<sub>6</sub>B<sub>12</sub> amorphous alloy via measuring magnetic reluctivity versus time after demagnetization for samples pre-annealed at elevated temperatures. Such annealing changes the sample microstructure and allows studying the progress in structural relaxation. Measurements were carried out at room temperature in weak magnetic field (0.5 A/m). According to the Neel approach reluctivity  $r(t)$  for a non-interacting system represents a simple exponential relaxation. In order to describe the observed non-exponential process we have generalized the Neel formalism by applying the so-called coupling model (universal response function) appropriate for strongly correlated systems. Numerical analysis of the experimental curves shows that with increasing annealing temperature the relaxation intensity, the relaxation time and the coupling parameter decrease monotonically. This result is in agreement with the idea of formation of thermally stable relaxed amorphous phase containing small iron clusters.



## **P-6-04**

### **INFLUENCE OF MAGNETIC ANNEALING ON THE MAGNETIC PROPERTIES IN Fe-Co-M-B (M=Nb, Zr AND Mo) NANOCRYSTALLINE ALLOYS**

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The technological driving force behind this study is the optimization of the alloy composition and heat treatment process in order to obtain FeCo-based nanocrystalline materials with improved soft magnetic properties. A special attention has been devoted to the study of the effects of annealing under presence of external magnetic field in order to produce controllable uniaxial anisotropy in the samples. We report on the effects of both longitudinal and transverse magnetic field applied during the heat treatment on the magnetic behaviour in the series of Fe-Co-M-B type (M=Nb, Zr and Mo) nanocrystalline alloys. Sheared loops with good field linearity were achieved for all investigated alloys after annealing in transverse magnetic field. The stronger response to the transverse field-annealing is observed for the alloys containing Nb and Zr. Here, the values of the induced anisotropy constant up to  $K_u \approx 1350 \text{ Jm}^{-3}$  can be reached. A heat treatment under the presence of longitudinal magnetic field results for the Mo-containing samples in squared hysteresis loops characterized by coercive field values in the range of 3 - 8  $\text{Am}^{-1}$ . These values are superior to those previously reported for FeCo-based nanocrystalline materials and they remain fairly stable also at elevated temperatures.

## **P-6-05**

### **STRUCTURE AND MAGNETIC PROPERTIES OF Fe(Mn)-Si-B-Nb-Cu ALLOYS**

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The aim of this work was to investigate the role of the partial iron substitution by manganese on structural and magnetic properties of amorphous and nanocrystalline ribbons with nominal composition of  $\text{Fe}_{73.5-x}\text{Mn}_x\text{Cu}_1\text{Nb}_3\text{Si}_{13.5}\text{B}_9$  ( $x = 1, 5, 9, 15$  at. %) prepared by single-roller melt spinning technique. Both, the glassy state of as-quenched samples and nanocrystalline samples after annealing were studied by X-ray diffraction (XRD) measurements using synchrotron radiation performed at HASYLAB/DESY and thus structural factors and atomic pair distribution functions could be calculated. No significant changes were observed in a short range atomic order that could be expected as a result of Mn substitution. Thermal stability of the as-prepared alloys was investigated by differential scanning calorimetry (DSC). The structural evolution of amorphous samples Fe(Mn)-Si-B-Nb-Cu within temperature annealing was studied by in-situ XRD measurements. DSC measurements and in-situ XRD experiments revealed the two-step crystallization process, temperatures  $T_{x1}$  and  $T_{x2}$  were influenced by Mn content (thermal separation between  $T_{x1}$  and  $T_{x2}$  completely vanished for  $x = 15$  at. %.) The influence of Mn substitution on magnetic properties was confirmed by measurements of coercivity and by thermomagnetic measurements.

