Program of the PCFES

Friday, July 5

Registration since 9.00

13.00 ***Opening***

13.15 – 15.15 Chair: H. Nakotte

L1 M.B. Maple
Superconductivity and heavy fermion behavior in $PrOs_4Sb_{12}$

L2 H. Harima
Fermi surface nesting in the filled skutterudite compounds

L3 E. Bauer
Heavy electron features of Pr-based Skutterudites

L4 T. Kawae
La concentration dependence of the ground state properties in $Pr_xLa_{1-x}Pb_3$

15.15 – 15.45 *Coffee break*

15.45 – 17.15 Chair: G. Zwicknagl

L5 B. Coqblin
Band filling effects in the Kondo lattice model

L6 M. Continentino
Griffiths phases in the strongly disordered Kondo necklace model

L7 P. Riseborough
Crystal field effects in $CeAl_3$

17.15 – 18.15 Chair: G. Oomi

L36 M. Doerr
Magnetic phase transitions of RCu_2 compounds in high magnetic fields

L37 A. Señas
Pressure effects on the magnetic inconmensurate structures

18.15 – 20.30 *Welcome party*

Saturday, July 6

8.30 – 10.30 Chair: W.E. Pickett

L10 T. Nishioka
Pressure-induced superconductivity of UGe_2

L11 D. Aoki
Superconductivity of the itinerant ferromagnet URhGe

L12 A. Shick
Superconductivity on the verge of magnetism

L13 J. Spalek
Coexistence of ferromagnetism and superconductivity induced by the Hund's rule coupling

10.30 – 11.00 *Coffee break*

11.00 – 13.30 Chair: E. Bauer

L14 H. von Löhneysen
Metals at a magnetic instability

L15 P. Gegenwart
Field tuning into a heavy electron quantum critical point

L16 J. Sereni
Scaling of thermal parameters at the magnetic instability of Ce-systems

L17 H. Michor
Heavy-Fermion- and NFL-behaviour in $CeNi_9X_4$ (X=Ge, Si)

L18 Z. Hossain
On the Existence of Eu-Based Heavy Fermion Compounds

15.30 – 17.00 ***Posters*** *with (soft)drinks*

17.00 – 19.00 Chair: M. Richter

L19 J. Kuneš
Bulk properties of light actinides: modified second variation method

L20 U. Nitzsche
Theoretical atomic volumes of the light actinides

L21 K. Kvashnina
RIXS (Resonant inelastic X-ray scattering) of Uranium compounds

L22 E. Colineau
Magnetic ordering in the $(U_{1-x}Np_x)_2Rh_2Sn$ system

Sunday, July 7

8.30 – 10.30 Chair: J.M. Mignot

L23 M. Kohgi
Physics of the low-carrier system Ce-monopnictides

L24 P.A. Alekseev
Neutron scattering study of the magnetic response in the YbB_{12} Kondo-insulator

L25 R.G.M. Caciuffo
Multipolar ordering in NpO_2 below 25 K

L26 A.S. Moskvin
Crystal-field fluctuations for 4f ions in high-T_c cuprates

10.30 – 11.00 *Coffee break*

11.00 – 13.00 Chair: P. Mohn

L27 M. Richter
Band anisotropy of rare-earth--transition-metal compounds: theory

L28 M. Rotter
Spontaneous magnetoelastic effects in Gadolinium compounds

L29 J.C. Gomez Sal
Disorder and low temperature effects in CeNiCu

L30 L. Durivault
Influence of the Kondo effect on the Ce-ordered magnetic moment existing in the compounds rich in germanium (50% at.) of the Ce-Ni-Ge system

13.00 – 15.00 ***Posters*** *with (soft)drinks*

17.30 ***Colloquium dinner*** *departure from the* ***Holiday Inn*** *hotel for* ***Château Detenice***

Monday, July 8

8.30 – 11.00 Chair: H. Eschrig

L31 L. Petit
5f electron localization-delocalization transition from UPd_3 to UPt_3

L32 G. Zwicknagl
The dual nature of 5f states and heavy quasiparticles in UPt_3

L33 H. Amitsuka
Two-phase separation in URu_2Si_2 studied by microscopic measurements under hydrostatic pressure and uniaxial stress

L34 N. Bernhoeft
The concept of a dynamical phase in magnetic order: implications for URu_2Si_2

L35 P. Coleman
Hidden orbital order in the heavy fermion metal URu_2Si_2

11.00 – 11.30 *Coffee break*

11.30 – 13.30 Chair: G. Oomi & L. Havela

L35 I. Goncharenko
Studies of magnetic orders under very high pressures

L36 S.R. Saha
Anomalous behaviors in f-electron systems studied by uniaxial pressure experiments

L37 T. Gouder
5f localization in Pu systems: ground state and final state effects in photoemission

L38 J. Tobin
A new paradigm for the determination of 5f electronic structure using spin-dependent photoelectron spectroscopy

15.00 – 15.45 ***Ernst Mach Medal Award Lecture***

L39 O.K. Andersen
From multiple-scattering theory to orbitals (NMTOs); applications to magnesium diboride and high-temperature superconductors

15.45 – 17.45 Chair: M. Continentino

L40 P.M. Oppeneer
Unconventional superconductivity in UPd_2Al_3 from realistic selfconsistent calculations

L41 T. Hotta
Role of orbital fluctuations for unconventional superconductivity in f-electron systems

L42 S. Kos
Effect of paramagnetic fluctuations on superconductivity in $CeCoIn_5$

L43 P. Pagliuso
Phase diagrams of $CeMIn_5$ heavy-fermion superconductors (M=Rh, Ir and Co)

17.45 ***Closing***

Tuesday, July 9

7.30 – 8.00 ***Uploading of bus for Krakow*** *at your hotels*

8.00 – 17.00 ***Trip to Krakow*** *with ample time for discussions*

L1
Superconductivity and heavy fermion behavior in $PrOs_4Sb_{12}$

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University of California, San Diego

