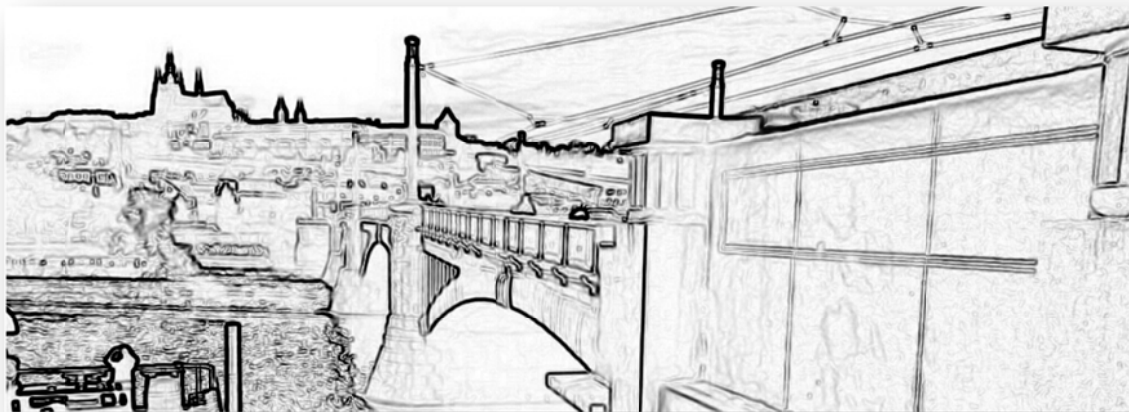


# 11<sup>th</sup> Prague Colloquium on f-Electron Systems



*Prague, 2<sup>nd</sup> – 5<sup>th</sup> July 2014*

## Program & Abstracts



## Welcome to PCFES!.....and some local information

Almost every second year since 1992 we organized the *Prague Colloquium on f-Electron Systems*, an exciting meeting covering topics in physics of actinides and lanthanides. Also this year we keep the tradition and we will have the pleasure to welcome you at 11<sup>th</sup> PCFES, an informal forum for presentations and discussions on the current issues of magnetism, strongly correlated systems, spectroscopies, materials science, as well as progress in theory. It should also provide ground for close interaction of students and other early-stage researchers with experienced specialists.

Regarding our venue, the Faculty of Mathematics and Physics belongs to the youngest faculties of the Charles University, which was founded in 1348 by the Roman Emperor and King of Bohemia, Charles IV. The Faculty itself was founded in 1952, splitting from the Faculty of Science. The building Ke Karlovu 5, where the PCFES sessions will take place, is now over 100 years old. Careful reconstructions succeeded to provide high functionality while meticulously preserving or restoring most of the details, carrying the spirit of the founders in early 1900's as well as following generations of professors and students. Part of the laboratories of the Department of Condensed Matter Physics (technology, X-ray diffraction, high-pressure lab) are located on the ground floor of the building. Neighbour building in the Ke Karlovu street, number 3, is the official and administrative seat of the Faculty. It is followed by the Church of the Virgin Mary and St. Charlemagne, built in the 14<sup>th</sup> century and known for its unique vaulted central dome without any support. Unfortunately it is not opened during working days. Those you stay till Sunday you can attend the Holy Mass at 9 a.m., 2.30-4.30 pm it is opened for sightseeing with a guided tour, if you wish, between 2.45-4.30 p.m.

Down the street, the redbrick Maternity hospital and even farther the Psychiatric hospital (with the Antonin Dvorak museum opposite in a cute small baroque palace) complete the list of useful addresses.

Besides the oral sessions, taking place in the lecture room F1, there will be posters on the 1st floor corridor. Presenters are requested to mount the posters as early as possible and keep them for the whole duration of PCFES to allow informal discussions. There is one dedicated poster session (Thursday evening), during which presenters are expected to be present at their posters. During PCFES, refreshment will be provided at coffee breaks and evenings. Lunches are left on you, depending on your preference you will find numerous small restaurants in the lively part of the town North of the Ke Karlovu street.

This year PCFES is organized just following the  *$\Psi$ -k Workshop Strong electron correlation effects in complex d- and f-based magnetic materials for technological applications* (<http://wsp-psik.fzu.cz/>), organized by the Theory group of the Institute of Physics, Academy of Sciences of the Czech Republic in the main Academy building Národní 3, Praha 1. So as to provide a mix zone, the last part of the  *$\Psi$ -k Workshop* (Wednesday afternoon) will be in the same time the introductory part of PCFES and will be at the Charles University. And the Workshop participants are invited for the welcome party of PCFES.

Information update on: <http://kflk.cz/pcfes/>

Please feel comfortable in Prague, we wish you most enjoyable and productive days.

PCFES Organizers

The 11<sup>th</sup> Prague Colloquium on f-Electron Systems takes place with the contribution of material and human potential of the Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague.



# Program

Wednesday, 2 July 2014

10.00 – 18.00 *Registration*

## Session I Theory

### Chairpersons

**L. Havela**

**Charles University in  
Prague**

14.20 – 14:30 *Welcome address*

Vladimir  
Sechovský  
Pavel Novák

Charles University in  
Prague  
Institute of Physics,  
ASCR

14.30 – 15:00 Crystal field and magnetism with Wannier functions: rare-earth intermetallics and low symmetry systems

15.:00 – 15.30 First principles study of valence and structural transitions in rare earth compounds under pressure

Leon Petit

Daresbury Laboratory,  
United Kingdom

15.30 – 16.00 *Coffee Break*

## Session II Theory

### Chairperson

**A. Shick**

**Institute of Physics,  
ASCR**

16.00 – 16:20 Rare-earth based pigments and colors from first principles

Jan Tomczak

TU Vienna

16.20 – 16.40 Charge localization in La, Pr and Nd substituted Sr hexaferites

Vojtěch Chlan

Charles University in  
Prague  
TU Vienna

16.40 – 17.00 Study of complex magnetic states and phase transitions with Lichtenstein method

Sergii  
Khmelevskiy  
Yaroslav  
Kvashnin

Uppsala University

17.00 – 17.20 Effective inter-site exchange interactions from DFT+DMFT

17.20 – 17.40 Interplay between Kondo effect and molecular quenching in magnetic molecules at metal substrates from first principles

David Jacob

MPI MP, Halle

18:00 – 21.00 *Welcome party*

Thursday, 3 July 2014

## Session III Theory - many body

### Chairperson

**P. Oppeneer**

**Uppsala University**

9.00-9.30 A novel *ab-initio* many body Green's function approach for the materials with correlated d- and f-electrons

Vladimir  
Antropov

Ames Lab, USA

9.30-10.00 Collective excitations, stability of the excitonic phase, and electronic ferroelectricity in the extended Falicov--Kimball model

Denis I. Golosov

Bar-Ilan University,  
Israel

10.00-10.30 Nonmagnetic ground state of PuO<sub>2</sub>

Jindřich Kolorenč

Institute of Physics,  
ASCR

10:30 – 11.00 *Coffee break*

## Session IV Theory

### Chairperson

**A. Shick**

**Institute of Physics,  
ASCR**

11.00 – 11:30 X-ray magnetic linear dichroism of UC - ab initio study

Dominik Legut

VSŽ - TU of Ostrava

11:30 – 12.00 Ising anisotropy of quasiparticles in URu<sub>2</sub>Si<sub>2</sub>: A signature of localized 5f states?

Peter Oppeneer

Uppsala University

12:00 – 14:00 *Lunch break*

## Session V Theory

### Chairperson

**J. Kolorenč**

**Institute of Physics,  
ASCR**

14:00 – 14:30 Magnetic anisotropy of Co-intercalated graphene on Ir(111)

Alexander B.  
Shick

Institute of Physics,  
ASCR

14:30 – 15:00 Strong quantum memory at resonant Fermi edges revealed by shot noise

Tomáš Novotný

Charles University  
Prague

15:00 – 15.30 *Coffee break*

## Session VI Cerium

### Chairperson

**A. Slebarski**

**University of Silesia,  
Poland**

15.30 – 16.00 Effect of Pressure on the Electronic Properties on Rare-earth and Uranium compounds

Fuminori Honda

Tohoku University,  
Japan

16.00 – 16.30 Incommensurately modulated crystal and magnetic structures in CeRuSn

Steffen Hartwig

Helmholtz-Zentrum  
Berlin

16.30 – 17.00 Single crystal growth and physical properties of the Ce<sub>n</sub>T<sub>m</sub>In<sub>3n+2m</sub> heavy fermion compounds

Marie  
Kratochvilova  
Milan Klicpera

Charles University in  
Prague  
Charles University in  
Prague

17.00 – 17.30 Electronic properties study of CePtIn single crystal

17.30 – 18.00 Pressure-induced superconductor CePtSi<sub>2</sub>

Tomohito Nakano

Niigata University,  
Japan

18:00 – 20.30 *Poster session and refreshment*

**Friday, 4 July 2014**

<b>Session VII Actinides</b>	<b>Chairperson</b>	<b>F. Honda</b>	<b>Tohoku University, Japan</b>
9:00 – 9:25	Thermodynamic properties of selected splat-cooled U-T alloys (T=Mo, Pd, Pt)	Nhu Tarnawska H Kim Ngan	Pedagogical University Krakow
9:25 – 9:50	Superconductivity and structure of U-Zr and U-Mo splats	Ilya Tkach	Charles University Prague
9:50 – 10:15	The influence of doping on magnetic properties of the UH <sub>3</sub> -based hydrides	Mykhaylo Paukov	Charles University Prague
10:15 - 10:40	Pressure-induced strengteing and subsequent suppression of the ferromagnetic interactions in UGa <sub>2</sub>	Alexandre Kolomiets	Charles University in Prague & Lviv Polytechnic University
10:40 – 11:10	Low-Temperature Magnetic Properties of Dilute Uranium Alloys (Th,U)Be <sub>13</sub>	Hiroshi Amitsuka	Hokkaido University, Japan
11:10 – 11:30	<i>Coffee break</i>		
<b>Session VIII superconductivity</b>	<b>Chairperson</b>	<b>H. Amitsuka</b>	<b>Hokkaido University, Japan</b>
11:30 – 12:00	Superconductivity of La <sub>3</sub> M <sub>4</sub> Sn <sub>13</sub> with M = Co, Rh, and Ru: A comparative study	Andrzej Slebarski	University of Silesia, Poland
12:00 – 12:30	Crystal structure and superconductivity in the cage compounds RV <sub>2</sub> Al <sub>20</sub>	Tomasz Klimczuk	TU Gdansk, Poland
12:30 – 14:00	<i>Lunch Break</i>		
<b>Session IX Theory</b>	<b>Chairperson</b>	<b>V. Antropov</b>	<b>Ames Lab, USA</b>
14:00 – 14:30	Pre-critical fluctuations in Nodal Kondo Insulators	Peter Riseborough	Temple University
14:30 – 15:00	Quantum critical metal YbRh <sub>2</sub> Si <sub>2</sub> : High magnetic fields and elevated temperatures	Gertrud Zwicknagl	TU Braunschweig
15:00 – 15:30	Theory of ultrafast magnetization dynamics	Karel Carva	Charles University in Prague
15:30 – 16:00	<i>Coffee break</i>		
<b>Session X Actinides</b>	<b>Chairperson</b>	<b>L. Havela</b>	<b>Charles University in Prague</b>
16:00 – 16:30	Structural, electronic, and magnetic characteristics of Np <sub>2</sub> Co <sub>17</sub> under extreme conditions	Itzhak Halevy	NRCN, Ben Gurion Univ. &, CALTECH, USA
16:30 – 17:00	Crystal structure and physical properties of novel U-Fe-Ge intermetallic compounds	Margarida Henriques	University of Lisbon, Portugal
17:00 – 17:30	Studies of UFeSb <sub>2</sub> uranium antimonide	Marian Reiffers	University of Presov, Slovakia
17:30 – 18:00	Single crystal growth and magnetism of the novel U <sub>2</sub> RhIn <sub>8</sub> compound	Attila Bartha	Charles University in Prague
18:00 – 23:00	<i>Barbeque and wine tasting evening</i>		

**Saturday, 5 July 2014**

<b>Session XI Rare earths</b>	<b>Chairperson</b>	<b>Nhu Tarnawska H Kim Ngan</b>	<b>Pedagogical University, Krakow</b>
9:00 – 9:30	Peculiar magnetic properties of selected RE-compounds with 221 composition	Silvie Mašková	Charles University in Prague
9:30 – 10:00	Relationship between magnetic structure and physical properties in Co- and Ca-doped EuFe <sub>2</sub> As <sub>2</sub> compounds	Lan Maria Tran	ILT & SR PAS, Wroclaw
10:00 – 10:30	<i>Coffee break</i>		
10:30 – 11:00	Electronic properties of a distorted kagome lattice antiferromagnet Dy <sub>3</sub> Ru <sub>4</sub> Al <sub>12</sub>	Denis Gorbunov	Institute of Physics, ASCR
11:00 – 11:30	Hydrogenation of W <sub>2</sub> CoB <sub>2</sub> -type structure intermetallics	Khrystyna Miliyanchuk	IF national University of Lviv
11:30 – 12:00	NMR study of ternary stannides of R <sub>3</sub> Co <sub>4</sub> Sn <sub>13</sub> (R = Ce, Pr, Yb)	C.S. Lue	National Cheng Kung Univ.
12:00 – 14:00	<i>Lunch Break</i>		
14:00 – 18:00	<i>Non-structured discussion and farewell party</i>		