## **P-6-06**

### **STRUCTURE AND MAGNETIC PROPERTIES OF Fe(Mn)-Si-B-Nb-Cu ALLOYS**

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The aim of this work was to study the influence of niobium substitution by vanadium in  $\text{Fe}_{73.5}\text{Cu}_1\text{Nb}_{3-x}\text{V}_x\text{Si}_{13.5}\text{B}_9$  ( $x = 1.5, 3$ ) alloys on their structure and magnetic properties. Amorphous ribbons were prepared by melt spinning method. The structural evolution of the alloys after annealing treatment was investigated by the in-situ XRD experiments using synchrotron radiation performed at DESY Hamburg. Thermal analysis of the samples was performed by DTA method. DTA confirmed the influence of vanadium on crystallization temperature of nanocrystalline phase- $T_{x1}$  and crystallization of borides- $T_{x2}$ . The higher vanadium content lowers crystallization temperature  $T_{x1}$ ,  $T_{x2}$ . Magnetic measurements show the influence of vanadium content on magnetic properties (coercivity, Curie temperature, saturation magnetic induction, Hall effect) of both amorphous and nanocrystalline alloys, respectively.

## **P-6-07**

### **LATTICE DYNAMICS OF MAGNETIC 3D METALS WITHIN THE KKR GREEN'S FUNCTION METHOD**

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We present a formalism for the calculation of the force-constant tensor within the KKR Green's function method. As a primary information the formalism gives the real-space force-constant tensor, i.e. the pairwise interaction parameters, on the basis of ab-initio electronic structure calculations. Accordingly, the technique is applicable in principle to any system as for example solids, surfaces and nanostructures.

First results of calculations of the force-constant tensor as well as phonon spectra of magnetic metals and alloys will be presented. The influence of magnetism on the elastic properties as well as phonon spectra will be analysed. The calculated phonon spectra were used to investigate the role of magnetism in structural stability of 3d transition metals and alloys.

## **P-6-08**

### **INFLUENCE OF MILLING AND COMPACTION PROCESSES ON MAGNETIC PROPERTIES OF FeCo POWDER**

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Magnetic and structural studies were performed on Fe<sub>50</sub>Co<sub>50</sub> material. The samples (disk-shaped, diameter: 10 mm, thickness: 2.5 mm) were fabricated by compaction of powder under pressure of 800 MPa for 5 minutes at 500°C. The powder was obtained by milling of Fe<sub>50</sub>Co<sub>50</sub> alloy swarf in high-energy planetary RETSCH PM4000 mill (ball to powder mass ratio: 6:1, rate per minute: 180). The milling time varied from 1 hour to 40 hours. In course of milling process the mean size of alloy pieces was decreasing from about 0.5 mm to 0.05 mm (SEM), what provided more compact structure after compression. Coercive field is minimal (1200 A/m) in the case of 10 hour milling time. Parameters of CEMS Mössbauer spectra are almost the same for all samples, what points to not significant changes of internal magnetic structure after milling and compacting.

## **P-6-09**

### **THE INFLUENCE OF MECHANICAL ALLOYING ON THE STRUCTURAL AND MAGNETIC PROPERTIES OF SmNi<sub>5</sub>**

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We have investigated the influence of mechanical alloying on structural changes and magnetic properties of the SmNi<sub>5</sub> compound. The decrease of intensity and broadening of the diffraction lines have been detected after milling as a consequence of the grain's size reduction, and amorphisation of the samples. This compound crystallizes in the hexagonal structure of CaCu<sub>5</sub>, is ferromagnetic with the Curie temperature of 30 K and the saturation magnetic moment of  $0.7\mu_B$  at 4.2 K. From our magnetic measurement results, we revealed that difference in a magnetization at 2 K between FC and ZFC is a characteristic behavior for cluster glasses. We suggest that the cluster glass is controlling mechanism in the mechanical alloyed powder.