The filled skutterudite compound $PrOs_4Sb_{12}$ exhibits superconductivity, with a superconducting critical temperature $T_c \approx 1.85$ K, that appears to involve heavy fermion quasiparticles with an effective mass $m^* \approx 50\ m_e$, where m_e is the free electron mass [1,2]. The magnetic susceptibility $\chi(T)$ exhibits Curie-Weiss behavior above 50 K, passes through a maximum at ~3 K, and approaches a finite value as $T \rightarrow 0$ K, indicative of a nonmagnetic ground state. Specific heat $C(T)$ data below 20 K can be represented by a pronounced Schottky anomaly with a peak at ~3 K, a Debye lattice contribution, and an electronic contribution $C_e = \gamma T$ with $\gamma \approx 0.5$ J/mol-K^2. Analysis of the $\chi(T)$ data suggests that the Pr^{3+} ground state in the cubic crystalline electric field is a Γ_3 nonmagnetic doublet that carries an electric quadrupole moment. Measurements of the nonlinear magnetic susceptibility of $PrOs_4Sb_{12}$ at low temperatures are consistent with a Pr^{3+} Γ_3 nonmagnetic ground state. Inelastic neutron scattering measurements yield a Pr^{3+} energy level scheme that agrees well with that inferred from the magnetic susceptibility and specific heat measurements. Analyses of the specific heat jump at T_c and the slope of the upper critical field $H_{c2}(T)$ curve near T_c provide estimates for m^* comparable to that extracted from γ. Structure in the specific heat jump at T_c suggests the possibility of two distinct superconducting phases, as observed in the heavy fermion superconductors UPt_3 and $U_{1-x}Th_xBe_{13}$. Magnetoresistance measurements indicate that a phase transition occurs in fields above 40 kOe and below ~1 K in the normal state of $PrOs_4Sb_{12}$. Electrical resistivity measurements under pressure to ~20 kbar reveal a linear decrease of T_c with pressure. The compound $PrOs_4Sb_{12}$ may be the first example of a Pr-based heavy fermion superconductor. Furthermore, it is possible that the heavy fermion state in $PrOs_4Sb_{12}$ is generated by screening of the Pr^{3+} Γ_3 quadrupole moments by the charges of the conduction electrons.

References:
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L2
Fermi surface nesting in the filled skutterudite compounds

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ISIR Osaka University, Japan

The filled skutterudite with a general formula RT_4X_{12} (R = Rare earth, Th or U; T = Fe, Ru or Os; X = P, As or Sb) crystallizes in a unique BCC structure of a space group Im_3 (Th_5, #204). The compounds have recently attracted much attention as improved thermoelectric materials and for the variety of the electrical and magnetic properties. Among them, $PrRu_4P_{12}$ shows a metal-insulator (M-I) transition at TMI = 60 K [1] and $PrFe_4P_{12}$ undergoes a non-magnetic ordering at TA = 6.5 K [2], resulting in a low carrier system, which exhibits a heavy-fermion states in applied magnetic field [3]. The filled skutterudite compound PrT_4P_{12} (T = Fe/Ru) is an uncompensated metal with Pr_{3+}, then it could not be an insulator or a semi-metal within the same primitive unit cell. The study of Fermi surface reveals that the main Fermi surface of $LaFe_4P_{12}$ is a distorted cube and the volume is almost a half of the BCC BZ with a sharp peak in the density of states, indicating that the nesting with $\boldsymbol{q}$ = (1, 0, 0) is likely in the skutterudite compounds. [4] In fact, structural phase transitions with $\boldsymbol{q}$ = (1, 0, 0) are observed below TMI and TA in $PrRu_4P_{12}$ [5] and $PrFe_4P_{12}$ [6], respectively. These experiments show that the unit cell becomes doubled from BCC to simple lattice, then they

could be a semi-metal or an insulator, though the atomic displacements remain undetermined experimentally.
We have performed bandstructure calculations for the doubled unit cell (34 atoms) by using the FLAPW-LDA+U method [7] with many types of lattice distortions. Then we have found solutions for an insulator only in $PrRu_4P_{12}$ with the space group Pm_3 (Th1, #200), in which P atoms are distorted by about 5 % of a lattice constant with G1 mode [8]. The result shows that the distortion coupled with anti-quadrupolar ordering of Pr 4f 2 states, which is discussed with *T* displacements [9], is not necessary for the M-I transition of $PrRu_4P_{12}$. The M-I transition is caused by the perfect 3 dimensional nesting of the Fermi surface consisting of the P_{12} molecular orbital with the symmetry xyz, which is the only one Fermi surface in the mother structure of $PrRu_4P_{12}$ [10].

References:
[1] C. Sekine et al.: Phys. Rev. Lett. 79 (1997) 3218.
[2] H. Sato et al.: Phys. Rev. B 62 (2000) 15125.
[3] H. Sugawara et al.: J. Magn. Magn. Mater. 226 -230 (2001) 48.
[4] H. Sugawara et al.: J. Phys. Soc. Jpn. 69 (2000) 2938.
[5] C.H. Lee et al.: J. Phys.: Condens. Matter 13 (2001) L45.
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[7] H. Harima: J. Magn. Magn. Mater. 226 -230 (2001) 83.
[8] S.H. Curnoe et al.: J. Phys. Chem. Solid in press (Proceedings of ISSP-Kashiwa2001, Kashiwa).
[9] S.H. Curnoe et al.: Physica B in press (Proceedings of SCES2001, Ann Arbor), H. Harima et al.: J.Phys. Soc. Jpn Supplement in press (Proceedings of ORBITAL2001, Sendai).
[10] H. Harima and K. Takegahara: Physica B in press (Proceedings of SCES2001, Ann Arbor).

L3
Heavy electron features of Pr-based Skutterudites

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Ternary skutterudites $RE_yTM_4X_{12}$ with RE = rare earth, TM = Fe, Co, Rh, Ru, … and X = P, As, Sb attracted much interest because of an enormously large figure of merit $Z = S^2/(\rho\lambda)$, being a basic requirement for thermoelectric applications. S, ρ, λ are the Seebeck coefficient, the electrical resistivity and the thermal conductivity, respectively. Furthermore, these filled ternary compounds exhibit a rich variety of ground state properties, whereby the magnetic behaviour is dominated by the particular 4f electronic configuration. Hence features like Kondo- and heavy fermion behaviour or various types of magnetic order, hopping conductivity and superconductivity were already found. Skutterudites based on Pr also evidence a number of outstanding characteristics. Among them are superconductivity in $PrRu_4As_{12}$, $PrRu_4Sb_{12}$ below 2.4 and 1 K, respectively, a metal to insulator transition in $PrRu_4P_{12}$ at T_{MI} = 60 K, as well as magnetic ordering at T_{ord} = 6.2 K in $PrFe_4P_{12}$. Kondo-like anomalies in transport phenomena were found for the latter and C_p/T for $T \rightarrow 0$ shows a huge value of about 1.4 J/molK^2. Moreover, de Haas van Alphen measurements indicated extraordinary heavy electrons and unusual features of the Fermi surface topology, suggesting strongly correlated electrons in this compound. Very recently, heavy fermion superconductivity was found in $PrOs_4Sb_{12}$ below about 1.8 K.
In the present contribution, the skutterudite $PrFe_4Sb_{12}$ is investigated with respect to structural, magnetic and transport properties. $PrFe_4Sb_{12}$ orders magnetically below 5.5 K and exhibits an unusually high electronic contribution to the specific heat C_p/T for $T \rightarrow 0$ of about 1000 mJ/molK^2, thus ranking this compound among strongly correlated electron systems. We attribute some of such extraordinary features of these cubic Pr compounds to crystal field splitting, providing the possibility of non-magnetic singlets, doublets and triplets as ground state and hence the possibility of an occurrence of quadrupolar Kondo interactions. Moreover, the feasibility of a field induced non-Fermi-liquid state is taken into consideration.