## List of posters

P-1	Oleksandr Bednarchuk	Single-crystal study on the antiferromagnetism in $\text{EuNiGe}_3$
P-2	Daniel Gralak	The hybridization of 5f- conduction electrons in $\text{URu}_{1-x}\text{Pd}_x\text{Ge}$
P-3	Hiroyuki Hidaka	Effects of Pressure on $\text{CeAg}$
P-4	Vladimir Karpasyuk	Structural and electromagnetic characteristics of $\text{La}-(\text{Sr,Ce})-(\text{Mn,Zn})-\text{O}$ manganites and the problem of charge compensation
P-5	Kamila Komadera	Magnetism of europium in superconducting $\text{EuFe}_{(2-x)}\text{Co}_{(x)}\text{As}_2$ studied by $^{151}\text{Eu}$ and $^{57}\text{Fe}$ Mössbauer spectroscopy
P-6	Agnieszka Kozub	Screening of magnetic moment at Co impurities in Cu hosts
P-7	Vasily Krylov	Screening effect of magnetic exchange in the U- and Gd-based intermetallic compounds
P-8	Chia Nung Kuo	Comparative study of ternary stannides of $\text{R}_3\text{Co}_4\text{Sn}_{13}$ (R = Ce, Pr, Yb)
P-9	Jana Lazurova	Magnetic Properties of $\text{NdFe}_{1-x}\text{Mn}_x\text{O}_3$
P-10	Silvie Maskova	Hydrogen absorption in $\text{UNiZn}$ and its similarity to $\text{UNiAl}$
P-11	Krzysztof Domieracki	Superconductivity in non-centrosymmetric compound $\text{ThPtSi}$
P-12	Zuzana Molcanova	Crystal growth and characterization of $\text{Ce-Ni-Ge}$ compounds
P-13	Shota Mombetsu	High-Frequency Ultrasonic Measurements of $\text{SmOs}_4\text{Sb}_{12}$ under Hydrostatic Pressure
P-14	Gendo Oomi	Application of Nd-ferromagnet to the elementary education of physics in university
P-15	Omosede Osafire	Strongly Correlated Four Electron Systems Away from Half Filling
P-16	Alexander Povzner	Hybridization features of the electronic structure and paramagnon mechanism of superconductivity
P-17	Chihiro Tabata	High-Resolution X-Ray Diffraction Study on $\text{URu}_2\text{Si}_2$
P-18	Zbigniew Tarnawski	Hydrogen induced interdiffusion in selected Vanadium and Titanium oxide thin films
P-19	Arkadij Volkov	Magnetic susceptibility and features of electronic structure $\text{Pu}??\text{Ga}_5$
P-20	Michał Winiarski	Extensive Studies of Antiferromagnetic $\text{GdM}_2\text{Al}_{20}$ (M = V, Ti, Cr)
P-21	Natalia Zaitseva	Anomalous influence of an external magnetic field on spin fluctuations and magnetorefractive effect in lanthanum manganites
P-22	Amir Zellati	Study the structural and superconducting properties of europium oxide nanoparticle added $\text{Bi}_{1.6}\text{Pb}_{0.4}\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_y$
P-23	Martin Zinner	XAS- and XMCD-Signatures of Kondo and Heavy Fermion Behaviour in the Surface Intermetallic $\text{CePt}_5/\text{Pt}(111)$
P-24	Itzhak Halevy	Structural investigation of $\text{Np}_2\text{Co}_{17}$ and analogue compounds under pressure
P-25	Rudolf Šýkora	Optical properties of a monoclinic insulator $\text{Cu}(\text{H}_2\text{O})_2(\text{en})\text{SO}_4$ , $\text{en}=\text{C}_2\text{H}_8\text{N}_2$
P-26	Karol Synoradzki	Electric resistivity of the $\text{Ce}(\text{Cu}_{1-x}\text{Ni}_x)_4\text{Mn}$ series

# Orals

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### **Crystal field and magnetism with Wannier functions: rare-earth intermetallics and low symmetry systems**

$\Psi$ -01

Pavel Novak

*Institute of Physics ASCR, Cukrovarnicka 10, Praha 6, Czech Republic*

Until recently no robust ab-initio method to calculate the crystal field of rare-earth ions in crystals was available. During the last two years we developed a scheme, which was successfully used to determine the crystal field parameters of trivalent RE ions in oxides with orthoperovskite and garnet crystal structure. These parameters were then inserted in atomic-like program which, besides the crystal field, takes into account the 4f-4f electron repulsion, spin-orbit and Zeeman interactions. The agreement of the calculated and experimental splitting of RE multiplets was very good (within meV) and also magnetism of the RE multiplet is correctly described.

The method uses the density functional theory based band structure calculation, followed by a transformation of the Bloch to the Wannier basis and expansion of the local Hamiltonian in terms of the spherical tensor operators. It contains a single adjustable parameter that characterizes the hybridization of RE(4f) states with the states of oxygen ligands. In the present contribution the method is applied to NdFe<sub>14</sub>B and to R:LaF<sub>3</sub> (R=Ce, Pr, ... Yb). In LaF<sub>3</sub> the rare earth site has a low symmetry and 27 crystal field parameters are needed to describe the crystal field.

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### **First principles study of valence and structural transitions in rare earth compounds under pressure.**

$\Psi$ -02

Leon Petit<sup>1</sup>, Axel Svane<sup>2</sup>, Martin Lueders<sup>1</sup>, Zdzislawa Szotek<sup>1</sup>, V Kanchana<sup>3</sup>, Ganapathy Vaitheeswaran<sup>4</sup>, and Walter Temmerman<sup>1</sup>

<sup>1</sup>*Daresbury Laboratory, Warrington WA4 4AD, United Kingdom*

<sup>2</sup>*University of Aarhus, DK-8000 Aarhus C, Denmark*

<sup>3</sup>*Indian Institute of Technology, Hyderabad-502 205, India*

<sup>4</sup>*University of Hyderabad, Hyderabad-500 046, India*

The self-interaction corrected (SIC) local spin-density (LSD) approximation is used to study the sequence of structural and electronic transitions that occur in rare earth compounds (rare earth mono-tellurides and EuO) under pressure. It emerges that at ambient conditions all the rare earth tellurides (RTe) are stabilized in the NaCl (B1) structure. The corresponding rare earth valency is nominally trivalent (R<sup>3+</sup>), with the exception of SmTe, EuTe, DyTe, TmTe, and YbTe, that are characterized by a divalent (R<sup>2+</sup>) ion, corresponding to a fully localized f-electron configuration. Under pressure the CsCl (B2) structure becomes energetically favourable. Whilst the trivalent RTe undergo an isovalent structural transition, the divalent RTe are characterized by a succession of structural and valence transitions, the order of which is determined by the degree of f-electron localization. This interplay between structural and electronic degrees of freedom becomes even more noticeable in EuO. Here, starting from the Eu<sup>2+</sup> ground state, an insulator to metal transition around 48 GPa leads to a valency increase in the B1 phase, followed at around 60 GPa by a structural transition to a B2 phase with an associated decrease in valency. This scenario is in line with the reentrant valence behaviour observed in recent pressure experiments.



Jan Tomczak<sup>1</sup>, Leonid Pourovskii<sup>2</sup>, Loig Vaugier<sup>2</sup>, Antoine Georges<sup>2</sup>, and Silke Biermann<sup>2</sup>

<sup>1</sup>*Institute of Solid State Physics, Wiedner Hauptstrasse 8-10, Wien, A-1040, Austria*

<sup>2</sup>*Centre de Physique Théorique, Ecole Polytechnique, France*

Many inorganic pigments contain heavy metals hazardous to health and environment. Much attention has been devoted to the quest for nontoxic alternatives based on rare-earth elements. However, the computation of colors from first principles is a challenge to electronic structure methods, especially for materials with localized f-orbitals. Here, starting from atomic positions only, we compute the colors of the red pigment cerium fluorosulfide as well as mercury sulfide (classic vermilion). Our methodology uses many-body theories to compute the optical absorption combined with an intermediate length-scale modelization to assess how coloration depends on film thickness, pigment concentration, and granularity. We introduce a quantitative criterion for the performance of a pigment. While for mercury sulfide, this criterion is satisfied because of large transition matrix elements between wide bands, cerium fluorosulfide presents an alternative paradigm: the bright red color is shown to stem from the combined effect of the quasi-2D and the localized nature of 4f states. Our work [1] shows the power of modern computational methods, with implications for the theoretical design of materials with specific optical properties.

[1] J. M. Tomczak, L. V. Pourovskii, L. Vaugier, A. Georges, and S. Biermann, PNAS 110 (3), 904 (2013).

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## Charge localization in La, Pr and Nd substituted Sr hexaferrites

Vojtěch Chlan<sup>1</sup>, Karel Kouřil<sup>1</sup>, Helena Štěpánková<sup>1</sup>, Kateřina Uličná<sup>1</sup>, Richard Řezníček<sup>1</sup>, and Jörg Töpfer<sup>2</sup>

<sup>1</sup>*Faculty of Mathematics and Physics, Charles University in Prague, V Holešovičkách 2, Prague, Czech Republic*

<sup>2</sup>*University of Applied Sciences Jena, Department of SciTec, Carl-Zeiss-Promenade 2, 07745 Jena, Germany*

In the M-type hexagonal ferrite SrFe<sub>12</sub>O<sub>19</sub> ferric cations form five magnetic sublattices, denoted as 2a, 2b, 4f<sub>IV</sub>, 4f<sub>VI</sub> and 12k. The magnetic structure is collinear: moments of 2a, 2b and 12k are parallel (4f<sub>IV</sub> and 4f<sub>VI</sub> antiparallel) to the overall magnetization with easy direction along the hexagonal c-axis. Substitution of divalent Sr for a trivalent one (La, Nd, Pr, Sm, Eu, Gd, ...) produces an excess valence electron and leads to changes in valence states of ferric ions. From measurements of magnetocrystalline anisotropy and total magnetic moment Lotgering [1] deduced that Fe<sup>2+</sup> should localize in octahedral 2a site at low temperatures and proposed that the increased magnetic anisotropy is due to single ion contribution of Fe<sup>2+</sup> in 2a sites. Since then the picture of full (or strongly preferred) Fe<sup>2+</sup>(2a) localization was supported by various local hyperfine methods, however, the mechanism of increased magnetic anisotropy can be experimentally clarified only indirectly. Theoretical description of the increased anisotropy is lacking, since the solution corresponding to Fe<sup>2+</sup>(2a) has not been achieved until now. The calculations of electronic structure resulted in a delocalized solutions with excess charge contained in the interstitial space or smeared over all iron sites [2-3].

Using electron structure calculations we model the Fe<sup>2+</sup> localization in 2a sites of La, Nd, and Pr hexaferrites. Orbital potential is employed to stabilize various orbital states, and thus obtain more than one scf solution. The desired localized solution is found to be energetically favourable compared to the delocalized one, for all used substituting trivalent atoms. This is also supported by <sup>57</sup>Fe nuclear magnetic resonance experiments where the intensity of Fe<sup>3+</sup>(2a) line decreases linearly with increasing concentration of trivalent large ion. The single-ion contribution to magnetocrystalline anisotropy of the hexaferrites is calculated using the force theorem approach, while the dipolar contribution is obtained by direct summation and is found to be much smaller. The results show that the localization is responsible for the increased anisotropy of LaM, compared to SrM. We discuss the details of the charge localization and the mechanism leading to increased anisotropy and also explain the strong decrease of anisotropy in LaM with increasing temperature (in contrast with constant character in case of SrM).

[1] F. K. Lotgering, J. Phys. Chem. Solids 35, 1663 (1974).

[2] P. Novák et al., Eur. Phys. J. 43, 509 (2005).

[3] M. Küpferling et al., J. Appl. Phys. 97, 10F309 (2005).

## Study of complex magnetic states and phase transitions with Lichtenstein $\Psi$ -05 method

Sergii Khmelevskiy

*CMS, Vienna University of Technology, Gusshausstrasse 25a, Vienna, 1040, Austria Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki t 8. H1111 Budapest, Hungary*

The first-principle calculations of the magnetic exchange constants using the magnetic force theorem (so-called Lichtenstein method) is allowed to investigate the microscopic mechanism of the complex magnetic phase formations and phase transitions. We illustrate this using as examples the complex non-collinear ground state in NpCoGe compound, predictions of novel type of meta-magnetic transition in (Mn,Cr)Au<sub>2</sub> alloy and evaluation of magnetic compensation temperature in DyCo<sub>5</sub> compound. On the basis of Lichtenstein method the state-of-the-art ab-initio calculations one may predict a novel materials with superior magnetic properties. The experimental invention of high-temperature antiferromagnets Mn<sub>2</sub>Au ( $T_{Neel} > 1200\text{K}$ ), which for over two decade has been regarded as non-magnetic compound, has been initiated by the theoretical predictions on the basis of Lichtenstein method. Another example is the prediction of the one-dimensional metallic ferromagnetism in MnB<sub>4</sub> will be discussed.

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## Effective inter-site exchange interactions from DFT+DMFT $\Psi$ -06

Yaroslav Kvashnin, Igor Di Marco, Oscar Grånäs, Corina Etz, and Olle Eriksson

*Uppsala University, Department of Physics and Astronomy, Lägerhyddsvägen 2, SE-75120 Uppsala, Sweden*

The inter-site exchange couplings ( $J$ 's) is one of the main quantities of magnetic materials. They define the Curie temperature, such an important property of a compound for its technological application. An ability to predict and tweak the  $J$ -parameters in various materials would be an essential step towards the design of new permanent magnets. Therefore, a great effort is made in the field of computational modelling. However, this task becomes even more challenging due to the fact that many of suitable compounds exhibit strong correlation effects.

In this talk I will present our recent implementation of the method for extracting exchange parameters in strongly correlated systems from first-principles calculations. We model the electronic structure with the help of the full-potential linear muffin-tin orbital code, developed in Uppsala [1]. The effects of electron correlations are studied within the same framework by means of charge self-consistent density functional theory + dynamical mean field theory (CSC DFT+DMFT) method [2]. In order to calculate the effective exchange parameters, we employ the linear-response-like approach by Lichtenstein *et al.* [3]. Combined all together, these methods allow us to investigate how  $J$ 's are affected by electron correlations at finite temperature.

In the last part of my presentation I will show some particular applications of the method. A special attention will be given to the case of SrRuO<sub>3</sub>. The impact of correlation effects and structural changes on the  $J$ -parameters in this system will be discussed.

[1] J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, and O. Grechnev, Springer Series in Solid-State Sciences pp. 1–195 (2010).

[2] O. Granäs, I. Di Marco, P. Thunstrom, L. Nordstrom, O. Eriksson, T. Bjorkman, and J. M. Wills, Computational Materials Science 55, 295 (2012).

[3] A. I. Liechtenstein *et al.*, J. Magn. Magn. Mater., 67, 65 (1987); M. I. Katsnelson and A. I. Liechtenstein, J. Phys. Condens. Matter, 16, 7439 (2004).

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## Interplay between Kondo effect and molecular quenching in magnetic molecules at metal substrates from first principles $\Psi$ -07

David Jacob

*Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany*

When a magnetic molecule is deposited on a metallic substrate or attached to metal leads, the Kondo effect can take place, thereby screening its magnetic moment. On the other hand strong coupling of the transition metal center to the organic ligands also leads to quenching of the spin. Using our DFT based ab initio approach for nanoscale devices explicitly taking into account the dynamic correlations originating from strong electronic interactions [1,2], we calculate the electronic structure and STM spectra of high spin complexes on metal surfaces. Our calculations reveal the complex interplay of the Kondo effect and molecular quenching processes in these systems. Furthermore we find that Kondo screening via the organic ligands leads to novel features in the spectral function near the Fermi level different from the usual Kondo peaks [3].

[1] D. Jacob, K. Haule and G. Kotliar, PRL 103, 016803 (2009)

[2] M. Karolak, D. Jacob and A. I. Lichtenstein, PRL 107, 146604 (2011)

[3] D. Jacob, M. Soriano and J.J. Palacios, PRB 88, 134417 (2013)

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## A novel *ab-initio* many body Green's function approach for the materials with correlated d- and f-electrons O-01

Vladimir Antropov and Andrey Kutepov  
Ames Laboratory, USDOE, Ames, IA, 50011

We propose a novel approach to improve *ab-initio* description of the materials with d- or f-electrons. The proposed approach is based on usage of perturbative many body Green's functions and its distinctive feature is that we include explicitly the *ab-initio* calculated vertex corrections. We discuss the place where this method should be placed in the hierarchy of different many body techniques. Then we show different tests of this method together with the results obtained using the local density approximation, quasiparticle GW approach and others. We consider in details possible calculations of the total energy using the proposed technique. A different highly accurate scheme of calculation of the perturbation energy is developed and tested for the case of spin orbital and magnetic perturbations. We demonstrate how proposed method improves a description of the electronic structure and the exchange splittings in numerous magnetic materials with f-electrons.