## **P-6-10**

### **PHASE DIAGRAMS FOR THE EVOLUTION OF POLYDOMAIN AND POLYVARIANT STATES IN TETRAGONAL FERROMAGNETIC MARTENSITES**

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A continuum model for equilibrium microstructures in ferromagnetic twinned martensites is developed [1] that couples micromagnetic domain theory with anisotropic crystal elasticity and is applicable for magnetic shape memory materials as the Ni-Mn-Ga Heusler alloys. The approach considers the twin variant redistribution in tetragonal martensites with no-slip condition at the twin boundaries, magnetic 180° domain structures within twins, and the rotation of magnetization within domains due to finite magnetic anisotropies. For two-variant twinned single crystals, we calculate equilibrium phase diagrams, strain and magnetization curves under combined applied magnetic fields and external stresses within the thermodynamic phase theory approximation. The limitations of the phase-theory approximations are discussed. For three-variant twinned microstructures, we show that magnetic charges arise internally at the twin boundaries. Work supported by DFG, SPP 1239 project A08.

[1] A.N. Bogdanov, A. DeSimone, S. Müller, U.K. Rößler, J. Magn. Magn. Mater. 261 (2003) 204.

## **P-6-12**

### **STRUCTURAL AND MAGNETIC PROPERTIES OF Cr TELLURIDE-SELENIDE ALLOYS**

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We present the results of theoretical study of magnetic and structural properties of Cr telluride-selenide alloys having trigonal crystal structure. Both ground state and temperature-dependent magnetic properties of the  $\text{Cr}_x(\text{Te}_\alpha\text{Se}_\beta)_2$  alloys have been investigated in a wide region of  $\alpha : \beta$  ratios with various Cr content. Theoretical results are compared with the experimental ones.

The ground state properties have been studied on the basis of electronic structure calculations using the Korringa-Kohn-Rostoker (KKR) band structure method. The substoichiometry and the disorder in the chalcogenide sub-lattice has been treated by means of the Coherent Potential Approximation (CPA) alloy theory. Magnetic properties at finite temperature have been studied by means of Monte Carlo simulations on the basis of a classical Heisenberg Hamiltonian and the exchange coupling parameters calculated from first principles. This approach allowed to determine the critical temperature in good agreement with experiment.

## **P-6-13**

### **STUDY OF MAGNETIC INHOMOGENEITY ON THE MAGNETOIMPEDANCE EFFECT OF SOFT MAGNETIC ALLOYS**

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In this paper, the rule of magnetic anisotropy and its inhomogeneity due to weakly interactions of magnetic heterogeneous structures with different magnetic properties in locally laser irradiated amorphous ribbons in the low frequency magnetoimpedance (MI) effect has been studied in details. This advances the classical model in which only the first-order anisotropy constant was taken into account and makes possible the study of the influence of the second-order anisotropy constant on the MI effect. This effect is caused by crystallization of magnetic materials at the surface and gradient temperature produced by locally irradiating mechanism of sample's surface in which various active magnetic media can be achieved. Interaction of different magnetic regions is interpreted by taking an average over all parts with various magnetic anisotropies in order to estimate the magnetic permeability and so the MI effect of the whole sample. The model can describe flattened peaks observed in the MI experiments and can describe the changes in the initial magnetization curves.

## **P-6-14**

### **ACTIVATION ENERGIES OF CRYSTALLIZATION IN AMORPHOUS $\text{RMn}_{4.5}\text{Ge}_{4.5}\text{Fe}_{1.5}\text{Al}_{1.5}$ ( $\text{R} = \text{La}, \text{Y}$ ) ALLOYS**