L4
La concentration dependence of the ground state properties in $Pr_{(1-x)}La_xPb_3$

Tatsuya Kawae
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We have studied the low temperature properties of $Pr_xLa_{1-x}Pb_3$ with the ground state of a non-Kramers $\bullet_3$ for $0 \leq x \leq 1$. The fluctuation of the quadrupolar moments of the $\bullet_3$ doublet in $PrPb_3$ is entrily depressed by antiferro-quadrupolar ordering (QPO) at $T = 0.4$ K. Both of $PrPb_3$ and $LaPb_3$ have the $AuCu_3$-type cubic structure with the lattice parameter a= 4.867 Å and 4.903 Å, respectively. Thus La ions can be substituted for Pr ions without the change of crystal symmetry for all the concentration.
From the concentration dependence of the specific heat, QPO is expected to occur only up to x ~ .02, indicating that QPO is very sensitive to the distortion of the CEF field.
For a wide range of Pr concentration for $0.1 \leq x \leq 0.9$ where the ordering is absent, the specific heat shows a T-linear variation with a large coefficient, which is similar to PrInAg2. The temperature dependence of the specific heat can be almost reproduced by the model for amorphous materials with a random configuration of two level system.
This means that the large C/T in PrxLa1-xPb3 is responsible for the superpose of the Schottky specific heat due to splitting of the •3 doublet by the distortion of CEF field. Moreover, the low-temperature properties of the specific heat for $0.9 \leq x$ will be reported in the presentation.

L5
Band filling effects in the Kondo lattice model

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We present here theoretical results for a Kondo lattice model with local spins ½ and icluding both the intrasite Kondo exchange and an intersite antiferromagnetic exchange interaction treated within an extended mean field approximation. We have computed both the Kondo temperature and the correlation temperature below which shortrange magnetic correlations appear. An “exhaustion” problem arises if the number of conduction electrons is not large enough to screen all the lattice spins and we describe here the case of a non-integer conduction band filling. The Kondo effect disappears for low band filling and/or strong intersite coupling and a phase diagram is presented as a function of both parameters. The magnetic susceptibility and the effective magnetic moments are also computed as a function of temperature. A comparison of our theoretical results with experimental results is given here for Cerium Kondo compounds.

L6
Griffiths phases in the strongly disordered Kondo necklace model

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We study the effect of strong disorder on the one-dimensional Kondo necklace model using a perturbative real-space renormalization group approach which becomes asymptotically exact in the

low energy limit. The phase diagram of the model presents a random quantum critical point separating two phases; the *random singlet phase* of a quantum disordered *XY* chain and the *random Kondo phase*. We also consider an anisotropic version of the model which for strong disorder maps on the random transverse field Ising model. The present results provide a microscopic basis for non-Fermi liquid behavior in disordered heavy fermions associated with the existence of Griffiths phases. Finally the properties of the system in the different regions of the phase diagram are obtained.

L7
Crystal Field Effects in $CeAl_3$

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The thermodynamic and magnetic properties of a single impurity Anderson model, describing Ce in an environment with hexagonal symmetry, is treated within the N.C.A. It is found that the properties of the system are described by a Kondo temperature of the six fold degenerate spin orbit multiplet at temperatures larger than the crystal field splitting, and a highly renormalized Kondo temperature at low temperatures. The inelastic neutron scattering spectra exhibits a quasi-elastic and inelastic component. The results are compared with the concentrated heavy fermion compound $CeAl_3$. The system is well described by the single impurity Anderson model at temperatures above 1 K, with the crystal field parameters determined by Goremychkin et. al. from inelastic neutron scattering experiments. The excellent agreement may be due to the small variation of the f occupation number with temperature in heavy fermion systems. However, the single impurity model fails to describe the peak in the ratio C(T)/T found in experiments. Thus, it is concluded that this peak is either due to the coherence of the lattice, or due to magnetic interactions that may be responsible for spin glass like ordering.

L8
5f localization in Pu systems: ground state and final state effects in photoemission

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The deposition of Pu on Mg substrate allowed to prepare pure Pu layers with controlled thickness down to 1 monoatomic layer, only weakly interacting with the substrate. High-resolution UPS and Pu-*4f* core-level spectra demonstrate the dramatic changes of electronic structure for Pu below 5 monolayers thickness. For the „thick“ layer one can see the spectral intensity representing a *5f* band, increasing up to the Fermi level cut-off. The reduced thickness leads to a new feature around 1.7 eV below E_F. This broad maximum is of *5f* origin, and corresponds roughly to the *5f* emission found in PuSb. Therefore we interpret it as due to the emission from *5f* states, which get localized due to the reduced Pu coordination number. Another set of experiments reveals how the electronic structure of Pu is sensitive to details of crystal structure at the surface. The valence band spectra of α-Pu, prepared by ion-etching at various temperatures, show a systematic development from the triangular form, characteristic for low-*T* surface preparation, into the δ-Pu type, with 3 peaks close to E_F, obtained at elevated temperatures. This supports the theoretical conjecture that the surface of α-Pu should have a δ-Pu character.

L9
A New Paradigm for the Determination of 5f Electronic Structure using Spin-Dependent Photoelectron Spectroscopy

James G. Tobin[1] and collaborators:
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Despite recent intensive experimental effort [1-3], the electronic structure of Pu, particularly δ-Pu, remains ill defined. An evaluation of our previous synchrotron-radiation-based investigation of α-Pu and δ-Pu [1] has lead to a new paradigm for the interpretation of photoemission spectra of U, Np, α-Pu, δ-Pu and Am. This approach is founded upon a model in which spin and spin-orbit splittings are included in the picture of the 5f states [4] and upon the observation of chiral/spin-dependent effects in non-magnetic systems. [5,6] By extending a quantitative model developed for the interpretation of core level spectroscopy in magnetic systems [7], it is possible to predict the contributions of the individual component states within the 5-f manifold. This has lead to a remarkable agreement between the results of the model and the previously collected spectra of U, Np, Pu and Am, particularly δ-Pu, [1-3,8] and to a prediction of what we might expect to see in future spin-resolving experiments. [9] This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

References:

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L10
Pressure-induced superconductivity of UGe_2