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## Collective excitations, stability of the excitonic phase, and electronic ferroelectricity in the extended Falicov--Kimball model O-02

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We consider the excitonic insulator state (often associated with electronic ferroelectricity), which arises on the phase diagram of an extended spinless Falicov--Kimball model (FKM) at half-filling. Within the Hartree--Fock approach, we calculate the spectrum of low-energy collective excitations in this state up to second order in the narrow-band hopping and/or hybridisation. This allows to probe the mean-field stability of the excitonic insulator. The latter is found to be unstable when the case of the pure FKM (no hybridisation with a fully localised band) is approached. The excitonic phase, however, may be stabilised further away from the pure FKM limit. In this case, the low-energy excitation spectrum contains new information about the properties of the excitonic condensate (including the strongly suppressed critical temperature). Our results on stability and degeneracies of the excitonic insulator phase imply that the presence of both hybridisation and narrow-band hopping is required for electronic ferroelectricity. When only one of these is present, the dielectric constant diverges, yet the electrostatic dipole interactions preclude the formation of spontaneous polarization.

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## Nonmagnetic ground state of PuO<sub>2</sub> O-03

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The correlated band theory implemented as a combination of the local density approximation with the exact diagonalization of the Anderson impurity model is applied to PuO<sub>2</sub>. We obtain an insulating electronic structure consistent with the experimental photoemission spectra, and a nonmagnetic ground state that is characterized by a noninteger filling of the plutonium f shell ( $n_f \approx 4.5$ ). Due to sizeable hybridization of the f shell with the p states of oxygen, the ground state is more complex than the four-electron Russell--Saunders <sup>5</sup>I<sub>4</sub> manifold split by the crystal field. The inclusion of hybridization improves the agreement between the theory and experiment for the magnetic susceptibility.

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## X-ray magnetic linear dichroism of UC - ab initio study O-04

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The full angular dependence of the x-ray magnetic linear dichroism (XMLD) on the crystalline orientation of the magnetization was investigated for the anti-ferromagnetic and ferromagnetic phase of uranium carbide. The anisotropic spectra were computed in the single electron picture within the framework of density functional theory at the  $M_{4,5}$  edges. The generalized gradient approximation as parametrized by Perdew-Burke-Ernzerhof was utilized for the exchange-correlation energy term. The correlated behavior of f-electron states were treated with Hubbard U technique. The XMLD spectra for selected magnetization direction and for a number of effective Hubbard U were examined.

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## Ising anisotropy of quasiparticles in $URu_2Si_2$ : A signature of localized 5f states? O-05

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The hidden order (HO) phase emerging below 17.5K in the heavy-fermion compound  $URu_2Si_2$  has drawn considerable attention. In spite of intensive experimental and theoretical investigations the origin of the arising electronic order could not be unambiguously explained [1]. Since the actinide 5f electrons can adopt localized or itinerant character, theories based on localized 5f behavior have been proposed as well as competing theories based on the assumption of itinerant 5f behavior; in the latter the existence of a Fermi surface instability is central.

Experimental evidence in favor of either localized, itinerant, or dual 5f behavior is crucial. Recent experiments drew attention to a previously unrecognized aspect of the HO quasiparticles (QPs). A g-factor anisotropy exceeding 30 was estimated, implying that HO emerges out of QPs with giant Ising anisotropy [2]. The Ising behavior of the near Fermi-energy QPs was reported to support the picture of localized 5f states, possibly having a small hybridization with conduction electrons [2]. This extreme magnetic anisotropy is central to the hastatic order theory in which a local  $5f^2$  crystal field doublet induces the Ising character [3]. For bandlike electrons, a g-factor of 2 with little anisotropy is expected which would definitely seem to exclude delocalized 5f behavior [2,3].

We show on the basis of relativistic DFT-based electronic structure calculations that the *bandlike* 5f electrons in  $URu_2Si_2$  exhibit surprisingly a colossal Ising behavior, a property which is truly exceptional for itinerant electrons. The calculated total moment vanishes steeply for directions away from the tetragonal c-axis, i.e. the moment displays a huge Ising anisotropy. The origin of the unique Ising anisotropy is found to be due to a combination of the peculiar nesting of Fermi surface states and the strong spin-orbit interaction. Our results have important consequences for models applicable to unveil the nature of the HO.

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Perpendicular magnetic anisotropy in cobalt-intercalated graphene on Ir(111) attracts interest due to possible applications for ultra-high density magnetic storage, and spin-torque magnetic random-access memories [1]. The magnetism, and the magnetic anisotropy energy (MAE) graphene/Co/Ir(111) are studied making use the first-principles density functional theory calculations, and the magnetic torque method. The structure relaxation is taken into account. At first, we show that monolayer Co/Ir(111) has a strong perpendicular MAE of 1.25 meV/Co, which is consistent with the experimental estimates [2]. This MAE is strongly affected by the structure relaxation, and originates mostly from the topmost Ir(111)-substrate layers magnetized by the overlayer of Co. The magnetic moments and the MAE are strongly affected by presence of graphene. For the placement of graphene in the hexagonal hollow positions over the monolayer Co ("hex"), the value of MAE is reduced and stays positive. For the placement with one of the C atoms on the top of Co ("top" position) the MAE changes the sign and becomes negative. The role of Coulomb correlations beyond DFT on the spin and orbital magnetic moments, and the MAE will be discussed.

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Studies of non-equilibrium current fluctuations enable assessing correlations involved in quantum transport through nanoscale conductors. They provide additional information to the mean current on charge statistics and the presence of coherence, dissipation, disorder, or entanglement. Shot noise, being a temporal integral of the current autocorrelation function, reveals dynamical information. In particular, it detects presence of non-Markovian dynamics, i.e., memory, within open systems, which has been subject of many current theoretical studies. We report on low-temperature shot noise measurements of electronic transport through InAs quantum dots in the Fermi-edge singularity regime and show that it exhibits strong memory effects caused by quantum correlations between the dot and fermionic reservoirs. Our work, apart from addressing noise in archetypical strongly correlated system of prime interest, discloses generic quantum dynamical mechanism occurring at interacting resonant Fermi edges.

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The wide variety of *f*-electron compounds provides an ample opportunity for systematic studies of electronic properties. In rare-earth and actinide compounds, various kinds of electronic ground states such as magnetic ordering, heavy fermion, and unconventional superconductivity are realized as a result of RKKY interaction, Kondo effect, hybridization etc. It is recognized that the electronic states in *f*-electron compounds can be tuned by pressure *P*. For example, in some Ce compounds, the magnetic ordering temperature  $T_{\text{ord}}$  decreases with increasing *P* and becomes zero at a critical pressure  $P_c$ , where a heavy fermion state and/or even pressure-induced superconductivity are formed. On the other hand, it is reported that non-magnetic Yb compounds are changed into the magnetically ordered state under high pressures. In the case of uranium compounds, it seems to me that pressure effect on electronic structures is more complicated. In order to investigate pressure effect on *f*-electron compounds, we extend our attention to several uranium compounds for studying wider pressure range.

CeIrGe<sub>3</sub>, which crystallizes in the BaNiSn<sub>3</sub>-type tetragonal structure without inversion symmetry, is an antiferromagnet with the Néel temperature  $T_{\text{N1}} = 8.5$  K. With increasing pressure,  $T_{\text{N1}}$  shows a step-like decrease up to 20 GPa and suddenly disappears above 22 GPa. At 20 GPa, unconventional superconductivity appears below 1.5 K [1]. The upper critical field  $H_{c2}(0)$  at 24 GPa reaches more than 10 T for  $H \parallel c$ -axis, reflecting the lack of inversion symmetry in the crystal structure. An antiferromagnet UIrSi<sub>3</sub> with  $T_{\text{N}} = 42$  K also crystallizes with the same structure as that of CeIrGe<sub>3</sub>. While, in case of UIrSi<sub>3</sub>,  $T_{\text{N}}$  monotonically increases with increasing pressure with a rate of 2.5 K/GPa up to 5 GPa. Pressure experiments on other uranium compounds will be presented and discussed.

This work was done in collaboration with Y. Onuki, R. Settai, and Y. Haga.

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## Incommensurately modulated crystal and magnetic structures in CeRuSn

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We have determined the crystal and magnetic structures of CeRuSn using single-crystal neutron and x-ray diffraction at various temperatures and magnetic fields up to 3T. CeRuSn adopts at 320K a crystal structure, which is related to a CeCoAl type of structure by doubling of the *c* lattice parameter. Between 290K and 150K the crystal structure shows a strong temperature dependence, but eventually becomes modulated along the *c* axis with a propagation vector close to  $q_{\text{nuc}} = (0\ 0\ 0.35)$  and *x* and *z* parameters varying at all elemental sites. A previously expected tripled (3*c*) type of structure can be rejected clearly. Magnetic property measurements and neutron diffraction data exhibit below  $T_{\text{N}} = 2.8$  (1) K an antiferromagnetic order of nearly collinear Ce moments. However, neutron single crystal diffraction shows distinctly an rearrangement of the spins at 0.9T ( $T=1.7$ K), which breaks the antiferromagnetic order. Without magnetic field these moments are forming ferromagnetically coupled pairs, which are confined in the *a-c* plane. Its propagation vector is  $q_{\text{mag}} = (0\ 0\ 0.175)$ , i.e. the magnetic unit cell is doubled along the *c*-axis and therefore commensurate with respect to the incommensurate crystal structure. As one moves along the *c*-axis the magnitudes of this moments are modulated between 0.11 and  $0.95\mu_{\text{B}}$ . However, the moment maxima correspond with the bond valence sum maxima, which contradicts theoretical expectations.

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## Single crystal growth and physical properties of the $\text{Ce}_n\text{T}_m\text{In}_{3n+2m}$ heavy fermion compounds

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The  $Ce_nT_mIn_{3n+2m}$  ( $n=1,2$ ;  $m=1,2$ ;  $T$ =transition metal) heavy fermion compounds are interesting in two aspects: (i) They are known to be on the verge of a magnetic to non-magnetic quantum critical point where unconventional superconductivity has been reported [1]. (ii) These materials crystallize in the tetragonal structures providing the possibility to tune the structural dimensionality from more 2D to 3D (115→218→103) [1,2], which makes them ideal candidates to investigate the influence of the parameter “dimensionality” with respect to quantum criticality [3].

We have successfully prepared single crystals of  $CePdIn_5$ ,  $Ce_2PtIn_8$ ,  $Ce_3PdIn_{11}$  and  $Ce_3PtIn_{11}$  compounds for the first time using In self-flux method [4]. These new compounds contribute to completion of the structure sequence running from the purely cubic  $CeIn_3$  to the more 2D  $CeTIn_5$  counterparts. X-ray and microprobe analysis confirmed the high quality of the single crystals. Series of bulk measurements down to low temperatures were performed, allowing a thorough study of the superconductivity and magnetism depending on the dimensionality [5]. The ground state properties will be discussed in the context of the already known  $Ce_nT_mIn_{3n+2m}$  compounds.

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## Electronic properties study of CePtIn single crystal

O-11

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The hexagonal intermetallic  $RTX$  compounds, where  $R$  is rare-earth element,  $T$  transition d-metal and  $X$  p-metal, crystallizing in ZrNiAl-type structure, form a large family of compounds with a variety of ground state properties. Most of these compounds order magnetically at low temperatures, often with complex magnetic structures, but there are also some compounds without magnetic transition down to very low temperatures. The presented study is focused on the electronic properties of newly prepared CePtIn single crystal.

CePtIn do not reveal magnetic order at least down to 60 mK. It lies on the border between a valence fluctuating CeNiIn with Kondo like behaviour and heavy-fermion antiferromagnet CePdIn. The electronic properties are strongly influenced by the chemical pressure, although the substitution of d-element is isostructural and isoelectronic. CePtIn behaves very complex at low temperatures, i.e. specific heat strongly increases with decreasing temperature, what ranks CePtIn among heavy-fermion compounds. Moreover, the non-Fermi-liquid behaviour has been observed.

The preparation of single crystal and its thorough characterization will be presented. The basic physical properties studied by means of magnetization, specific heat, electrical resistivity and magnetoresistance are discussed with respect to the other  $CeTIn$  compounds, and especially then the noticeable similarity of physical properties of CePtIn and  $CeNi_{0.4}Pd_{0.6}In$  and  $CeNi_{0.6}Pd_{0.4}In$  compounds.

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Recently, a correlation between valence fluctuations and superconductivity has attracted attention. The ternary heavy fermion compound CePtSi<sub>2</sub> exhibits a pressure-induced superconductivity, which is suggested to be mediated by valence fluctuation similar to the case in CeCu<sub>2</sub>(Si,Ge)<sub>2</sub>[1]. CePtSi<sub>2</sub> has an orthorhombic CeNiGe<sub>2</sub>-type crystal structure (space group *Cmcm*), and exhibits an antiferromagnetic (AFM) ordering below the Néel temperature  $T_N = 1.8$  K. With increasing pressure,  $T_N$  decreases and disappears above  $\sim 1$  GPa. Instead of AFM phase, the superconducting one appears between 1.4 and 2.1 GPa with  $T_c \sim 0.15$  K. Recently, we succeeded in preparing single crystal of CePtSi<sub>2</sub> and CePt(Si<sub>0.8</sub>Ge<sub>0.2</sub>)<sub>2</sub> using an In-flux method[2], and measured its electrical resistivity under pressures.

At ambient pressure,  $\rho(T)$  of CePt(Si<sub>0.8</sub>Ge<sub>0.2</sub>)<sub>2</sub> for excitation current direction  $J // a$ -axis shows the maxima at  $T_1 = 6.3$  K and  $T_2 = 50$  K due to the Kondo effect affected by the crystalline electric field. The antiferromagnetic transition was evidenced by an inflection point at  $T_N \sim 4.4$  K, indicating an increase of  $T_N$  due to a negative pressure effect by Ge substitution. In contrast to the case for  $J // a$ -axis,  $\rho(T)$  for  $J // b$ -axis exhibits a clear peak at  $T_N$ . With increasing pressure up to 2 GPa, these characteristic temperatures slightly decrease. On the other hand,  $T_1$  and  $T_2$  increase above 4.5 GPa and merge above 6 GPa. We will report details and comparison with CePtSi<sub>2</sub>.

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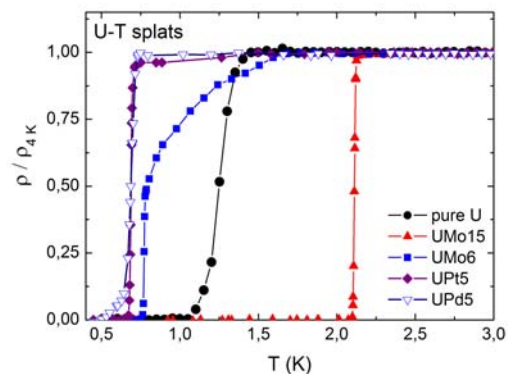
## Thermodynamic properties of selected splat-cooled U-T alloys (T=Mo, Pd, Pt)

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Using Mo doping in a combination with splat-cooling technique we are able to stabilize the high-temperature cubic  $\gamma$ -U structure down to low temperatures. The pure  $\gamma$ -U structure was obtained in alloys with  $\geq 13$  at.% Mo [1-4]. Those  $\gamma$ -U materials exhibit a conventional BCS superconductivity with e.g.  $T_c \approx 2.1$  K and critical field exceeding 5 T for 15 at.% Mo (UMo15). The alloys with  $< 10$  at.% Mo exhibit the mixed cubic  $\gamma$ - and orthorhombic  $\alpha$ -phase.