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The multicomponent  $\text{RMn}_{6-x}\text{Ge}_{6-x}\text{Fe}_x\text{Al}_x$  ( $0 \leq x \leq 6$ ) system with  $\text{R}=\text{La}, \text{Y}$  and Dy is derived from a ternary compounds combining transition metals (TM) Fe and Mn, rare-earths element (R), and metalloid or other metal (M) Ge and Al. Some compositions of this series with Dy were already obtained in fully amorphous state. Also for La and Y amorphization is attainable in the same range of compositions. Alloys with La and Y atoms are used as nonmagnetic analogues for Dy in further heat capacity and resistivity measurements analysis. Here we report results obtained with x-ray diffraction (XRD) and differential scanning calorimetry (DSC). DSC curves were recorded at different constant heating rates from 10 to 50 K/min. Crystallization process in  $\text{LaMn}_{4.5}\text{Ge}_{4.5}\text{Fe}_{1.5}\text{Al}_{1.5}$  sample occurs in higher temperatures than in samples with Dy and Y and is characterized by the two well defined effects at the first exothermic event. This event is not taken into consideration but it has to be underlined that this effect is also observed for Dy and Y containing samples. Activation energies for primary crystallization were calculated from the Kissinger relation and thermal stability of  $\text{LaMn}_{4.5}\text{Ge}_{4.5}\text{Fe}_{1.5}\text{Al}_{1.5}$  alloy reaches values of about 780 kJ/mol which exceeds considerably those for Dy and Y compositions.

## **P-6-15**

### **STRUCTURE AND MAGNETIC PROPERTIES OF Fe<sub>11</sub>Ni<sub>70</sub>Zr<sub>7</sub>B<sub>12</sub> ALLOY**

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Structure and magnetic properties of melt-spun Fe<sub>11</sub>Ni<sub>70</sub>Zr<sub>7</sub>B<sub>12</sub> alloy have been studied by means of X-ray diffraction (XRD), vibrating-sample magnetometry (VSM), differential scanning calorimetry (DSC) and Mössbauer spectroscopy (MS). The aim of the present paper is an investigation of the influence of Cr<sub>23</sub>C<sub>6</sub>-type phase appearance on magnetic properties of FeNi based alloys. Melt-spun sample crystallizes into metastable (FeNi)<sub>23</sub>B<sub>6</sub> structure at 450°C with probable *fcc*-austenite as the additional phase. Structure identification by XRD is complicated because of overlapped positions of austenite and metastable boride Bragg picks. Magnetization in amorphous Fe<sub>11</sub>Ni<sub>70</sub>Zr<sub>7</sub>B<sub>12</sub> alloy is about 12 Am<sup>2</sup>/kg at 300 mT external field and is induced by Ni atoms. From the shape of hysteresis loop one may conclude about the existence of paramagnetic and ferromagnetic components. For isothermally annealed (640°C for 1 hour) sample magnetization value increases. This is connected with crystallization process and occurs due to incorporation of Fe atoms into crystalline phase. According to MS measurements annealed sample contains only 13 percent of paramagnetic fraction.

## **P-6-16**

### **HETEROGENEOUS NUCLEATION IN Fe<sub>41</sub>Ni<sub>40</sub>Zr<sub>7</sub>B<sub>12</sub> MELT: MODELING AND EXPERIMENT**

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A numerical approach to description of the cooling and crystallization processes in a melt-spinning technique has been proposed. Based on the values of the thermodynamic and kinetic parameters which control crystallization of metallic glasses upon heating, we predict the largest critical thickness of the melt layer crystallizing by heterogeneous nucleation. The dominant contribution of this type of nucleation to the Fe<sub>41</sub>Ni<sub>40</sub>Zr<sub>7</sub>B<sub>12</sub> melt crystallization has been confirmed and the most probable values of the heterogeneous sites density and wetting angle have been estimated.

## ***P-7-01***

### **MAGNETIC LOGIC WITH PERPENDICULAR ANISOTROPY**

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In magnetic logic the direction of the magnetisation in sub-micron patterned ferromagnets is identified with Boolean logic 1 or 0. As first demonstrated Magnetic Logic with perpendicular magnetic anisotropy promises low power non-volatile computing, massively parallel character and fast operation and thus has the potential to become a key technology for logic circuits. NOT-gate and domain wall generator are presented. Both structures use nucleation strategy. First results showed problems with control nucleation processes in the magnetic nanostructures. Magneto-optic Kerr effect was used for the observations magnetic logic device.