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The ferromagnetic material UGe_2 exhibits superconductivity in the pressure range between ~1 and ~1.6 GPa. The ferromagnetism disappears nearly at ~1.6 GPa, therefore the superconducting phase appears completely in the ferromagnetic phase. It seems to be assumed that both ferromagnetism and superconductivity arise from 5*f* electrons in U atom and coexist homogeneously. We have measured dc magnetizations and ac magnetic susceptibilities χ_{ac} at pressures up to ~1.8 GPa and at temperatures down to ~0.4 K. The susceptibility measurements have indicated that the superconducting shielding current is imperfect. At low pressures less than P_0~1 GPa, the Curie temperature T_{Curie} which is characterized by a peak in $\chi_{ac}(T)$ coincides with a temperature T_m below which the spontaneous magnetization appears. Above P_0, on the other hand, T_{Curie} deviates from T_m. The difference between T_{Curie} and T_m becomes large as pressure increases. In addition, the zero-field-cooled and field-cooled magnetization curve separate below T_m. Furthermore, the peak in $\chi_{ac}(T)$ broadens abruptly above P_0. From these results we suggest that tiny ferromagnetic clusters

are formed below T_m and they show superparamagnetic behavior, and that not only the superconductivity but also the ferromagnetism are inhomogeneous in the real space.

L11
Superconductivity of the itinerant ferromagnet URhGe

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We studied superconducting properties of an itinerant ferromagnet URhGe. Experimental evidence for the coexistence of ferromagnetism and superconductivity is presented. In this superconductivity, the spin-triplet is the unique pairing category, because the spin-singlet state, in which opposite spin electrons are paired, is no longer energetically favorable, owing to the strong internal field. The key signature of spin-triplet superconductivity is a strong suppression of the superconducting critical temperature by magnetic/non-magnetic impurities. We present the impurity dependence of the critical temperature. The superconductivity is completely destroyed when the mean free path falls below the superconducting coherence length. We also report a search for new ferromagnetic superconductors.

L12
Superconductivity on the verge of Magnetism

A. Shick
Institute of Physics ASCR

The coexistence of superconductivity with magnetism has recently re-emerged as a central topic in condensed matter physics. I will discuss two U-based ferromagnetic superconductors UGe_2 and URhGe. The {it ab initio} relativistic electronic structure calculations reveal very unusual microscopic properties of these materials, in which the coexisting superconducting and ferromagnetic phases are formed by the same electrons.
The consistent picture of the magnetic properties and electronic structure of the UGe_2 will be shown to require inclusion of correlation effects beyond the local spin density approximation (LSDA). I will show that the "LSDA + Hubbard U" (LSDA+U) approach reproduces magnetic properties and yields the largest Fermi surface sheet of the Fermi surface, which is comprised primarily of spin majority states. This occurence and the quasi-two-dimensional geometry of the Fermi surface, support the likelihood of magnetically mediated p-wave triplet pairing in UGe_2.
The URhGe is very different. I will show that LSDA provides better description for magnetic ground state properties than LSDA+U. It will be also shown that the canted magnetic structure of URhGe can originate from non-collinear arrangement of U atom orbital magnetic moments, while the spin magnetic moments are ferromagnetically ordered. The Fermi surface analysis will be presented and the possibility for phonon-mediated s-wave superconductivity in URhGe will be discussed.

L13
Coexistence of ferromagnetism and superconductivity induced by the Hund's rule coupling

Jozef Spalek
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We discuss general implications of the local spin-triplet pairing among correlated fermions that is induced by the Hund's rule coupling in orbitally degenerate systems. The quasiparticle energies, the magnetic moment, and the supercinducting gap are determined for principal superconducting phases (A, A1). The phase diagram, as well as the evolution in an applied magnetic field near the Stoner

threshold is provided for a model two-band system. The appearance of the spin-polarized pin-triplet superconducting phase makes the Stoner threshold a hidden critical point.

L14
Metals near a magnetic instability

H. v. Löhneysen
Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany and
Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

The groundstate of a number of metals, notably those with strong electronic correlations such as heavy fermion systems or weak itinerant magnets, is in close proximity to a magnetic instability. The transition from a Pauli-paramagnetic to a magnetically ordered state can be tuned by chemical composition, pressure, or magnetic field. Often pronounced deviations from Fermi-liquid behavior are observed, which are commonly referred to as non-Fermi-liquid (NFL) behavior.
The scenario of incipient magnetic order is exemplified by $CeCu_6$ with a nonmagnetic groundstate, and long-range incommensurate antiferromagnetism in $CeCu_{6-x}Au_x$ for $x > x_c = 0.1$. The magnetic instability can be tuned by alloying or applying external pressure p. At the quantum critical point (QCP), where the Néel temperature T_N vanishes, the specific heat C varies as $C/T \sim a \ln(T/T_0)$, independent of whether T_N is tuned to zero by variation of x or p, and one observes a linear resistivity contribution $\Delta\rho \sim T$. These NFL features can be explained by quasi two-dimensional critical fluctuations, as observed for $x = 0.1$ with inelastic neutron scattering. In addition, unusual dynamic scaling laws are found in the vicinity of the QCP in $CeCu_{6-x}Au_x$ which are incompatible with simple spin-fluctuation scenarios.
Here we compare in detail the QCP tuned by alloying with new data for x = 0.2, inducing a magnetic instability by a magnetic field. The observation that in case the specific heat and the resistivity at the critical field can be described by the three-dimensional spin fluctuation the latter scenario finds its correspondence in Lorentzian quasi-elastic linewidths observed with inelastic neutron scattering.
The archetypal weak ferromagnet $ZrZn_2$ has long been considered a candidate for p-wave superconductivity if samples can be made sufficiently pure. We recently found evidence for superconductivity in $ZrZn_2$ single crystals of unpredicted purity. Surprisingly, super-conductivity (with $T_c \approx 0.3$ K) exists over the entire pressure range where ferromagnetism exists, and vanishes when ferromagnetism is suppressed at sufficiently high pressure.

L15
Field tuning into a heavy electron quantum critical point

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In $YbRh_2Si_2$ pronounced Non-Fermi liquid (NFL) effects are observed in thermodynamic, magnetic and transport properties above a weak antiferromagnetic (AF) phase transition at $T_N = 70$ mK. The AF order is suppressed to $T_N \rightarrow 0$ either by i) the application of small critical magnetic fields B_{c0} or ii) a slight expansion of the crystal lattice by substituting 5% of the Si atoms by Ge in $YbRh_2(Si_{1-x}Ge_x)_2$. In both cases the NFL behavior extends to lowest temperatures. For $B > B_{c0}$ (with $B_{c0} = 0$ for x=0.05) we observe a weakly polarized Landau FL at lowest temperatures which fulfills the Kadowaki-Woods relation $A/\gamma^2 = const$ between the coefficients A of the resistivity and γ of the specific heat. The $1/(B-B_{c0})$ divergence of A(B) indicates singular scattering at the whole Fermi surface and a divergence of the heavy quasiparticle mass at the quantum critical point.