In this work we present our study of superconductivity in the mixed  $\alpha+\gamma$  alloys, i.e. with 6 at.% Mo (UMo6) and 5 at.% Pd and Pt doping (UPd5 and UPt5). A smooth decrease below 1.5 K and a sharp drop at 0.6 K in the resistivity was observed for UMo6, while a single sharp drop was revealed at  $T_c \approx 0.8$  K for UPd5 and UPt5 (shown in the Figure). With applying the magnetic fields, the resistivity jumps move to lower temperatures. The superconductivity transitions were revealed by only one broad peak at  $T_c$  in the C-T curves.



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## Superconductivity and structure of U-Zr and U-Mo splats.

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Uranium can exist in three allotropic phases, namely:  $\alpha$  - (orthorhombic),  $\beta$  - (tetragonal) and  $\gamma$  - (body-centered cubic).  $\gamma$ -uranium phase is thermodynamically stable in the high temperature range 1048-1408 K. The metastable  $\gamma$ -phase can be retained at room temperature by doping with Mo or Zr and using splat cooling technique. Structure investigation by XRD shows that  $\gamma$ -U phase increases while  $\alpha$ -U phase decreases with increasing dopant concentration. Samples with 11-12 at.% Mo revealed the modified tetragonal structure of the cubic phase (the  $\gamma^0$  phase). A pure  $\gamma$ -phase was observed for samples with concentrations  $\geq 13$  at.% Mo. For U-Zr splat samples we observed pure  $\gamma$ -phase for concentrations  $\geq 30$  at.% Zr. EBSD structure investigation confirmed XRD results.

Splat samples become superconducting at low temperatures. Transitions to superconducting state were observed by the sharp drop of resistivity. U-Zr splats become superconducting with critical temperatures close to 0.7 K which is smaller than for U-15at.% Mo (2.1 K). Superconductivity was also investigated by measuring low temperature heat capacity and resistivity in magnetic fields. The superconducting transition temperature shifts to lower values with the applied magnetic field. Critical field for U-30 at.% Zr splat (3 T) is smaller than for U-15 at.% Mo splat (6 T) but still much larger than for pure U splat (0.4 T). Such difference can indicate two types of superconductivity. One type related to  $\alpha$ -U, not necessarily intrinsic, which has lower  $T_c$  and critical field. The other type, belonging to  $\gamma$ -U phase, has a higher  $T_c$  and much higher critical field.

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## The influence of doping on magnetic properties of the $\text{UH}_3$ -based hydrides.

O-15

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The  $\gamma$  phase of Uranium is more suitable for applications than  $\alpha$ -U as more malleable, ductile and stable with respect to irradiation effects and corrosion. The *bcc* structure of uranium, which corresponds to the  $\gamma$  phase, is stable at high temperatures. It is possible to get a metastable  $\gamma$ -phase at room temperature by means of doping. A splat cooling technique gives a possibility to reduce the necessary concentration of doping elements. Stabilization of pure *bcc* phase suppresses the  $\alpha$ -U phase, which can be easily hydrogenated at low  $\text{H}_2$  pressures. We have been testing the hydrogenation of the  $\gamma$ -U alloys and we found out that high pressures ( $> 4$  bar  $\text{H}_2$ ) are needed to form hydrides. The  $\text{UMo}_x$  alloys lead to the  $\text{UH}_3\text{Mo}_x$  hydrides, which are amorphous, although their structure seems to be derived from the cubic  $\beta$ - $\text{UH}_3$  type. Their Curie temperature can reach 200 K.  $\text{UZr}_x$  alloys yield the  $\text{UH}_3\text{Zr}_x$  hydrides, crystallizing in the  $\alpha$ - $\text{UH}_3$  type, which is for pure  $\text{UH}_3$  only a metastable transient phase. They reveal that magnetic properties of  $\alpha$ - $\text{UH}_3$  and  $\beta$ - $\text{UH}_3$  are practically identical, despite rather different nearest U-U spacing (360 pm and 330 pm, respectively).

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The pressure effect on the magnetic exchange in UGa<sub>2</sub> was studied by the resistivity measurements on the single crystal under quasi-hydrostatic conditions. The Curie temperature of UGa<sub>2</sub> monotonously increased from the ambient pressure value of  $T_C = 124$  K up to 154 K at  $p = 14.2$  GPa and then started to decrease at notably higher rate ( $-7$  K/GPa vs.  $+2.1$  K/GPa) reaching  $T_C = 147$  K at  $p = 15.2$  GPa. At 20 GPa, after the structural transition at 16 GPa, UGa<sub>2</sub> is no longer magnetic. The observed variation of the ordering temperature can be described by the two-band model of the non- $f$  band hybridized with the weakly delocalized  $5f$  states. The character of the latter ones is indicated by the low Sommerfeld coefficient  $\gamma = 10$  mJ/mol·K<sup>-2</sup>, high uranium moments of about 3  $\mu_B$ /f.u., and the magnon contribution to the electric resistivity. According to the said model the increase of the  $5f$ -ligand hybridization should facilitate the magnetic exchange up till the point when the wash-out of the magnetic moment leads to a non-magnetic state altogether. The decrease of the magnon gap and the weakening of the spin-disorder scattering with pressure in UGa<sub>2</sub> are consistent with such picture. So far the pressure-induced increase of the ordering temperature was registered in very few uranium compounds and the saturation of the  $T_{ord}$  is even rarer.

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## Low-Temperature Magnetic Properties of Dilute Uranium Alloys (Th,U)Be<sub>13</sub>

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We have performed measurements of specific heat  $C$ , magnetic susceptibility  $\chi$ , and electrical resistivity  $\rho$  down to 1.8 K on single-crystalline Th<sub>1-x</sub>U<sub>x</sub>Be<sub>13</sub> with compositions  $x = 0, 0.01, 0.07,$  and  $0.11$  in order to investigate the single-U-site properties. The main experimental results are summarized as follows: (i) The single-U-site contribution to  $\rho(T)$  exhibits a broad maximum at  $\sim 70$  K and obeys a  $T^2$  law with an enhanced coefficient of  $A \sim 0.1(1)$   $\mu\Omega\text{cm}/\text{K}^2\text{molU}$  below  $\sim 20$  K. (ii)  $\chi(T)$  follows a Curie-Weiss law above  $\sim 100$  K with an effective moment of  $\mu_{\text{eff}} \sim 3.7(3)$   $\mu_B/\text{U}$  and a Curie-Weiss temperature of  $\theta_p \sim -50(5)$  K, while as  $T$  is lowered below  $\sim 20$  K it shows a tendency to saturate at a value of  $\sim 0.025(5)$  emu/molU. (iii) The low- $T$   $C(T)/T$  is enhanced roughly in proportion to  $x$  with a rate (estimated at 1.8 K) of  $\sim 0.15(2)$  J/K<sup>2</sup>molU. The negative  $d\rho/dT$  and the Curie-Weiss behavior with a negative  $\theta_p$  indicate the presence of Kondo effects in the high-temperature range above  $\sim 70$  K, while a decrease in  $\rho(T)$  at lower temperatures apparently different from the usual single-impurity Kondo behavior. We found that as  $T \rightarrow 0$ , the dilute system behaves as a (moderately heavy) local Fermi liquid (LFL). The non-Fermi-liquid (NFL) behavior, which is observed in UBe<sub>13</sub> [1-3] and discussed in terms of the quadrupole Kondo model [4], cannot be seen in the dilute system. We will discuss the observed LFL behavior and its relationship to the NFL state in pure UBe<sub>13</sub> in comparison with the theoretical models which predict the competition (or crossover) between the Kondo-Yosida singlet and the CEF singlet states in the  $f^2$  configuration [5-6].

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## Superconductivity of La<sub>3</sub>M<sub>4</sub>Sn<sub>13</sub> with M = Co, Rh, and Ru: A comparative study

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The discovery of superconductivity in  $\text{La}_3\text{M}_4\text{Sn}_{13}$  [1] has attracted considerable attention and provided an avenue by which to better understand the relationship between superconductivity and magnetism in the presence of strong electron correlations. We report the electric transport and thermodynamic properties of the skutterudite-related  $\text{La}_3\text{M}_4\text{Sn}_{13}$  superconductors, where  $\text{M} = \text{Co}, \text{Rh}, \text{and Ru}$ . Applying an external pressure to  $\text{La}_3\text{Rh}_4\text{Sn}_{13}$ , the resistive superconducting critical temperature  $T_c$  decreases, while the critical temperature of  $\text{La}_3\text{Co}_4\text{Sn}_{13}$  is enhanced with increasing pressure. The positive pressure coefficient  $dT_c/dP$  correlates with a subtle structural transition in  $\text{La}_3\text{Co}_4\text{Sn}_{13}$  [2] and is discussed in the context of lattice instabilities. Specific heat data show that  $\text{La}_3\text{M}_4\text{Sn}_{13}$  are typical BCS superconductors. However,  $\text{La}_3\text{Rh}_4\text{Sn}_{13}$  and  $\text{La}_3\text{Ru}_4\text{Sn}_{13}$  also exhibit a second superconducting phase at higher temperatures  $T_c^*$  ( $T_c < T_c^*$ ), which is characteristic of inhomogeneous superconductors. We calculate the specific heat for an inhomogeneous superconducting phase, which agrees well with experimental  $C(T)$  data for  $\text{La}_3\text{Rh}_4\text{Sn}_{13}$ . We also found that an applied pressure reduces this second superconducting phase. We show evidence of nanoscale inhomogeneity as a bulk property of  $\text{La}_3\text{Rh}_4\text{Sn}_{13}$  and  $\text{La}_3\text{Ru}_4\text{Sn}_{13}$  in the sense that the samples exhibit electronic disorder over length scale similar to the coherence length which cannot be removed by any standard annealing procedure. Such a substantial nanoscale electronic inhomogeneity is characteristic of the bulk  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  high- $T_c$  materials and some heavy fermions with unconventional superconductivity (e.g.,  $\text{CeIrIn}_5$  or  $\text{PrOs}_4\text{Sb}_{12}$ ).

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## Crystal structure and superconductivity in the cage compounds $\text{RV}_2\text{Al}_{20}$ O-19

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Series of compounds with the stoichiometry  $\text{RV}_2\text{Al}_{20}$  ( $\text{R}=\text{rare earth}$ ) were synthesized by arc melting method in a high purity Ar atmosphere. The lattice constant, determined from Rietveld refinement, increases with increasing radii of the rare earth metal, which is located inside a CN16 Frank-Kaspar polyhedra formed by 16 Al atoms. The smallest  $a=1.44978$  nm is observed for  $\text{ScV}_2\text{Al}_{20}$ , whereas the largest lattice parameter  $a=1.4617$  nm is observed for  $\text{LaV}_2\text{Al}_{20}$ . We used magnetic susceptibility, resistivity, and heat capacity measurements to characterize the superconducting state in  $\text{MV}_2\text{Al}_{20}$ , where  $\text{M} = \text{Sc}, \text{Y}$  and  $\text{Lu}$ . Superconducting critical temperature is 1.0 K, 0.57 K and 0.6 K for  $\text{ScV}_2\text{Al}_{20}$ ,  $\text{YV}_2\text{Al}_{20}$ ,  $\text{LuV}_2\text{Al}_{20}$ , respectively. Influence of the size of M atom (and possibly rattling effect) on superconductivity in this important class of materials will be discussed.

I will also show preliminary data obtained on actinide based  $\text{AV}_2\text{Al}_{20}$  ( $\text{A} = \text{U}, \text{Np}, \text{Pu}$ ).

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We present a theoretical description of pre-critical fluctuations for an antiferromagnetic instability in a Kondo Insulator and its extensions to Kondo Insulators with nodes in the gap. In the paramagnetic state and for excitation energies greater than the gap energy, the pre-critical fluctuations resemble antiparamagnons in a metal in that they form a broad resonance which softens as the momentum is varied towards the wave vector  $Q$  characterizing the antiferromagnetic instability. However, at the momenta for which the resonance coincides with the gap, the spectrum undergoes a dramatic change. Below the gap energy, the excitations exist with a sharp dispersion relation below the edge of the electron-hole continuum. However, as the antiferromagnetic wave vector  $Q$  is approached, the dispersion relation has a finite excitation energy. As the temperature is lowered towards the critical temperature, the dispersion softens all the way to zero. We describe the excitations in a Kondo Insulator or Kondo semi-metal in which there are nodes in the gap. We extend the theory of Miyake and Ikeda to describe the orientational dependence of the spectrum of magnetic excitations in Kondo semi-metals and apply this to  $\text{CeFe}_{10}\text{Al}$ .

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## Quantum critical metal $\text{YbRh}_2\text{Si}_2$ : High magnetic fields and elevated temperatures

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We present results on the evolution with magnetic field and temperature of the Fermi surface in the heavy fermion compound  $\text{YbRh}_2\text{Si}_2$  whose B-T-phase diagram exhibits numerous anomalies [1]. In this material, the antiferromagnetic order below 70mK can be suppressed by a small magnetic field. In the vicinity of this transition, signatures for a quantum critical point (QCP) have been observed. There is an extended regime of non-Fermi liquid behavior fanning out above the QCP in the B-T-plane. The focus of the calculations presented here is the evolution of the heavy quasiparticles in high magnetic fields and at elevated temperatures where the moment screening due to the Kondo effect is weakened. The quasiparticle bands in high magnetic fields are determined by means of the Renormalized Band method [2,3]. The progressive de-renormalization of the masses in the magnetic field as well as the many-body enhancement of the Zeeman splitting are accounted for using field-dependent quasiparticle parameters deduced from Numerical Renormalization Group studies [4] and Perturbational Scaling Theory[5]. The calculations predict Lifshitz transitions at well-defined values of the external magnetic field which lead to anomalies in various transport properties [6,7]. The low-energy part of the T-dependent 4f spectral function reproduces recent ARPES data [8]. Implications for the interpretation of the  $T^*$ -line are discussed.

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Magnetization can be changed by means of a very strong laser light on the femtosecond timescale. This effect has a high application potential but it is also very interesting from the theoretical point of view due to reaching a previously unexplored nonequilibrium states of magnetic materials. We discuss here microscopic mechanisms proposed to explain the observed ultrafast demagnetization.

A special attention is paid to the Elliott-Yafet electron-phonon spin-flip (EY-SF) scattering [1]. We have calculated the spin-flip Eliashberg function for three ferromagnetic metals Fe, Co and Ni [2]. We consider both thermalized very hot electron distributions, as well as highly non-equilibrium electron distributions that are expected to be present immediately after the fs laser excitation. Based on this we evaluate the contribution of this process to the demagnetization [3] and discuss the physical relevance of the usually employed approximations.

Another proposed explanation is based on spin dependent electron diffusion employing different spin-dependent lifetimes of excited electrons [4]. A number of experimental findings support this explanation, including an ultrafast increase of magnetization or THz emission.

Recently an interesting magnetization dynamics has been observed in systems with 2 ferrimagnetically ordered sublattices. A complete reversal of magnetization in GdFeCo alloy can be achieved with a linearly-polarized laser pulse, without the help of external field, circular polarization of the laser pulse or any other direct source of angular momentum – similarly to the ultrafast demagnetization process. We calculate exchange interaction between the components of the compound as well as the intraatomic exchange between Gd 4f and 5d orbitals to allow mapping the problem to an effective orbital-resolved Heisenberg Hamiltonian. A subsequent simulation based on the Landau-Lifschitz-Gilbert equation has reproduced the switching behavior [5].