Magnetic Domain-Wall Logic; D.A. Allwood, G. Xiong, C.C. Faulkner, D. Atkinson, D. Petit, and R.P. Cowburn, *Science*, 309, 1688-1692 (2005)





## **O-8-01**

### **MAGNETIC HEATING BY TUNABLE ARRAYS OF NANOPARTICLES IN CANCER THERAPY**

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Detailed knowledge about the temperature distribution achieved in the target area is essential for the development of magnetic hyperthermia treatments. However, the temperature inhomogeneity was found in all local hyperthermia studies. As a consequence of the impossibility of guaranteeing the temperature and thus the thermal dose distribution, hyperthermia is never applied as a single treatment modality. We suggest a model that enables the calculations and optimization of the spatial-time distribution of the temperature in the target volume (i.e. tumor) caused by magnetically heated elements: i) arrays of clusters of iron oxides magnetite ( $\text{Fe}_3\text{O}_4$ ) magnetic nanoparticles (MNPs), and ii) arrays of magnetic needles. In order to find the spatial-time temperature distribution in tumor, the bioheat transfer equation is solved for the two above mentioned arrays of magnetically heated sources embedded in tumor. The temporal and spatial temperature distributions were calculated with regards to the effect of blood perfusion in tumor. It is shown that a matrix of magnetic micro-needles injected in tumor could provide rather uniform tumor heating with the center-edge temperature difference less than 30C at any times during the magnetic hyperthermia treatments. The temperature profiles can be suitably adjusted by a proper choice of the MNPs arrangement.

## **P-8-01**

### **MAGNETIC CHARACTERIZATION OF TAXOL LOADED MAGNETIC PLGA-NANOSPHERES**

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Magnetically controlled drug targeting is one of the various possibilities of drug targeting. One of these technologies is based on encapsulation established drug with magnetic fluids in polymer with aim to concentrate drug in the area of interest by means of magnetic field. The Poly(D,L/lactide-co-glycolide acid) (PLGA) nanospheres loaded with magnetic fluids and anticancer drug Taxol by the nanoprecipitation method were prepared. The morphology and the particle size distributions of the prepared nanospheres were investigated by transmission electron microscope (TEM) and scanning electron microscope (SEM) that confirmed the spherical shape of prepared nanospheres with size 250 nm. The magnetic properties of the Taxol loaded magnetic polymer nanospheres were studied using magnetometer (SQUID) at the temperatures from 4.2 K to 300 K. The obtained results showed superparamagnetism of the prepared nanospheres with the blocking temperature  $T_B = 100$  K and the saturation magnetization  $M_S = 0.48$  emu. The prepared magnetic labeled PLGA nanospheres showed suitable response to the external magnetic field.

## **P-8-02**

### **FINITE-TEMPERATURE, INTERACTION DRIVEN PHASE TRANSITION IN THE THREE-DIMENSIONAL BOSE-HUBBARD MODEL**

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We discuss the finite-temperature phase diagram in the three-dimensional Bose-Hubbard model, relevant for Bose-Einstein condensates in optical lattices, by employing U(1) quantum rotor approach and the topologically constrained path-integral that includes a summation over U(1) topological charge. The effective action formalism allows us to formulate a problem in the phase only action and obtain analytical formulas for the critical lines beyond mean-field theory.