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L16
Scaling of thermal parameters at the magnetic instability of Ce-systems

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The magnetic phase diagrams of Ce systems show instability regions where low energy excitations dominate the specific heat (C_{el}/T) and entropy (ΔS) temperature dependence, when the transition (T_N) is depressed by alloying (z) or pressure (p).
It is found that T_N (z,p) vanishes in different manners: i) by approaching a quantum critical point at $T_N \rightarrow 0$; ii) at finite temperature, and iii) with T_N being independent of z or p variation. We show that in each case C_{el} / T and ΔS are scaled by different dependencies on the two characteristic energies: ordering ($\sim T_N$) and/or 4f-band hybridization (T_0), which are driven by z and/or p in different forms.
Three cases are clearly identified: i) $C_{el}(z,p)/ T$ and ΔS scale with $\Delta T = T - T_N(z,p)$, being T_0 only system dependent); ii) there is a unique function for $C_{el} /T(T>T_N)$, independent of T_N and T_0(also only system dependent), and iii) where $\Delta S(T > T_N)$ is scaled by T/T_0, whereas T_N only depends on the system. We discuss and compare these three types of phase diagrams and the respective behaviours of T_N and T_0.

L17
Heavy-Fermion- and NFL-behaviour in $CeNi_9X_4$ (X=Ge, Si)

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The compounds $CeNi_9X_4$ (X = Ge, Si) have a tetragonal crystal structure (space group I4/mcm) that is derived from the cubic $NaZn_{13}$ structure type. In the case of $CeNi_9Si_4$ resistivity, magnetic susceptibility and specific heat measurements reveal Kondo-lattice behaviour with a T^2 temperature dependence of the electrical resistivity ($A \sim 0.01$ $\mu\Omega cm/K^2$) as well as a Sommerfeld value $\gamma = 160$ $mJ/molK^2$. The Kadowaki-Woods ratio $A/\gamma^2 \sim 0.4 \times 10^{-6}$ $\mu\Omega cm(molK/mJ)^2$ indicates weak RKKY coupling and a non-magnetic ground state. The magnetic contribution to the specific heat is well described by the Coqblin-Schrieffer model with an effective J=5/2 ground state and a characteristic temperature $T_0 \approx 180K$.
$CeNi_9Ge_4$ on the other hand, exhibits non-Fermi liquid (NFL) properties, i.e. an approximately logarithmic divergence of the low temperature heat capacity $C(T) \sim - T \ln T$ in the temperature range 80 - 1000 mK, indicating the proximity of a quantum critical point. Hydrostatic pressure and magnetic field recover the Fermi-liquid state. Furthermore, resistivity measurements down to 5 mK show a cross-over from a coherent to an incoherent regime at about 700 mK.

L18
On the Existence of Eu-Based Heavy Fermion Compounds

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Ternary Ce and Yb based intermetallic compounds exhibit a variety of interesting properties such as intermediate valence, Kondo effect, Non Fermi Liquid behavior, heavy fermion behavior, heavy fermion superconductivity etc. Most of these phenomena emerge since the 4f-level lies close to the fermi level which enhances the hybridization between the 4f-electrons and the conduction electrons in Ce and Yb compounds. Some of the Eu-based compounds show intermediate valence phenomena

which is a clear proof that the hybridization could be quite strong in Eu compounds as well. However, we do not find any Eu-based compounds exhibiting heavy fermion behavior in the literature. Our current research effort is directed towards finding Eu-based heavy fermion compounds. We have investigated polycrystalline samples of $EuCu_2(Ge_{1-x}Si_x)_2$, since this is an ideal system to tune the strength of hybridization using chemical pressure. $EuCu_2Ge_2$ shows AF transition with T_N ~14 K. With Si doping the T_N shows an enhancement, passes through a maximum before disappearing at the critical concentration $x_c = 0.65$. The resistivity behavior of samples with x =0.5 and x =0.6 are similar to those of Kondo lattice or heavy fermion antiferromagnet. For x =0.7, the magnetic order is suppressed and the sample shows evidence for moderate heavy fermion behavior ($\gamma \sim 200$ mJ/mol K^2) which is the first Eu-based heavy fermion compound. For $x \geq 0.75$, the magnetic properties are typical of the valence fluctuating compounds. A particularly interesting result is the coexistence of magnetic order and valence fluctuation in the sample with x = 0.6. The experimental results will be discussed in the light of existing theoretical work on the subject.

L19
Bulk Properties of Light Actinides: Modified Second Variation Method

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The second variation method is a common and efficient way of treating the spin-orbit coupling within electronic structure codes. While it works satisfactorily for most elements, it was demonstrated recently to be inadequate for light actinides. The problem was traced back to insufficient description of the 6p states, resulting in a poor convergence of the total energies with respect to the computational parameters. We present a simple way to overcome this deficiency and demonstrate its effect on the stability of the calculation. The results obtained for bulk properties of light actinides (Th-Pu) are compared to those obtained with methods using full Dirac formalism.

L20
Theoretical atomic volumes of the light actinides

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The uttermost importance of relativistic effects for the electronic structure of f-elements and -compounds is demonstrated on a number of examples. Most electronic structure schemes rely on approximativ treatments of relativity, e.g. on a basis constructed from spin eigenstates (second variation method). Recently, severe problems with this method regarding the calculation of atomic volumes for heavy elements were reported [1]. The relativistic FPLO-method solves the full 4-component Dirac equation [2], circumventing the mentioned approximation. Using this method atomic volumes and bulk moduli of all light actinides have been calculated. A critical comparison with data from the literature is given.

Reference:
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[2] I. Opahle, PhD thesis, TU Dresden, 2001.

L21
RIXS (Resonant inelastic X-ray scattering) of Uranium compounds

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In the design of nuclear waste final repository systems one includes many safety measures in order to insure stable long-term conditions in the vicinity of the spent fuel containers. For example,

effects of possible future penetration of ground water into the canister need to be studied in details in order to prevent possible leaching process. The Uranium in the waste comes as UO_2, which has low solubility in water. However, it is possible that some UO_2 can transform into UO_3 under certain conditions. UO_3 is a more soluble compound that can be leached out by groundwater. The presence of iron in the canister walls is expected this course of events. Details understanding of the mechanism involving uranium reactions is therefore important. For the study of these mechanisms we arrange model systems for different uranium compounds in contact with water and iron. The systems are studied by X-ray Absorption and Emission Spectroscopy. These include advances in experimental technique, using synchrotron radiation and theoretical methods, based of atomic multiplied calculations.