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## Structural, electronic, and magnetic characteristics of Np<sub>2</sub>Co<sub>17</sub> under extreme conditions.

O-23

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A previously unknown neptunium-transition-metal binary compound Np<sub>2</sub>Co<sub>17</sub> has been synthesized and characterized by means of powder x-ray diffraction, <sup>237</sup>Np Mössbauer spectroscopy, superconducting-quantum-interference- device magnetometry, and x-ray magnetic circular dichroism (XMCD). The compound crystallizes in a Th<sub>2</sub>Ni<sub>17</sub>-type hexagonal structure with room-temperature lattice parameters  $a = 8.3107(1) \text{ \AA}$  and  $c = 8.1058(1) \text{ \AA}$ . Magnetization curves indicate the occurrence of ferromagnetic order below  $T_C > 350 \text{ K}$ . Mössbauer spectra suggest a Np<sup>3+</sup> oxidation state and give an ordered moment of  $\mu_{\text{Np}} = 1.57(4) \mu_B$  and  $\mu_{\text{Np}} = 1.63(4) \mu_B$  for the Np atoms located, respectively, at the 2b and 2d crystallographic positions of the  $P6_3/mmc$  space group. Combining these values with a sum-rule analysis of the XMCD spectra measured at the neptunium  $M_{4,5}$  absorption edges, one obtains the spin and orbital contributions to the site-averaged Np moment [ $\mu_S = -1.88(9) \mu_B$ ,  $\mu_L = 3.48(9) \mu_B$ ]. The ratio between the expectation value of the magnetic-dipole moment and the spin magnetic moment ( $m_{\text{md}}/\mu_S = +1.36$ ) is positive as predicted for localized 5f electrons and lies between the values calculated in intermediate-coupling (IC) and  $jj$  approximations. The expectation value of the angular part of the spin-orbit-interaction operator is in excellent agreement with the IC estimate. The ordered moment averaged over the four inequivalent Co sites, as obtained from the saturation value of the magnetization, is  $\mu_{\text{Co}} \cong 1.6 \mu_B$ . The experimental results are discussed against the predictions of first-principles electronic-structure calculations based on the spin-polarized local-spin-density approximation plus the Hubbard interaction.

The structural behavior of Np<sub>2</sub>Co<sub>17</sub> is investigated by means of high pressure diamond-anvil-cell compression measurements and is compared with that of the isostructural compounds Lu<sub>2</sub>Co<sub>17</sub> and Lu<sub>2</sub>Ni<sub>17</sub>. The Th<sub>2</sub>Ni<sub>17</sub>-type hexagonal crystal structure is preserved with no measurable discontinuous volume collapses up to the highest achieved pressure,  $p = 43 \text{ GPa}$ .

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## Crystal structure and physical properties of novel U-Fe-Ge intermetallic compounds

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A systematic study of the ternary system U-Fe-Ge at 900°C has revealed several new intermetallic phases. Among them are the compounds U<sub>34</sub>Fe<sub>4-x</sub>Ge<sub>33</sub> and U<sub>3</sub>Fe<sub>2</sub>Ge<sub>7</sub>. Their electronic properties clearly demonstrate the crucial role of the 5*f*-ligand hybridization, besides the 5*f*-5*f* overlap, in determining the magnetic properties.

The new ternary phase U<sub>34</sub>Fe<sub>4-x</sub>Ge<sub>33</sub> ( $x = 0.68$ ) crystallizes in its own tetragonal structure type (space group *I4/mmm*), with lattice parameters  $a = 10.873(5)$  Å and  $c = 25.274(3)$  Å. Structure refinement disclosed six inequivalent U atoms, occupying sites with dissimilar coordination, the Ge atoms staying on seven positions and Fe on two positions, one of the Fe sites with a partial occupancy. U<sub>34</sub>Fe<sub>4-x</sub>Ge<sub>33</sub> undergoes a ferromagnetic-type transition below  $T_C = 28$  K. Mössbauer spectroscopy shows that the Fe atoms have no ordered moments so that the magnetism is ruled by the U sub-lattice. The Sommerfeld coefficient of the electronic specific heat is  $\gamma = 131$  mJ/(mol<sub>U</sub> K<sup>2</sup>), whereas the estimated magnetic entropy at  $T_C$  is  $0.22 R \ln 2$ . The electrical resistivity exhibits an upturn below  $T_C$  that shifts towards higher temperatures with the applied magnetic field. This behavior may be related to some disorder in the non-magnetic lattice and/or partial ordering of the magnetic lattice.

Single crystals of the new ternary compound U<sub>3</sub>Fe<sub>2</sub>Ge<sub>7</sub> were synthesized by solution growth method using tin flux. It crystallizes in the orthorhombic La<sub>3</sub>Co<sub>2</sub>Sn<sub>7</sub>-type (space group *Cmmm*) with lattice parameters determined from single-crystal X-ray diffraction as  $a = 4.171(5)$  Å,  $b = 24.990(5)$  Å and  $c = 4.157(5)$  Å. Structure refinement indicated two crystallographically inequivalent positions for U atoms. U<sub>3</sub>Fe<sub>2</sub>Ge<sub>7</sub> orders ferromagnetically at  $T_C = 64$  K. Both the U and Fe sub-lattices display an ordered magnetic moment. The compound exhibits a strong uniaxial anisotropy, the magnetic moments lie along the  $c$  axis with the spontaneous magnetic moment  $M_s = 3.3 \mu_B/\text{f.u.}$  at 2 K. A strong anisotropy is present in the ( $ab$ ) plane as well. A S-shape anomaly is observed along the  $a$  axis in an applied magnetic field. The estimated Sommerfeld coefficient is  $\gamma = 52$  mJ/(mol<sub>U</sub> K<sup>2</sup>).

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UFe<sub>1-x</sub>Sb<sub>2</sub> is a ternary uranium phase that crystallizes in the tetragonal HfCuSi<sub>2</sub>-type structure (SG. P4/nmm), the U and Fe atoms being located in one position (2c and 2b, respectively), while Sb occupies two sites (2a and 2c). This phase is closely related to the USb<sub>2</sub> binary compound (Cu<sub>2</sub>Sb-type structure, SG. P4/nmm), which is a layered structure with Sb(I), U and Sb(II) sheets stacked along the c axis: UFe<sub>1-x</sub>Sb<sub>2</sub> can be seen as formed from USb<sub>2</sub> by inserting an additional Fe layer between the planes that compose the Sb(II) sheets. UFeSb<sub>2</sub> is the limit compound in of this homogeneity range, being reported the identification of its crystal structure (HfCuSi<sub>2</sub>-type), unit cell parameters and electrical resistivity as a function of temperature. The binary antimonide USb<sub>2</sub> orders antiferromagnetically below T<sub>N</sub> = 206 K, the refinement of its magnetic structure from neutron diffraction data showing a sequence of alternating (↑↓↑) U ferromagnetic layers and a magnetic moment of ~1.9μB/U. In UFeSb<sub>2</sub> the lowest U-U distance (4.327 Å, corresponding to the a cell parameter) is well above the Hill limit, pointing to a strong chance of magnetic ordering for the U sublattice, similarly to the USb<sub>2</sub> case. However, it is not excluded the possibility of a Fe magnetic contribution, which leads to the existence of two potential magnetic sublattices in UFeSb<sub>2</sub>. Indeed, the reported resistivity data shows a maximum at ~40 K that can be related to a magnetic transition. Here we present the synthesis and a detailed study on the UFeSb<sub>2</sub> compound, by powder X-ray diffraction, electrical resistivity, magnetoresistance, magnetization, specific heat and Mössbauer spectroscopy measurements. A UFeSb<sub>2</sub> polycrystalline sample was prepared by arc-melting, followed by annealing at 750°C for one week. The Rietveld refinement confirms that UFeSb<sub>2</sub> crystallizes in the HfCuSi<sub>2</sub>-type structure and indicates that the majority of the sample consists of UFeSb<sub>2</sub> (98.2 w%) and that only minor amounts of FeSb<sub>1+x</sub> and α-Fe (1.7 and 0.1 w%, respectively) exist. All the nearest neighbor atoms of U are at distances close to or higher than the metallic radii sum, pointing to the possibility of a non negligible U magnetic moment. However, the very short Fe-Sb1 distances indicate strong interactions between these atoms and a probable collapse of the Fe magnetic moments. The low temperature electrical resistivity versus temperature results is similar to those previous reported, showing a maximum at ~40K under zero applied magnetic field. At higher fields the maximum broadens and shifts to higher temperatures, as expected for a ferromagnetic-type transition. The temperature dependence of the UFeSb<sub>2</sub> specific heat shows only a very small anomaly at T<sub>C</sub>, pointing to itinerant magnetism. At low temperatures the specific heat follows C<sub>p</sub> = γT + βT<sup>3</sup>, with γ = 51(1) mJ/mol.K<sup>2</sup> and β = 0.55(1) mJ/mol.K<sup>4</sup> (θ<sub>D</sub> = 152 K). The γ value points to a relatively high density of electronic states at the Fermi level and classifies this compound as an enhanced correlated system.

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## Single crystal growth and magnetism of the novel U<sub>2</sub>RhIn<sub>8</sub> compound

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We report on thermodynamic, magnetization and transport properties of the novel compound U<sub>2</sub>RhIn<sub>8</sub>. Single crystals have been synthesized for the first time using In self-flux method. Single crystal X-ray diffraction revealed that the compound crystallizes in the tetragonal Ho<sub>2</sub>CoGa<sub>8</sub> structure type with lattice parameters *a* = 4.6163 Å and *c* = 12.0144 Å. In contrast to its nonmagnetic counterpart U<sub>2</sub>RhGa<sub>8</sub> [1], U<sub>2</sub>RhIn<sub>8</sub> undergoes an antiferromagnetic phase transition at T<sub>N</sub> = 117 K. The Sommerfeld coefficient is slightly enhanced yielding γ = 47 mJ.mol<sup>-1</sup>.K<sup>-2</sup>. The behavior of U<sub>2</sub>RhIn<sub>8</sub> strongly resembles the properties to the related URhIn<sub>5</sub> [2] with respect to magnetization and resistivity. The magnetic susceptibility χ(*T*) shows a strong anisotropy with effective magnetic moment corresponding approximately to that of free U-ion and with unusually large, negative Curie temperature reaching almost -800 K along *H* || *a* and -230 K along *H* || *c*. This weak temperature dependence of χ(*T*) might be attributed to the mainly itinerant nature of 5*f* electrons. While applied magnetic field leaves the evolution of T<sub>N</sub> unaffected up to 14 T, it is enhanced upon applying hydrostatic pressure. The overall phase diagram will be discussed in the context of magnetism in related URhX<sub>5</sub> and UX<sub>3</sub> (*X* = In, Ga) [2, 3].

[1] S. Ikeda *et al.*, J. Phys.: Condens. Matter **15** (2003) S2015-S2018

[2] Y. Matsumoto *et al.*, Phys. Rev. B **88**, 045120 (2013) and references therein

[3] D. Kaczorowski *et al.*, Physica B 230-232 (1997) 35-38

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## Peculiar magnetic properties of selected RE-compounds with 221 composition

Magnetic properties of RE<sub>2</sub>T<sub>2</sub>X series (T = late transition metal, X = p-metal) are interestingly complicated. RE atoms form a triangular motif within the tetragonal crystal structure bringing magnetic frustration into the system. The crystal structure resembles 2D Shastry-Sutherland lattice [1]. We have prepared for the first time single crystals of some of the representatives of RE<sub>2</sub>Pd<sub>2</sub>In series and studied details of magnetic behavior as a function of temperature and magnetic field. The ordering temperatures of RE<sub>2</sub>Pd<sub>2</sub>In compounds follow reasonably well the de Gennes scaling. We have found from measurements on single crystals that magnetic properties of these compounds are highly anisotropic showing several metamagnetic transitions in various crystallographic directions. Another representative of 221-series which will be presented is Nd<sub>2</sub>Ni<sub>2</sub>In. Neutron diffraction indicated AF ordering of Nd moments in the basal plane below  $T = 8.5$  K, where most likely a first-order phase transition appears. A detailed study of magnetic properties on a single crystal revealed that magnetic field applied along  $c$  induces a full alignment of Nd moments in  $< 0.2$  T, and field cycling exhibits a hysteresis and a remanent magnetization.

[1] B. Shastry and B. Sutherland, *Physica B+C* 108 (1981) 1069.

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## Relationship between magnetic structure and physical properties in Co- and Ca-doped EuFe<sub>2</sub>As<sub>2</sub> compounds

O-28

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Co- and Ca-doped EuFe<sub>2</sub>As<sub>2</sub> materials crystallize in the tetragonal ThCr<sub>2</sub>Si<sub>2</sub>-type structure (space group I4/mmm) at room temperature. At low temperatures, the compounds display richness of physical phenomena, e.g., tetragonal-orthorhombic distortion at  $T_{SD}$ , charge-density-wave ordering at  $T_{SDW}$ , antiferromagnetic ordering at  $T_N$ , and coexistence of magnetism and superconductivity below  $T_c$ . In this contribution we focus on single crystals of Eu(Fe<sub>0.89</sub>Co<sub>0.19</sub>)<sub>2</sub>As<sub>2</sub> and Eu<sub>0.73</sub>Ca<sub>0.27</sub>(Fe<sub>0.87</sub>Co<sub>0.13</sub>)<sub>2</sub>As<sub>2</sub>, that were grown by the conventional tin-flux method. We performed measurements of ac-susceptibility, electrical resistivity, magnetoresistance, single-crystal neutron diffraction and Mössbauer spectroscopy. The obtained data indicate that the studied compounds undergo successive phase transitions at  $T_{SD}/T_{SDW} = 80, 70$  K,  $T_N = 16.5, 12$  K,  $T_c = 5.2, 12$  K, respectively. Moreover, the bulk properties reveal a peculiar behaviour, in particular when magnetic field is applied perpendicularly to the  $c$ -axis. In a such configuration, there appears unexpectedly magnetic field-induced superconductivity in Eu(Fe<sub>0.89</sub>Co<sub>0.19</sub>)<sub>2</sub>As<sub>2</sub> and re-entrance phenomenon of the resistivity in Eu<sub>0.73</sub>Ca<sub>0.27</sub>(Fe<sub>0.87</sub>Co<sub>0.13</sub>)<sub>2</sub>As<sub>2</sub>. These unusual features can be understood if taking into account the relationship between magnetic structure determined by the microscopic techniques and superconducting pairing in these materials.