## **P-8-03**

### **PONDEROMOTIVE ACTION OF THE VECTOR POTENTIAL**

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A symmetric closed magnetic circuit, placed along the axis of the copper ring with sliding contacts is rotated, when the current flows through the contacts. The ponderomotive action may be explained by the interaction of the electric current and the magnetic vector potential  $\mathbf{A}$  induced by the magnetization. Within the framework of the classical electrodynamics it is shown, that an elementary volume is exposed along with magneto-dipole moment the moment of force  $\mathbf{N}^A = c^{-1}[\mathbf{J}^{\text{eff}}\mathbf{A}]$ , where  $c$  is the light velocity,  $\mathbf{J}^{\text{eff}}$  is the effective current density. The moment  $\mathbf{N}^A$  is similar to the moment of force  $[\mathbf{v}\mathbf{p}]$  into the equation of dynamic of the orbital angular momentum  $d\mathbf{L}/dt = [\mathbf{v}\mathbf{p}] + \mathbf{N}$ . The vector  $\mathbf{A}/c$  is considered as potential impulse of an electromagnetic field per unit of charge. The reality of the  $\mathbf{A}$  is evident from Aaronov-Bom effect. The volume integration of the  $N_z^A$  gives us the total moment of force which acting on the ring from magnetic circuit  $N_z^A = (\Phi J_0 / 2\pi c) F$ , where  $\Phi$  is the magnetic flux,  $J_0$  is the total current into the semiring. The function  $F$  is determined by geometric of the motor. Using typical magnitudes of the parameters one obtains  $(N_z^A)_{\text{max}} / J_0 \approx 135 \text{ dyne-cm/A}$ . The numerical values of the  $(N_z^A)_{\text{max}}$  are corresponded to the experimental values. Furthermore the theoretical angular dependence of the relative moment of force quality describes experimental dependence.

## ***P-8-04***

### **DYNAMICS OF PHAGOSOME WITH INTERNALIZED MAGNETIC NANOPARTICLES**

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Cytomagnetometry using magnetic nanoparticles is effective in probing the mechanisms of intracellular motion and rheological properties of the cytoplasm in living cells. We propose a model to describe intracellular magnetic field-driven motion of endosomes and phagosomes with internalized magnetic nanoparticles (MNPs). Utilizing different types of creep functions ( $J(t)$ ) measured for a living cell, we calculate the time dependences of the phagosome displacement and velocity. In particular, it is found that for a power-law  $J(t)$  the velocity as a function of time exhibits a wide plateau after which it falls to zero. For experimentally reachable magnetic field gradients the maximal phagosome velocity is found to be dozens micrometers per second which is two orders of magnitude larger than typical organelles velocities in living cells. The proposed model allows us to find the viscoelastic parameters of cytoplasm by experimentally detecting the phagosome displacements and then by fitting the obtained time dependence to those calculated for a given creep function. For application in cancer therapy we discuss the possibilities of cell cytoskeleton destroying by a high speed moving phagosome under pulses of gradient magnetic fields.



## Postdeadline abstract: P-5-33

### MAGNETISM OF SOFT-LANDED CADMIUM ATOMS ON NICKEL SURFACE

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Applying elaborate preparation techniques, isolated radioactive Cadmium atoms were positioned at different sites on a ferromagnetic Nickel surface [1]. The magnetic hyperfine fields and the electric field gradient were measured by the perturbed angular correlation (PAC) spectroscopy of gamma-radiation. The experiments were performed in ultra-high vacuum at the on-line mass separator ISOLDE of CERN/Geneva. The magnetic fields at Cd were found to depend on the number of neighbouring Nickel atoms (coordination number NN) and exhibited a change of sign between NN=5 and NN=4. The results were confirmed by calculations using the Greens function embedding methods and can be explained by a polarization in the s-conduction band [2]. The field gradients, which are a representation of the electric charge distributions, were interpreted to develop from asymmetric populations of p-sublevels [3]

[1] Y. Manzhur, W.-D Zeitz, M. J. Prandolini, W.D. Brewer, P. Imielski, J. Schubert, K. Johnston, and ISOLDECollaboration, European Physical Journal B59 (2007), 277-283

[2] P. Mavropoulos J. Phys.: Condens. Matter 15 (2003) 8115-8122

[3] V. Bellini, S. Cottenier, M. Çakmak, F. Manghi and M. Rots, Phys. Rev B 70 (2004) 155418



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