L22
Magnetic ordering in the $(U_{1-x}Np_x)_2Rh_2Sn$ system

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In the An_2T_2X family, the Rh compounds show singular exceptions to the general tendency. On one hand Np_2Rh_2Sn does not order magnetically [1] whereas the uranium counterpart U_2Rh_2Sn orders antiferromagnetically at 25K with a 5f moment $\mu_{ord} \approx 0.53\mu_B$ [2,3]. On the other hand, the U moment is oriented along the c-axis, in contradiction with the usual rule followed by all other U_2T_2X compounds and stating that the magnetic moment be perpendicular to the shortest U-U distance.
We have undertaken the investigation of the $(U_{1-x}Np_x)_2Rh_2Sn$ intermediate system by ^{237}Np Mössbauer spectroscopy and SQUID magnetization for $0<x<1$. It is inferred from the quadrupolar interaction parameter that the Np moments point in the direction of the main principal axis of the electric field gradient (EFG) for x=0.25 and they rotate of $\sim\pi/2$ as x increases to 0.75. If we assume that Np and U moments are aligned, it is deduced that i) the EFG main principal axis is oriented along the c-axis ii) the Np moment lie close to the basal plane for high x concentrations. The ordering temperature and the magnetic moment weaken as x increases and finally disappear for x = 0.9. The concomitant decrease of the isomer shift, affected by the delocalization of 5f electrons, points out the key role of hybridization in the magnetic properties of this system. These results are consistent with our magnetization measurements.
We can then suggest that the unusual orientation of U moments in U_2Rh_2Sn results in weaker 5f-ligand hybridization, allowing the occurrence of (weak) magnetic order in U_2Rh_2Sn whereas Np_2Rh_2Sn is near to a magnetic instability.

L23
Physics of the low-carrier system Ce-monopnictides

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The origin of the unusual magnetic properties of Ce-monopnictide, CeX (X=P,As,Sb,Bi), whose carrier density is very low, is discussed on the basis of the physical picture obtained from recent neutron and X-ray scattering experiments. It is revealed that the unusual properties of the compounds are characterized as the appearance of $\bullet_8$ like Ce ions with a large magnetic moment of about $2\bullet_B$ among Ce ions with $\bullet_7$ crystal field ground state. The $2\bullet_B$ Ce ions appear in the form of ferromagnetic sheets of (001) planes with various sequence of stacking sandwiching $\bullet_7$ Ce planes in the ordered state. The formation of the $2\bullet_B$ Ce in the $\bullet_7$ Ce lattice is ascribed to the combined effects of strong p-f mixing and carrier localization due to the low carrier density.

L24
Neutron scattering study of the magnetic response in YbB_{12} Kondo-insulator

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We report a neutron scattering study of the magnetic response in YbB_{12} and $Yb_{1-x}Lu_xB_{12}$ alloys at temperatures between 10 K and 200 K. Measurements were performed on several time-of-flight spectrometers providing a wide range of energies and resolutions. The crystal field (CF) parameters for Yb^{3+}have been obtained experimentally from measurements of the CF splitting of Er^{3+} ions introduced as impurities into the Yb sublattice.

At low temperature ($T \approx 15$ K), the magnetic excitation spectrum of YbB_{12} exhibits a spin gap with an energy of about 15 meV. At higher energies, the spectrum consists of two narrow peaks at 15 and 20 meV, and a broader one at 38 meV. With increasing temperature the spectral shape begins to transform already around 50 K. Above 100 K drastic changes are observed: *i*) the two peaks at lower energies transform to a single excitation at about 23 meV; *ii*) a sizable quasielastic signal develops in the gap and simultaneously the 38 meV peak seems to be suppressed. These transformations are ascribed to a crossover from the Kondo-insulator state to a single-ion regime of spin-fluctuations at higher temperatures. The high-resolution data unambiguously confirm that no intrinsic quasielastic magnetic scattering exists in YbB_{12} at low temperature, whereas a broad signal, with a width $\Gamma/2 \approx 10$ meV, appears for $T \geq 50$ K. This value of the width provides a microscopic estimate of the single-ion Kondo energy.

In the solid solutions, the breakdown of coherence on the Yb sublattice mainly results in a reduction of the of 15-20 meV structure in the low-temperature limit, but no filling of the gap at low temperature nor any sizeable change in the high-temperature spectral shape have been observed up to 25% Lu concentration. The CF parameters of YbB_{12} derived from the Er^{3+} excitation spectrum in $Er_{0.1}Yb_{0.9}B_{12}$ yield an estimate of the splitting of the Yb^{3+} ground state multiplet ($J = 7/2$) of about 10 meV, which is on the same order of magnitude as the spin-gap.

This suggests that CF effects could play a role in the unconventional magnetic response of YbB_{12}, which is not explained satisfactorily by existing Kondo-insulator models.

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L25
Multipolar ordering in NpO_2 below 25 K

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We report the results of Resonant X-ray Scattering experiments performed at the $M_{4,5}$ Np edges in NpO_2. Below T_0 = 25 K, the development of long-range order of Np electric quadrupoles is revealed by the growth of superlattice Bragg peaks at positions forbidden in the space group of the disordered phase. The electronic transition is not accompanied by crystallographic distortions, neither internal nor external, so the symmetry of the system remains cubic. The polarization and azimuthal angle dependence of the intensity of the resonant peaks is well reproduced assuming Templeton scattering from a triple-q longitudinal antiferro-quadrupolar structure. Electric quadrupole order in NpO_2 could be driven by the ordering at T_0 of magnetic octupoles of $\bullet_5$ symmetry, splitting the Np ground state quartet and leading to a singlet ground state with zero dipole magnetic moment.

L26
Crystal-field fluctuations for 4f ions in high-T_c cuprates

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Neutron spectroscopy of crystal field (CF) excitations for 4f ions in cuprates like $Y_{1-x}R_xBa_2Cu_3O_{6+y}$ represents one of the powerful tools to probe quasiparticle dynamics over a wide range of time scales. In particular, the CF lifetime measurements provide the information concerning the dynamic susceptibility at the frequency of the CF transition. Conventional approach to the interpretation of linewidth measurements in cuprates is based on the assumption of the predominant contribution of spin-fluctuations through the 4f-3d exchange interaction. This mechanism predicts the ratio of the effective matrix elements for the Stark transitions to be governed by the Lande factors as follows

$$\left|\frac{v_{ij}^{ex}(J)}{v_{ij}^{ex}(J')}\right| \cong \frac{(g_J - 1)}{(g_{J'} - 1)}$$

However, A. Mukherjee et al. [1] when studying the system $Y_{1-x}R_xBa_2Cu_3O_{6+y}$ (R=Er, Ho, Tm) found $\left|\frac{v_{ij}(\mathrm{Tm})}{v_{ij}(\mathrm{Ho})}\right| \cong 2$, instead of theoretically expected $\frac{(g_{\mathrm{Tm}} - 1)}{(g_{\mathrm{Ho}} - 1)} = \frac{2}{3}$, and $\left|\frac{v_{ij}(\mathrm{Tm})}{v_{ij}(\mathrm{Er})}\right| \cong 4.5$, instead of expected $\frac{(g_{\mathrm{Tm}} - 1)}{(g_{\mathrm{Er}} - 1)} = \frac{5}{6}$.