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A geometrical frustration often results in complex spin structures of solids due to the presence of conflicting interactions which separately favor different ground states. In this work, a Dy<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub> single crystal was grown for the first time and its electronic properties studied. Dy<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub> crystallizes in the hexagonal crystal structure ( $a = 877.4$  pm,  $c = 953.0$  pm) of the Gd<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub> type (space group  $P6_3/mmc$ , two formula units per elementary cell). The Dy atoms are arranged in distorted kagome nets. The onset of a long-range magnetic order of Dy moments occurs at 7 K. The compound has a non-collinear antiferromagnetic structure with a propagation vector  $(1/2\ 0\ 1/2)$ . The configuration of the Dy moments is consistent with the monoclinic Shubnikov group  $C_2/c$ . Each Dy atom carries an ordered magnetic moment  $M_{Dy}$  of about  $10\ \mu_B$  at  $T = 1.5$  K. The largest component of  $M_{Dy}$  is projected onto the  $c$  axis. The Ru magnetic moment, if exists, is below the error bar,  $0.5\ \mu_B$ , of the refinement. The  $\gamma$  coefficient in the temperature linear term of the specific heat is strongly enhanced to  $500\ \text{mJ mol}^{-1}\ \text{K}^{-2}$  taking into account the localized nature of Dy magnetism. An additional contribution originates from spin fluctuations induced in the  $4d$  subsystem of Ru by the exchange field acting from the Dy  $4f$  moments. The magnetic structure of Dy<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub> is a result of a compromise between the RKKY exchange interactions and the crystal field-induced anisotropy. In an applied magnetic field, the Zeeman energy should be taken into account. An intricate interplay among the three contributions leads to a complex behavior of Dy<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub> in a magnetic field manifested by first-order field-induced magnetic transitions below 8 T: one along  $[100]$ , two along  $[120]$  and two along the  $[001]$  axis. The transitions reflect a rotation of the magnetic moments from the initial antiferromagnetic state to a non-collinear ferromagnetic state. No more magnetization jumps are observed up to 60 T. The transitions are accompanied by large positive magnetoresistance (45-60%). The large positive effect is explained by changes in the conduction electron spectra through the jumps as the conduction electrons interact with localized magnetic moments.

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## Hydrogenation of W<sub>2</sub>CoB<sub>2</sub>-type structure intermetallics

**O-30**

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The hydrides of the compounds with the stoichiometry  $R_2T_2X$ , where  $R$  is rare-earth metal or uranium,  $T$  is a  $d$ -element, and  $X$  is a  $p$ -element, are intensively studied. So far, the particular attention has been paid to the compounds crystallizing with the tetragonal Mo<sub>2</sub>FeB<sub>2</sub> structure type. It has been shown that the compounds with the rare-earth metals can easily absorb up to 8 H atoms per formula unit, whereas the uranium compounds reach the stoichiometry just up to 2 hydrogen atoms per formula unit, but their physical properties are extremely sensitive to the concomitant lattice expansion.

Here we concentrate on H absorption in the other possible structure. The W<sub>2</sub>CoB<sub>2</sub> structure type is orthorhombic (space group  $Immm$ , Pearson symbol  $oI10$ ). The analysis of the crystal structure showed that it contains at least two types of interstitials favourable for accommodating hydrogen atoms, *i.e.* tetrahedra  $R_3T$  (Wyckoff position  $8I$ ) and  $R_2T_2$  ( $4f$ ).

Intermetallic compounds Gd<sub>2</sub>Ni<sub>2</sub>Al and Gd<sub>2</sub>Ni<sub>2</sub>Sn have been synthesized by arc-melting from pure metals under an argon atmosphere. Hydrogenation was performed at room temperature under the hydrogen pressure below 1 bar after the surface activation by heating the sample in dynamic vacuum. The kinetics of the absorption differs for both compounds. In the case of Gd<sub>2</sub>Ni<sub>2</sub>Sn, the process starts slowly after approx. 12 hours at room temperature. Further thermal treatment up to 200°C results in the final composition of the hydride Gd<sub>2</sub>Ni<sub>2</sub>SnH<sub>5.3</sub>. Surprisingly, in the case of Gd<sub>2</sub>Ni<sub>2</sub>Al, hydrogenation starts in only about 60 s and is completed even at room temperature. The final composition is Gd<sub>2</sub>Ni<sub>2</sub>AlH<sub>5.5</sub>. It should be noted that the equilibrium pressure is extremely low, since all the hydrogen could be absorbed even at the lowest pressure.

The crystal structure of the obtained hydrides, studied by X-ray powder diffraction method, undergoes dramatic changes upon hydrogenation. The broadening of diffraction peaks indicates certain amorphization of the sample. Several possible structure models can be considered for the hydrides, all yielding the cell volume expansion of 16%. The orthorhombic and monoclinic structure models will be discussed.

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## NMR study of ternary stannides of R<sub>3</sub>Co<sub>4</sub>Sn<sub>13</sub> ( $R = \text{Ce, Pr, Yb}$ )

**O-31**

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We report a systematic study of ternary stannides of  $R_3\text{Co}_4\text{Sn}_{13}$  ( $R = \text{Ce}, \text{Pr}, \text{Yb}$ ) by means of the  $^{59}\text{Co}$  nuclear magnetic resonance (NMR) spectroscopy. Distinctive NMR features associated with the anomalous phase transition have been identified for  $\text{Ce}_3\text{Co}_4\text{Sn}_{13}$  and  $\text{Pr}_3\text{Co}_4\text{Sn}_{13}$  at  $T^* \sim 155$  K and  $\sim 130$  K, respectively. For both materials, relative weak  $^{59}\text{Co}$  quadrupole splittings are consistently found below  $T^*$ , implying that the electrical field gradient (EFG) sensed by the Co site decreases undergoing this phase transition. Such an observation could be attributed to the local distortion of the Sn(2) atom from its initial position below  $T^*$  which consequently leads to significant modification of the electronic structures around the Fermi surfaces. For  $\text{Yb}_3\text{Co}_4\text{Sn}_{13}$ , however, the NMR results show the absence of the similar phase transition. The  $^{59}\text{Co}$  NMR Knight shift and spin-lattice relaxation rate  $1/T_1$  clearly indicate that  $\text{Yb}_3\text{Co}_4\text{Sn}_{13}$  is a Pauli-type paramagnet. From the Korringa relation (constant  $T_1T$ ), we thus estimated Co  $3d$  Fermi-level density of states  $N_d(E_F) \sim 3.95$  states/eV f.u. for this compound.

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Recently, europium-based intermetallics have become the focus of intense research activity due to a variety of their interesting physical properties. Among them are ternary phases with the composition EuTGe<sub>3</sub> (T = Pd, Pt) which have been reported to order antiferromagnetically at low temperatures and exhibit some anomalous behaviors in the ordered state [1,2]. In this contribution, we report on the formation and the bulk physical properties of another representative of this series, namely EuNiGe<sub>3</sub>. This novel germanide was obtained in the form of sizeable single crystals using In-flux method. X-ray diffraction and electron microprobe studies indicated single-phase and homogeneous material with the crystal structure of tetragonal BaNiSn<sub>3</sub>-type (space group I4mm) and the lattice parameters  $a = 4.3491(3)$  Å and  $c = 9.9087(15)$  Å. Magnetic susceptibility, heat capacity and electrical resistivity measurements were carried out on oriented single-crystalline specimens in wide ranges of temperature and magnetic field strength. Mössbauer spectra were collected at two different temperatures on powdered single crystals. The compound was found antiferromagnetic (AF) below  $T_N = 13.5$  K. In the paramagnetic region, the reciprocal magnetic susceptibility measured along the [100] and [001] axes follows a Curie-Weiss law with the effective magnetic moment  $\mu_{\text{eff}} = 7.68$  and  $7.74 \mu_B$ , respectively. These values are close to that expected for a divalent Eu ion ( $7.90 \mu_B$ ). The obtained positive paramagnetic Curie temperatures  $\theta_p = 6.8$  and  $6.4$  K for [100] and [001], respectively, indicate the predominance of ferromagnetic exchange interactions, despite the long-range AF order that sets in  $T_N$ . Some characteristic features in the [100] and [001] components of the magnetic susceptibility suggest that the magnetic structure in EuNiGe<sub>3</sub> consists of ferromagnetically coupled a-b planes that are stacked antiferromagnetically along the c direction. The heat capacity, Mössbauer spectroscopy and electrical resistivity data confirm the magnetic phase transition at  $T_N$ . With decreasing temperature in the ordered state, a gradual removal of the eight-fold degeneracy of the  $^8S_{7/2}$  multiplet of the Eu<sup>2+</sup> ions takes place due to increasing magnetic exchange field. This effect manifests itself as a small hump in the temperature variation of the specific heat. The compound exhibits metallic conductivity governed mainly by scattering on phonons in the paramagnetic region, and on AF magnons in the antiferromagnetically ordered phase.

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[2] N. Kumar, P. Kumar Das, R. Kulkarni, A. Thamizhavel, S.K. Dhar, and P. Bonville, J. Phys.: Condens. Matter 24 (2012) 036005

**Email of the presenting author: [O.Bednarchuk@int.pan.wroc.pl](mailto:O.Bednarchuk@int.pan.wroc.pl)****The hybridization of 5f-conduction electrons in URu<sub>1-x</sub>Pd<sub>x</sub>Ge**

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The ternary UTM compounds, where T = d-electron transition metals and M = p-electron metalloids, show a wide variety of magnetic behaviour, depending on the T and M ions involved. It was established that a hybridization between the 5f- and conduction electrons is the main factor determining the physical properties of UTM at low temperatures. In fact the hybridization has to fulfill a dual role; both destroys the localized U moments and mediates exchange interaction between the magnetic moments. In this work the series of compounds URuG-UPdGe may exemplify the important role of the hybridization, since with increasing the d-electrons numbers there occurs a change from a nonmagnetic state in URuGe to a ferro/antiferromagnetic one in UPdGe. Interestingly, recent works on the solid solutions URu<sub>1-x</sub>Rh<sub>x</sub>Ge have shown that before the ferromagnetism appears, the system exhibits non-Fermi liquid (nFL) behaviour around the magnetic quantum critical point (QCP) at  $x \sim 0.62$ . Moreover, it has been pointed out that spin-fluctuations as a precursor take place before the system brings nearer QCP.

Since, similar evolution in the ground state might be expected for URu<sub>1-x</sub>Pd<sub>x</sub>Ge, We present a systematic study of the URu<sub>1-x</sub>Pd<sub>x</sub>Ge solid solutions by means of X - ray diffraction, dc-magnetization, specific heat and electrical resistivity. The studied alloys ( $0.1 \leq x \leq 0.9$ ) crystallize in the orthorhombic TiNiSi - type structure with space group Pnma. Analysis of the X-ray diffraction data using Rietveld refinement method reveals the Vegard's law behaviour of the unit cell volume through the b - and - c axis parameters exhibit an anomaly around  $x = 0.7$ . It is found that the magnetic behavior of URu<sub>1-x</sub>Pd<sub>x</sub>Ge strongly depends upon the Pd substitution. The compositions with  $x < 0.3$  are nonmagnetic down to 2 K. In the concentration range  $0.3 < x < 0.8$  the magnetic ground state is antiferromagnetic with a maximum value of  $T_N = 32$  K at  $x = 0.7$ . The  $x = 0.9$  composition alike UPdGe undergoes two successive magnetic phase transitions: antiferromagnetic at  $T_N = 35$  K and ferromagnetic at  $T_C = 31$  K. In the nonmagnetic-magnetic crossover region ( $x \sim 0.3$ ) the magnetic and electron transport properties display non Fermi liquid behavior. The observed development of magnetism corresponds well to changes in the degree of 5f electron localization as well as in the Kondo interactions, resulting mainly from increased 5f conduction electron hybridization.

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CeAg has a CsCl-type body-centered cubic structure, and exhibits ferroquadrupole (FQ) and ferromagnetic (FM) transitions at  $T_Q = 16$  K and  $T_C = 5.5$  K at ambient pressure, respectively. It is also known that by applying pressure, two successive structural phase transitions from cubic to tetragonal and from tetragonal to an unidentified structure are induced at around 0.2 and 2 GPa, respectively. On the other hand, the pressure dependence of  $T_C$  above 2 GPa has long been controversial in the previous reports. In the present study, we have measured the temperature dependence of electrical resistivity  $\rho(T)$  in hydrostatic pressures ranging up to 4 GPa in order to construct a detailed pressure-temperature phase diagram. We found that two successive transitions in  $\rho(T)$  curves in a low temperature region below 10 K of the unidentified structural phase ( $P > 2.1$  GPa), whereas the compound shows only the FM transition in the tetragonal phase ( $0.2 < P < 2.1$  GPa). Both the transitions in the unidentified phase decrease with increasing pressure, suggesting the presence of pressure-induced quantum critical points above 5 GPa.

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## Structural and electromagnetic characteristics of La-(Sr,Ce)-(Mn,Zn)-O P-04 manganites and the problem of charge compensation

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In the present work experimental data are shown for the influence of double partial substitution of Zn for Mn and of Ce for Sr in  $\text{La}_{0.65}\text{Sr}_{0.35}\text{MnO}_{3+\gamma}$  manganite on the structure, magnetic and electrical properties of obtained materials. Polycrystalline samples were prepared by ceramic processing. The starting components (dried  $\text{La}_2\text{O}_3$ ,  $\text{SrCO}_3$ ,  $\text{MnO}_2$ ,  $\text{CeO}_2$ ,  $\text{ZnO}$  powders) were weighed out in stoichiometric proportions to obtain the compounds of  $\text{La}_{0.65}\text{Sr}_{1-c}\text{Ce}_c\text{Mn}_{1-x}\text{Zn}_x\text{O}_{3+\gamma}$  system ( $c=0.05$ ;  $x=0$ ; 0.05; 0.10). They were mixed and ground in a ball mill with addition of alcohol. Pellets compacted of the obtained charge mixture were then preliminarily burned at 1273 K for 4 h. This operation was followed by grinding, introducing a binder (an aqueous solution of polyvinyl alcohol), pressing the samples, and burning out the binder. The final sintering step was performed at 1473 K for 10 h, and the samples were cooled together with the furnace. Then, in order to provide stoichiometric oxygen content, the samples were annealed at 1223 K and partial pressure of oxygen  $P_{\text{O}_2}=10^{-1}$  Pa for 96 h. All samples were of rhombohedral structure, but had the impurity of  $\text{CeO}_2$  phase, and the amount of this phase was increased from 0.5 to 1.9% with the zinc content. The separation of  $\text{CeO}_2$  means that in manganites the content of cerium “c” is less than 0.05, so that rare-earth sublattice contains cation vacancies. The unit cell volume ( $v$ ) of rhombohedral phase was nonmonotonic function of “x”. The value of  $v$  for all compositions rose after annealing due to increasing of  $\text{Mn}^{3+}$  concentration at the expense of  $\text{Mn}^{4+}$  content. Curie temperature and saturation magnetization ( $\sigma_s$ ) decreased with concentration of Zn increase as a result of diamagnetic dilution of octahedral sublattice, but after annealing  $\sigma_s$  rose. Of great interest is the fact that, despite of no single-phase structure and high concentration of defects, compounds with  $x=0.05$  had a narrow temperature interval of “ferromagnetic-paramagnetic” transition ( $\sim 5$  and 4 K before and after annealing, accordingly). All samples exhibited metallic type of temperature dependence of resistivity at appropriate low temperature regions. Maximum absolute value of negative magnetoresistance (MR) reached 127% for magnetic field strength 9 kOe at 166 K in annealed sample with  $x=0$ , and as-sintered sample revealed anomalous behavior of  $|\text{MR}|$ , namely its decline at low temperatures. Possible approach to the interpretation of established regularities is discussed taking into account valent and spin state of the ions, steric factor, properties of cation vacancies, double exchange interaction and various mechanisms of charge compensation, including formation of singly charged oxygen ion. From indirect data it may be noted that in manganites Ce was in  $\text{Ce}^{4+}$  state.