This clear disagreement evidences against exchange mechanism. We argue that the main contribution to the broadening of the linewidth of CF transitions for 4f ions in high-Tc cuprates results from the crystal-field fluctuations. Indeed, a simple assumption of the dominant contribution of the quadrupolar term (k=2) yields for the abovementioned ratio $\left|\frac{v_{ij}(\mathrm{Tm})}{v_{ij}(\mathrm{Ho})}\right| \cong \left|\frac{\alpha_{\mathrm{Tm}}}{\alpha_{\mathrm{Ho}}}\right|$ where α_R is the Stevens parametr. Expected ratios $\left|\frac{v_{ij}(\mathrm{Tm})}{v_{ij}(\mathrm{Ho})}\right| \cong 4.5$, and $\left|\frac{v_{ij}(\mathrm{Tm})}{v_{ij}(\mathrm{Er})}\right| \cong 4.0$ appear to agree with respective experimental values. Thus, we conclude that the crystal-field fluctuations induced by the charge and/or orbital fluctuations in copper-oxygen subsystem may be the main origin of the broadening of the linewidth of CF transitions for 4f ions in high-Tc cuprates.

References:
[1] A. Mukherjee, A.T.Boothroyd, D.McK.Paul et al., Phys. Rev. B **49**, 13089 (1994).

L27
Band anisotropy of rare-earth--transition-metal compounds: theory

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The band contribution to the magnetocrystalline anisotropy energy (MAE) of RCo_5 (R = Y, La, Pr, Nd, Sm, Gd) and Y_2T_{17} (T = Fe, Co) has been calculated within the local spin density approximation with orbital polarization corrections. The dependence of MAE on lattice geometry and composition is discussed and compared with available experimental data. We disprove the frequently assumed independence of the band contribution to MAE on the rare earth constituent.

L28
Spontaneous magnetoelastic effects in Gadolinium compounds

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The spontaneous magnetoelastic effects in Gd compounds are reviewed showing that the strain dependence of the magnetic two ion exchange interactions leads to significant effects. These effects are equal in magnitude to well established single ion contributions in other rare earth compounds with non vanishing orbital momentum (coming from the strain dependence of the crystal field). In some cases the exchange contribution can produce giant magnetostriction (GMS) or induce structural phase transitions. In order to extract the influence of the Gd-Gd exchange interactions, we consider only Gd compounds with partner elements showing no or only weak induced magnetic moments.The current status of the theory is presented and compared to measurements performed by temperature dependent x-ray diffraction and results of dilatometric measurements.

L29
Disorder and low temperature effects in $CeNi_{1-x}Cu_x$

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We will discuss the magnetic and the transport properties of the system at very low temperatures down to 100 mK, by means of specific heat, magnetization and muon spectroscopy. we discuss the adequate scenario to understand this system , where localized magnetic moments appears at least from x=1 to x=0.2. The existence of magnetic clusters, which give rise to "cluster glass" behavior or to long range magnetic structures, originates peculiar histeresis loops or specific heat temperature dependences. Muon spectroscopy give us indications about the nature of these magnetic clusters. The effect of thermal treatments on the magnetic properties are also analyzed. The evanescence of localized magnetic moments occurs close to the x=0.1 composition.

L30

Influence of the Kondo effect on the Ce-ordered magnetic moment existing in the compounds rich in germanium (≥50% at.) of the Ce-Ni-Ge system

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The magnetic properties of $RE_xT_yX_z$ intermetallic compounds, with RE = Rare Earth or Actinide, T = 3d, 4d or 5d transition metal and X = Si, Ge or Sn result from the interactions between the localized f electrons and the conduction electrons (competition between the demagnetising Kondo and the magnetic RKKY interactions). During the last decade, a lot of series of compounds were studied, like ternary compounds of type RET_2X_2, to show the influence of each atomic element on the various physical properties. En route to more systematic investigations, we have studied the Ce-Ni-Ge system (where 20 ternary compounds were taken in evidence [1]) in order to determine the influence of chemical composition on the Ce-ground states. At our knowledge, this study is the first realised in a same phase diagram.

L31

5f electron localization-delocalization transition from UPd_3 to UPt_3.

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The electronic structures of URh_3, UPd_3, UPt_3 and UAu_3 are calculated with the self-interaction-corrected local-spin-density approximation. We find that only in URh_3 the f-electrons are fully delocalized. UPt_3 has one f-electron localized at each U site, whilst a localized f^2 configuration of the U-ion is found for UPd_3. It is predicted that upon application of pressure, UPd_3 will acquire the f^1 configuration and possibly exhibit heavy-fermion behaviour. We find that UAu_3 is characterized by the same mixed localized-delocalized f-electron manifold as UPd_3.

L32

The dual nature of 5f states and heavy quasiparticles in UPt_3

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We propose a microscopic description of heavy quasiparticles in U-based compounds. It is based on the assumption that some of the 5f states may be itinerant while others remain localized. Band-structure calculations based on this assumption reproduce the observed deHaas-vanAlphen frequencies of UPt_3 very well. The observed enhancement of the quasiparticle effective masses over the band mass results from the local Coulomb interaction of the itinerant f-states with their localized counterparts.

The theory reproduces the observed deHaas-vanAlphen cross sections and effective masses very well. We discuss various microscopic mechanisms which may lead to the partial localisation of the 5f states in actinide compounds.

L33
Two-phase separation in URu_2Si_2 studied by microscopic measurements under hydrostatic pressure and uniaxial stress

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The heavy-fermion superconductor URu_2Si_2 ($T_c \sim 1.2$ K) shows at $T_o = 17.5$ K a phase transition which has been attributed to antiferromagnetic (AF) order with a saturation moment of $\sim 0.03\ \mu_B$/U. However, so small a value cannot simply be reconciled with large anomalies observed at T_o in various thermodynamic quantities. Moreover, the staggered internal fields corresponding to the AF order have never been detected by NMR. In this contribution, we report our recent investigations on this puzzling phase, on the basis of neutron scattering, NMR and μSR measurements performed under hydrostatic pressure and uniaxial stress. We show that the small staggered moment is ascribed to a small volume fraction of the AF order with a normal size ($\sim 0.25\ \mu_B$/U) of the saturation moment, which spatially competes with some different "hidden order parameter". The *5f* electronic states that may lead to the two order parameters are also discussed.