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# Magnetism of europium in superconducting $\text{EuFe}_{2-x}\text{Co}_x\text{As}_2$ studied by $^{151}\text{Eu}$ and $^{57}\text{Fe}$ Mössbauer spectroscopy P-05

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The compound  $\text{EuFe}_{2-x}\text{Co}_x\text{As}_2$  was investigated by means of the  $^{57}\text{Fe}$  and  $^{151}\text{Eu}$  Mössbauer spectroscopy versus temperature (4.2 – 300 K) for  $x=0$  (parent),  $x=0.34 - 0.39$  (superconductor) and  $x=0.58$  (over-doped). It was found that spin density wave (SDW) is suppressed by Co-substitution, however it survives in the region of superconductivity, but iron spectra exhibit some non-magnetic component in the superconducting region. Europium orders magnetically regardless of the Co concentration with the spin re-orientation from the  $a$ -axis in the parent compound toward  $c$ -axis with the increasing replacement of iron by cobalt. The re-orientation takes place close to the  $a$ - $c$  plane [1]. Some trivalent europium appears in  $\text{EuFe}_{2-x}\text{Co}_x\text{As}_2$  versus substitution due to the chemical pressure induced by Co-atoms and it experiences some transferred hyperfine field from  $\text{Eu}^{2+}$ . Iron experiences some transferred field due to the europium ordering for substituted samples in the SDW and nonmagnetic state both, while the transferred field is undetectable in the parent compound. Superconductivity coexists with the 4f-europium magnetic order within the same volume. It seems that superconductivity has some filamentary character in  $\text{EuFe}_{2-x}\text{Co}_x\text{As}_2$  and it is confined to the non-magnetic component seen by the iron Mössbauer spectroscopy.

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## Screening of magnetic moment at Co impurities in Cu hosts

P-06

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We present theoretical investigation of the electronic structure for cobalt impurities located in the bulk and on the surface of copper. We emphasize on systematic description of the many-body ground state and excitation spectra. The impurities are described within the framework of the multi-orbital Anderson impurity model (AIM), that is parametrized to match the LDA electronic structure. The AIM is then solved using the Lanczos method. We analyze the effect of spin-orbit interaction and the lowered symmetry due to the surface on the formation of the magnetic and non-magnetic ground states. The results are compared to those obtained using the continuous-time quantum Monte Carlo method [1].

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For the whole region of  $x$ , the  $^{119}\text{Sn}$  Mössbauer spectra of  $\text{UCuGe}_{1-x}\text{Sn}_x$  compounds ( $x=0.01 - 1.0$ ) represent a superposition of two magnetic sextets with two sets of hyperfine parameters. Two subspectra with significantly different values of the magnetic hyperfine fields ( $B_{\text{hf}}$ ),  $B_1$  and  $B_2$ , correspond to the two local magnetic states: low-field (LF) and high-field (HF). The LF-component corresponds to the  $^{119}\text{Sn}$  atoms which interact only with the three nearest uranium magnetic moments. The magnetic exchange of this group of  $^{119}\text{Sn}$  atoms with the other three more distant uranium moments is shielded by the Cu-layer and does not contribute to  $B_1$ . The HF-component  $B_2$  corresponds to other group of  $^{119}\text{Sn}$  atoms which have a magnetic exchange with all six uranium ions around the tin atoms. The structural (Ge-Cu) and (Sn-Cu) defects or vacancies in Cu-layers of the  $\text{UCuGe}_{1-x}\text{Sn}_x$  compounds lead to disruption of the shielding Cu-layer and creation of bonds of the Sn atoms with all the six uranium ions. In the ferromagnetic (FM) and antiferromagnetic (AFM) Gd - X (X is a p-, s-element) compounds, the  $B_{\text{hf}}$  values on  $^{119}\text{Sn}$  nuclei extrapolated to 0 K can be expressed as  $B_{\text{hf}} = \Delta B \times N$ , where  $\Delta B = -4.5(5) \text{ T}/\mu_{\text{Gd}}$  is a contribution of each Gd-moment to  $B_{\text{hf}}$ , and  $N$  is the number of uncompensated Gd magnetic moment in the nearest neighborhood of tin atoms. In the AFM  $\text{GdCuSn}$ ,  $\text{GdAgSn}$ , and  $\text{GdCuGe}$  compounds crystallizing in the hexagonal GaGeLi-type of structure, the hexagonal layers of atoms Gd, Cu(Ag) and Sn(Ge) alternate in the sequence Gd-Sn(Ge)-Cu(Ag)-Gd along the  $c$  axis. The tin atoms are surrounded by six atoms of Gd (3Gd atoms are located in the lower layer and 3Gd ones in the more distant upper layer). We have found that  $B_{\text{hf}}$  on the  $^{119}\text{Sn}$  nuclei in  $\text{GdCuSn}$  and  $\text{GdAgSn}$  is oriented along the  $c$ -axis. The  $B_{\text{hf}}$  values at 5 K are equal to 5.31(1) T and 5.04(2) T, respectively. These values correspond to the contribution of only one Gd magnetic moment to the  $B_{\text{hf}}$  on  $^{119}\text{Sn}$  nuclei. It is possible if only the three nearest Gd magnetic moments are involved in the magnetic exchange with the Sn atoms, the contributions from two of them mutually compensate. The three more distant Gd moments are shielded by a Cu-layer. The Cu-vacancies and partial Cu-Ge disorder in the compound  $\text{GdCuGe}$  lead to penetration of the magnetic exchange from three more distant Gd atoms through the Cu-layer. Therefore for the part of the  $^{119}\text{Sn}$  probe nuclei in  $\text{GdCuGe}$ ,  $B_{\text{hf}}$  is formed by two uncompensated Gd magnetic moments and reaches of 10 T. The investigation of  $B_{\text{hf}}$  on the  $^{119}\text{Sn}$  probe nuclei in uranium and RE-based compounds have shown that in the compounds with layered crystal structure the screening effect of the magnetic exchange interaction by layers of p-or s-, d-nonmagnetic atoms is observed.

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## **Comparative study of ternary stannides of $R_3\text{Co}_4\text{Sn}_{13}$ ( $R = \text{Ce}, \text{Pr}, \text{Yb}$ )**

**P-08**

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We report a systematic study of ternary stannides of  $R_3\text{Co}_4\text{Sn}_{13}$  ( $R = \text{Ce}, \text{Pr}, \text{Yb}$ ) by means of the specific heat and  $^{59}\text{Co}$  nuclear magnetic resonance (NMR) measurements. Distinctive phenomena associated with the structural phase transition have been identified for  $\text{Ce}_3\text{Co}_4\text{Sn}_{13}$  and  $\text{Pr}_3\text{Co}_4\text{Sn}_{13}$  at  $T^* \sim 155 \text{ K}$  and  $\sim 130 \text{ K}$ , respectively. For both materials, relative weak  $^{59}\text{Co}$  quadrupole splittings are consistently found below  $T^*$ , implying that the electrical field gradient (EFG) sensed by the Co site decreases undergoing this phase transition. Such an observation could be attributed to the local distortion of the Sn(2) atom from its initial position below  $T^*$  which consequently leads to significant modification of the electronic structures around the Fermi surfaces. For  $\text{Yb}_3\text{Co}_4\text{Sn}_{13}$ , however, the specific heat and NMR results show the absence of the structural-related phase transition. The  $^{59}\text{Co}$  NMR Knight shift and spin-lattice relaxation rate  $1/T_1$  clearly indicate that  $\text{Yb}_3\text{Co}_4\text{Sn}_{13}$  is a Pauli-type paramagnet. From the Korringa relation (constant  $T_1T$ ), we thus estimated Co  $3d$  Fermi-level density of states  $N_d(E_F) \sim 3.95 \text{ states/eV f.u.}$  for this compound.

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Magnetic properties of NdFeO<sub>3</sub> are mostly determined by three magnetic interactions (Fe-Fe, Fe-Nd and Nd-Nd), which are present in this material. Magnetic ordering of Fe<sup>3+</sup> ions creates a canted antiferromagnetic ordering below the Néel temperature at about  $T_{NI} = 690$  K. Upon cooling the magnetic moments of Fe<sup>3+</sup> exhibit reorientation from the *a*-axis to the *c*-axis in the spin reorientation region (103-165 K). Low temperature heat capacity measurements revealed a Schottky anomaly at about 2 K and a sharp maximum at  $T_{N2} = 1.05$  K. Neutron diffraction measurements confirmed magnetic ordering for Nd-Fe sub lattice below 1 K and long-range ordering due to Nd-Nd interaction below 0.4 K.

Our study of magnetic properties was performed on NdFe<sub>x-1</sub>Mn<sub>x</sub>O<sub>3</sub> single crystals with *x* from 0.0 to 0.4, which were grown by the optical floating zone technique (OFZT). Prepared crystals were characterized by powder diffraction, SEM and EDX analysis, X-ray and magnetic properties. All samples adopt orthorhombic crystal structure (space group Pbnm).

In the case of sample with *x* = 0.1 the Néel temperature decreases from 691 K to 621 K. The spin reorientation is indicated by steep decrease of magnetization in the range between 150 K and 125 K but the relatively flat curve down to 15 K is unusual in comparison with NdFeO<sub>3</sub>. The rise of magnetization below 15 K indicates increasing Nd-Fe magnetic interactions and the anomaly at about  $T_{max} = 11$  K is generated by doping. Magnetic fields smeared out the anomaly confirming its magnetic origin. The Schottky-type anomaly is shifted to higher temperatures reaching value  $T_{sh} = 2.76$  K.

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## Hydrogen absorption in UNiZn and its similarity to UNiAl

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We have found a new UTX (T = late transition metal, X = p-metal) compound with interesting hydrogen absorption properties. UNiZn crystallizes in the hexagonal ZrNiAl type of structure (*P*-62*m*). It was found to have a paramagnetic ground state. Magnetic susceptibility is low ( $10^{-8}$  m<sup>3</sup>/mol) but temperature dependent. UNiZn can be considered as a spin fluctuator with its magnetic properties between two limiting cases, Pauli paramagnet and magnetically ordered material.

Hydrogenation of UNiZn was found to be very sensitive to the temperature. The high-temperature synthesis (773 K) leads to so called HDDR process (hydrogenation-disproportionation-desorption-recombination). Upon hydrogenation the sample was decomposed to β-UH<sub>3</sub>, Zn and other unidentified phases. After the hydrogen is desorbed, the initial UNiZn compound is restored.

On the other hand, the low-temperature hydrogenation (437 K) is irreversible. The UNiZn compound can absorb 2.35 H/f.u at this temperature and hydrogen pressure *p* = 120 bar. This value of absorbed hydrogen reveals similarity to already studied UNiAl compound [1,2] which can absorb 2.3 H/f.u or similar amount of D. The similarity of hydrogen absorption process in UNiZn and UNiAl will be discussed.

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[2] H.N. Bordallo et al., Physica B **276-278**, 706 (2000).

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The thorium-based silicide ThPtSi crystallizes with an orthorhombic crystal structure of the LaPtSi-type (space group I4<sub>m</sub>d) that lacks an inversion center. Its low-temperature physical properties were studied by means of magnetization, electrical resistivity and heat capacity measurements, performed down to 0.35 K in magnetic fields up to 1 T. The compound was found to exhibit bulk superconductivity below  $T_c = 3.3$  K with an upper critical field of about 0.8 T. The key parameters of the superconducting state, derived from the experimental data, indicate a BCS-type coupling of Cooper pairs.

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## **Crystal growth and characterization of Ce – Ni – Ge compounds**

**P-12**

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In our paper we study metallurgical aspects of CeNiGe<sub>x</sub> samples preparation. The polycrystalline samples with  $x = 1, 3$  and  $6$  were prepared by arc melting under argon atmosphere in a mono arc furnace. The phase analysis of prepared samples was performed by methods of optical and scanning electron microscopy (SEM) including second electron (SE) and backscattered electron (BE) images. The energy dispersive X-ray (EDX) analysis was used for qualitative and quantitative determination of phases in the samples. The crystal structure was determined from X – ray powder diffraction experiments. Among as prepared samples only CeNiGe sample is a single phase sample. This compound crystallizes in orthorhombic crystal structure (space group  $Pnma$ ) with lattice parameters  $a = 0.72418$  nm;  $b = 0.43078$  nm;  $c = 0.72408$  nm. Remaining samples CeNiGe<sub>3</sub> and CeNiGe<sub>6</sub> are not single phase and contain several phases including CeNiGe<sub>2</sub>, CeNiGe<sub>3</sub>, Ge and CeO<sub>2</sub>. The presence of the oxide was successfully removed by re-melting of Ce and removing the oxides from the surface of the charge before melting. All compounds were re-melted 5-times in order to obtain better homogeneity of the samples. CeNiGe<sub>3</sub> and CeNiGe<sub>6</sub> were sealed in quartz tubes and expose to the heat treatment at 800°C for 14 days in order to obtain one phase samples. The main goal of our study is crystal growth of a single crystal from Ce – Ni – Ge system.

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## **High-Frequency Ultrasonic Measurements of SmOs<sub>4</sub>Sb<sub>12</sub> under Hydrostatic Pressure**

**P-13**

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We have performed ultrasonic measurements on the filled-skutterudite compound SmOs<sub>4</sub>Sb<sub>12</sub> under hydrostatic pressure up to 1.2 GPa with ultrasonic frequencies up to 250 MHz. The elastic constant  $C_{11}$  of the present compound shows ultrasonic dispersion (UDs), which will be caused by the “Rattling” of the Sm-ion, at  $\sim 20$  K and  $\sim 60$  K with the frequency of  $\sim 100$  MHz under ambient pressure [1]. Thus, the present study provides new information of hydrostatic pressure dependences of the UD and its relation to the heavy-electron state of this compound [2]. As increasing pressure, the UD of higher temperatures shifts to lower temperatures, which indicates a decrease of activation energy and/or an increase of relaxation time of the thermally-activated ionic motions. On the other hand, the UD of lower temperature gradually disappears as increasing pressure. We have also found that the elastic response around the phase transition temperature  $T_0$  is drastically changed under hydrostatic pressure. Under 1.2 GPa, the  $C_{11}$  shows rapid decrease of  $\sim 3\%$  in the unknown low-temperature ordered phase below  $T_0$ , which is quite larger than the change of  $\sim 0.2\%$  under ambient pressure [1]. The relatively large elastic anomaly implies that a lattice distortion occurs due to the transition under hydrostatic pressure. The  $C_{11}$  also shows Curie-type softening below 80 K down to  $T_0$ . The amount of change of the softening also increases as increasing pressure, which suggests that 4f-electron state become localized as increasing hydrostatic pressure. The present results strongly suggest that the quadrupole degrees of freedom play an important role in the phase transition.

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## **Application of Nd-ferromagnet to the elementary education of physics in university**

**P-14**

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It has been well known that the ferromagnet is used in physics education not only in the university but also in the elementary, secondary and high school. In the elementary education of physics in the university and college it is well established that the demonstration experiment (DE) in the lecture produces a good result on the deep understanding of physics for students. The DE is usually conducted by the cooperation of teachers with students, which is so-called bidirectional lecture. The DE should have a background of physics which is easily understandable by students. The electromagnetic induction phenomena are the most basic and important concept for the study of physics. In the present work, we made an attempt to construct a lecture using such DE of electromagnetic induction using Nd ferromagnet. When we move the ferromagnet near the conductor, an eddy current may be induced in the conductor, which is proportional to the magnitude of spontaneous magnetization of ferromagnet. We show this phenomenon is applied to the cooking utensil in our daily life. We will show the details of the lecture and its process.

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## Strongly correlated four electron systems away from half filling

P-15

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Exact analytical results for ground-state energy of four electrons in the nearly half-filled band of the one-dimensional single band Hubbard model is presented. The two cases treated covers odd and even lattices showing that the procedure employed is suitable for obtaining vital ground-state information from even and odd lattices.

A simplified modification of the Lanczos technique, which is relatively analytical, was used. An analytical grouping method that aids eradication of double counting was developed and applied to reduce the number of iterations required for convergence. This can also be found useful in small lattices in one dimension. Results obtained explain variations in ground-state energy in the: (a) strong coupling limit, (b) weak coupling limit, and (c) no interaction.

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## Hybridization features of the electronic structure and paramagnon mechanism of superconductivity

P-16

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Important feature of the electronic structure of strongly correlated superconducting compounds of transition and rare earth metals (e.g. lanthanum cuprate) due to the effects pd-hybridization. Within the framework, the periodic pd-Anderson model has been shown the possibility of appearance partially filled narrow band of heavy fermions on the edge or inside the hybridization gap. We calculated the magnetic susceptibility, spin-spin correlator for different values of the Hubbard interaction and the number of electrons. It was found that the decrease of the Hubbard interaction constants (value pd-hybridization is constant) leads to negative values of mode-mode coupling constants and the possibility of Cooper doubling through exchange paramagnons with d-symmetric order parameter. The estimates of the critical temperatures are consistent with the experimentally observed values for  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . Increase of Hubbard constant leads to the expulsion of the heavy-fermions band inside the hybridization gap, changing the sign of the mode-mode coupling constant and the appearance of ferromagnetic solutions.

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## High-Resolution X-Ray Diffraction Study on $\text{URu}_2\text{Si}_2$

P-17

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The heavy-fermion superconductor URu<sub>2</sub>Si<sub>2</sub> (ThCr<sub>2</sub>Si<sub>2</sub>-typed body-centered tetragonal, I4/mmm) shows an enigmatic second-order phase transition at  $T_0 = 17.5$  K, whose order parameter has been unidentified for more than 25 years [1-3]. The order is referred to as the “Hidden Order (HO)”, and a number of efforts have been made to solve the mystery of the HO in both experimental and theoretical researches. Quite interestingly, recently performed measurements of magnetic torque and cyclotron resonance on this compound have suggested that a four-fold rotational symmetry is broken into two-fold in the HO phase [4,5]. Although this may lead to a crystal-lattice deformation from the tetragonal to the orthorhombic structure below  $T_0$ , no evidence of such a lowering of the crystal symmetry has been found in the previous thermal-expansion measurements and X-ray and neutron diffraction experiments. However, there might be a tiny lattice distortion missed in those measurements. The dilatometry using a large crystal is unsuitable for detecting lattice distortions, if the crystal distortion forms a multi-domain structure. Diffraction technique, on the other hand, is free from such a difficulty, but the sensitivity of a change in lattice spacing  $d$  is normally  $\Delta d/d \sim 10^{-4}$ , which is much lower than that of the dilatometry technique,  $\sim 10^{-7}$ . We performed high-resolution X-ray diffraction experiments in order to see whether a symmetry lowering of the crystal lattice of URu<sub>2</sub>Si<sub>2</sub> actually occurs or not in the HO. We achieved a resolution of  $\Delta d/d \sim 1.3 \times 10^{-5}$  (FWHM) by using a combination of a high-resolution monochromator and a backscattering geometry in the present experiments. We conclude from the careful measurements that there is no development of orthorhombicity greater than  $\Delta d/d \sim 3 \times 10^{-5}$  below  $T_0$ .

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## Hydrogen induced interdiffusion in selected Vanadium and Titanium oxide thin films

P-18

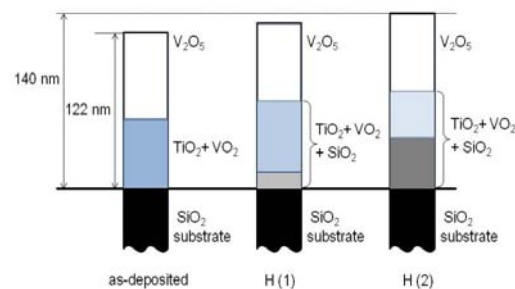
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From our previous study of the effect from the hydrogen absorption on film structure of Ti/TiO<sub>2</sub>/Ti thin films [1,2], we have found out that a hydrogen concentration of about 40 at.% and 15 at.% was found respectively for the top Ti and the bottom Ti layer and that the hydrogen can penetrate through the second layer TiO<sub>2</sub> without accumulation there.

In this work we focus on the effect from hydrogen-absorption on selected thin films of TiO<sub>2</sub>-V<sub>2</sub>O<sub>5</sub> systems. In the case if on the surface is the V<sub>2</sub>O<sub>5</sub> layer, the hydrogen charging effect is much enhanced indicated by a large increase of the total film thickness (up to 15% upon hydrogen charging of 6 hours). In the case if on the surface is the TiO<sub>2</sub> layer, no hydrogen is accumulated in the films. However, in all cases a large reduction of V<sub>2</sub>O<sub>5</sub> is observed upon hydrogen charging. After 6 hrs charging, a complete transition of V<sub>2</sub>O<sub>5</sub> into VO<sub>2</sub> can be obtained. The influence of hydrogenation on the structure and composition of one film V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub>/SiO<sub>2</sub> was illustrated in the figure.



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## Magnetic susceptibility and features of electronic structure PuCoGa<sub>5</sub>

P-19

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Self-consistent procedure has been developed for calculation of the electron density of states, electron-electron interaction parameters and magnetic susceptibility, based on the method of LDA + U + SO. Within this framework, we analyze the possible solutions of the equation of magnetic state, investigate the spin fluctuations arising due to the Hubbard interaction of the d- and f-electrons. For describing electron-electron interaction, we use the Hubbard–Stratonovich transformation, which reduces the problem of many-body to the study of non-interacting d- and f-electrons in fluctuating exchange and charge fields. The ferromagnetic ground state of the f- and d-electrons is thermodynamically unstable according to the calculated electronic structure. Significant spin

anharmonism has been detected, which leads to a maximum of the magnetic susceptibility depending on temperature near starts superconductivity in normal phase.

Spin-spin correlation functions are calculated. It is found that spin fluctuations in the d-subsystem increased due to exchange interaction d- and f-electrons. Herewith the radius of the spin correlations in the d-subsystem is considerably smaller than for f-electrons. It is expected that the spin fluctuations can lead to the formation of Cooper pairs of d-electrons.

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## Extensive Studies of Antiferromagnetic $GdM_2Al_{20}$ ( $M = V, Ti, Cr$ )

P-20

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Intermetallic cage compounds with  $CeCr_2Al_{20}$ -type structure (1-2-20 compounds) have recently attracted a significant scientific interest due to their versatility towards the chemical composition and a variety of physical phenomena that can be observed when various atoms are introduced instead of Ce, Cr and Al, like magnetic ordering [1,2], heavy fermion [3] and Kondo lattice behaviour [4] as well as low-frequency *rattling* phonon associated superconductivity [5].

In this study, a series of gadolinium containing intermetallic cage compounds of general formula  $GdM_2Al_{20}$  ( $M = V, Ti, Cr$ ) was synthesized using the arc-melting technique and characterized for their physical properties by means of electrical resistivity, magnetic susceptibility, Hall coefficient, and specific heat measurements. Antiferromagnetic transition was observed and extensively studied in all three compounds.

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## Anomalous influence of an external magnetic field on spin fluctuations and magnetorefractive effect in lanthanum manganites

P-21

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We study the influence of magnetic field on the electron spectrum and optical conductivity hybridized p-and d-electrons in the strong Coulomb correlations in the conditions of the magnetic phase transition in lanthanum manganites. We use the Hamiltonian of the generalized Hubbard model, complete terms, responsible for the hybridization of strongly correlated d-electrons with p-electrons. Electron Green's functions were calculated by the method of generating functional by using transformations which reduce the problem of many-electron to the study motion of non interaction electrons in the internal stochastic exchange and charge fields. It is shown that inside the hybridization gap arises narrow zone of heavy fermions. Scattering of electrons this band on the fluctuations of internal stochastic fields leads to their localization (similar to the result of Anderson for a crystal with "vertical" disorder). Within the developed concepts we got maximum temperature dependence of the spin stiffness in the near vicinity of the Curie point, which causes anomalously strong suppression of spin fluctuations by a magnetic field and leads to a large magnetorefractive effect. At the same time due to short-range order of the spin occurs slight change in the fundamental absorption edge as compared to the ferromagnetic region.

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## Study the structural and superconducting properties of europium oxide nanoparticle added $Bi_{1.6}Pb_{0.4}Sr_2Ca_2Cu_3O_y$

P-22

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The europium oxide nanoparticles addition effect on structural, DC electrical resistivity, critical current density, and AC magnetic susceptibility properties of polycrystalline  $Bi_{1.6}Pb_{0.4}Sr_2Ca_2Cu_3O_y$  samples are investigated. For this study, four bulk polycrystalline samples with general formula of  $Bi_{1.6}Pb_{0.4}Sr_2Ca_2Cu_3O_y + xEu_2O_3$  (where  $x = 0.0, 0.3, 0.5, 1.0$  wt%) were prepared by chemical sol-gel method. X-ray diffraction, and SEM were used for structural characterization of the samples. DC electrical resistivity, critical current, and AC magnetic susceptibility were measured. XRD analysis showed that both (Bi,Pb)-2223 and Bi-2212 phases coexist in the samples having orthorhombic crystal structure. Bi-2223 phase concentration increases with increasing europium

nanoparticle concentration. DC electrical resistivity,  $J_c$ , and AC susceptibility measurements reveal that adding europium nanoparticles to BSCCO improves superconducting properties of this system and enhances its critical current density due to the improvement of the grain connectivity with europium nanoparticle addition.

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## **XAS- and XMCD-Signatures of Kondo and Heavy Fermion Behaviour in the Surface Intermetallic CePt<sub>5</sub>/Pt(111)** **P-23**

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We explore the detection of magnetic signatures of Kondo and heavy fermion physics by X-ray spectroscopy and study the anisotropic paramagnetic Ce-4f response in CePt<sub>5</sub>, prepared on Pt(111). Temperature dependent X-ray absorption spectra yield impurity Kondo temperatures of the order of  $T_K \approx 150$  K. For  $T > 20$  K the magnetic behaviour is readily understood in terms of a hexagonal crystal field (CF), acting on weakly interacting, considerably screened Ce-4f moments. Nevertheless, Kondo screening is less pronounced than predicted within the non-crossing approximation [1] on the basis of the experimental  $T_K$ . We therefore resort to a more empirical Hamiltonian to analyze the Ce-4f susceptibility. Distinct CF parameters for ‘inner’ and ‘surface’ atoms are required to obtain quantitative agreement, well in line with complementary structural information from energy dependent electron diffraction results (LEED-IV). The paramagnetic response displays a remarkable anomaly ( $T^* \approx 20$  K), which we shall discuss as signalling the transition towards the coherent heavy fermion state. Well below  $T^*$  we find Ce-4f saturation moments much smaller than the free ion values. Their occurrence, too, can be understood to be characteristic of the coherent state and associated with a Lifshitz transition as predicted theoretically [2]. X-ray spectroscopy thus proves valuable for investigating strongly correlated electron systems in case sufficiently well-defined surfaces can be obtained.

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The structural behavior of  $\text{Np}_2\text{Co}_{17}$  is investigated by means of high pressure diamond-anvil compression measurements and is compared with that of the isostructural compounds  $\text{Lu}_2\text{Co}_{17}$  and  $\text{Lu}_2\text{Ni}_{17}$ . The  $\text{Th}_2\text{Ni}_{17}$ -type hexagonal crystal structure is preserved with no measurable discontinuous volume collapses up to the highest achieved pressure,  $p = 43$  GPa. For  $\text{Np}_2\text{Co}_{17}$ , fits to the Birch-Murnaghan and Vinet equations of state give values of the isothermal bulk modulus and its pressure derivative of  $B_0 = 286$  GPa and  $B'_0 = 3$ , revealing that this Np compound is a highly incompressible solid with stiffness comparable to that of superhard covalently bonded materials. For the  $\text{Lu}_2\text{T}_{17}$  ( $T = \text{Co}, \text{Ni}$ ) compounds, the measured bulk modulus changes from  $B_0 = 137$  GPa for  $T = \text{Co}$  to  $B_0 = 257$  GPa for  $T = \text{Ni}$ . The isothermal equation of state for the studied compounds are in excellent agreement with the results of *ab initio* fully-relativistic, full potential local spin-density functional calculations. Theoretical estimates of the bulk modulus are given also for  $\text{Np}_2\text{Ni}_{17}$ , for which  $B_0$  is predicted to assume values intermediate between those measured for  $\text{Lu}_2\text{Ni}_{17}$  and  $\text{Np}_2\text{Co}_{17}$ .

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## Optical properties of a monoclinic insulator $\text{Cu}(\text{H}_2\text{O})_2(\text{en})\text{SO}_4$ , $\text{en}=\text{C}_2\text{H}_8\text{N}_2$ P-25

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$\text{Cu}(\text{H}_2\text{O})_2(\text{en})\text{SO}_4$  was recently identified as a quasi-one-dimensional  $S=1/2$  antiferromagnetic insulator [1]. The structure possesses a monoclinic symmetry with the angle  $\beta$  of  $105.5^\circ$ . We measured the system's optical functions, by means of Mueller ellipsometry, and here compare these with results obtained from DFT-based (GGA+U) *ab-initio* calculations. We concentrate on the static limit,  $\omega \rightarrow 0$ .

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## Electric resistivity of the $\text{Ce}(\text{Cu}_{1-x}\text{Ni}_x)_4\text{Mn}$ series

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Measurements of electrical resistivity for polycrystalline alloys in the  $\text{Ce}(\text{Cu}_{1-x}\text{Ni}_x)_4\text{Mn}$  system have been done in order to investigate the spin-glass like behaviour. Electric resistivity measurements were performed using a standard four-probe DC technique in the temperature range 2–300 K. It was found that  $\text{Ce}(\text{Cu}_{1-x}\text{Ni}_x)_4\text{Mn}$  exhibits a large broad maximum in the  $\rho(T)$  dependence around 50-150 K. For all samples we have observed an increased residual resistivity. Using the Matthiessen's rule and the  $\text{LaCu}_4\text{Al}$  compound as a nonmagnetic analog we have obtained the magnetic part of the resistivity.  $T^{3/2}$  temperature dependence typical of the spin-glass systems has been found at low temperatures for some samples. The characteristic temperature dependence of the resistivity is sensitive to the Ni content and the maximum is suppressed while changing the composition from  $\text{CeCu}_4\text{Mn}$  to  $\text{CeNi}_4\text{Mn}$ .

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