L34
The concept of a dynamical phase in magnetic order: implications for URu_2Si_2

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The non Fermi liquid state, where the thermodynamic properties of the metals are non longer describable in terms of quasiparticle exciations in the sense of Landau Fermi liquid theory, has attracted considerable theorectical and experimental attention over the past decade. An alternative perspective, based on the concept of dynamical heterogeneities will be discussed. This suggests an empirical way to define a 'Non fermi liquid' parameter which may be of use in mapping out phase diagrams and an analysis of inelastic neutron scattering and thermodynamic data to be carried out within a self consistent framework.

L35
Hidden orbital order in the heavy fermion metal URu_2Si_2

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When matter is cooled from high temperatures, collective instabilities develop among its constituent particles that lead to new kinds of order. An anomaly in the specific heat is a classic signature of this phenomenon. Usually the associated order is easily identified, but sometimes its nature remains elusive. The heavy fermion metal URu_2Si_2 is one such example, where the order responsible for the sharp specific heat anomaly at $T_0 = 17$ K has remained unidentified despite more than seventeen years of effort. In URu_2Si_2, the coexistence of large electron-electron repulsion and antiferromagnetic fluctuations leads to an almost incompressible heavy electron fluid, where anisotropically paired quasiparticle states are energetically favoured. Here we develop a proposal for the nature of the hidden order in URu_2Si_2. We show that incommensurate orbital antiferromagnetism, associated with circulating currents between the uranium ions, can account for the local fields and entropy loss observed at the 17 K transition. We make detailed predictions for the outcome of neutron scattering measurements based on this proposal, so that it can be tested experimentally.

L36
Studies of magnetic orders under very high pressures

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Sign and values of exchange interactions, electronic band structure, and crystal field splitting are the basic parameters of any magnetic or strongly correlated electronic system. All these parameters are very sensitive to interatomic distances. Experiments under applied pressures is the only way to vary interatomic distances in a controlled way without changing chemical composition. High-pressure studies offer unique opportunities to test microscopic models and to search for new, highly exotic magnetic phenomena.We describe recent developments for magnetic neutron diffraction under very high pressures. Neutron diffraction is the most suitable tool to study spin arrangements. Progress in neutron and high pressure techniques allowed us to reach pressures up to 50 GPa, by 1-2 orders of magnitude higher than in previous neutron works. We give an overview of our recent high-pressure results. In rare - earth chalcogenides we observed a "resonant" ferromagnetic exchange induced by pressure. In frustrated Laves phases RMn_2 (R=Gd, Ho, Tb) we found new pressure induced magnetic phases and unusual "short range order - long range order" magnetic transitions. At the end, we discuss prospects for magnetic studies in Mbar pressure range.

L37
Anomalous behaviors in f -electron systems studied by uniaxial pressure experiments

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Heavy-Fermion metamagnetism, anomalous phase transition of non magnetic origin, Non Fermi liquid like anomaly, etc., are attractive problems in f electron systems. The hybridization between conduction and f –electrons including its anisotropy in that hybridization and the crystal electric field (CEF) level scheme play the key roles in all these problems. Uniaxial pressure experiments have a potential in studying the anisotropy in hybridization and the effect of crystal symmetry breaking. We have studied anisotropy on some unique systems under uniaxial pressure (Pu). Anisotropic effect of Pu has been observed on a metamagnetic anomaly (MA) in $CeRu_2Si_2$. It reveals an increase (decrease) in the 4d-4f hybridization which can be explained by the decrease (increase) of the nearest Ce-Ru distance by Pu along c-axis (a-axis). We have observed a sign that the anisotropic nature of hybridization, which is believed to play an important role in the MA, can be controlled by Pu. The filled skutterudite compounds ($RETr_4Pn_{12}$: RE= rare earth, Tr= Fe, Ru, Os, and P= pnictogen) which exhibit a variety of novel phenomena and a potential for thermoelectric application for the next generation, have been studying by Pu. Very anisotropic effect of Pu has been observed in new Pr-based heavy Fermion $PrFe_4P_{12}$. It is originated partly from the effect of symmetry breaking on the non magnetic ground state responsible for quadrupole interactions, which is believed to play an important role in the anomalous behaviors. In the anomalous heavy Fermion semimetal $CeRu_4Sb_{12}$, the change in the frequency of the Shubnikov-de Hass oscillations have been observed under Pu, indicating the elongation of the Fermi surface parallel to Pu.

L38

Pressure effects on the magnetic character of $TbM_{1-x}Cu_x$ (M= Pt & Ni)

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High pressure and controlled chemical substitution studies become complementary methods in the understanding of the basic magnetic interactions in solids. They provide a powerful tool for giving new insights to former theoretical magnetic models by establishing the influence of electronic and crystalline variations on the magnetic order of such compounds. In this work, we present the neutron diffraction studies under pressure up to 65 kbar on the series $TbPt_{1-x}Cu_x$ and $TbNi_{1-x}Cu_x$. At ambient pressure, a change from a ferromagnetic behavior to an antiferromagnetic one induced by increasing Cu concentration can be observed in both systems, while there is no volume variation in the Pt-based series and with a change of 4% in the Ni-based one. For those compounds with lower Cu contents non collinear ferromagnetic structures were determined (-CxFz for the Pt-based series and FxCz for the Ni one), whereas incommensurate magnetic structures appeared for Cu concentrations higher than 35%. We found that the applied pressure favours antiferromagnetism in both series by inducing an inner moment reorganisation. In this sense, the antiferromagnetic component of the non-collinear ferromagnetic structures is enhanced with pressure. In addition, in the antiferromagnetic compounds the strong decrease of the intensity of the first peak in the diffraction pattern associated to the incommensurate structures seems to indicate an evolution to a pure antiferromagnetic phase in the cell.

L39

Magnetic phase transitions of $R\text{-}Cu_2$ compounds in high magnetic fields

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Some of the RCu_2 compounds (R = Ce,Pr,Tb,Dy) with an easy a-axis show an irreversible change of the easy magnetization axis into the c-direction in high magnetic fields. This metamagnetic "axis conversion" is caused by a strong magnetoelastic coupling in the ac-plane. It is accompanied by giant magnetostriction effects in the order of some percent. With $NdCu_2$ a similar magnetic behaviour was found for the first time in a system with an easy axis perpendicular to the ac-plane. Magnetization measurements were carried out in pulsed fields up to 50 T. The results give an evidence that the conversion is caused by an effective quadrupolar coupling as in the other RCu_2 compounds. The experiments were extended to $SmCu_2$ which shows magnetic phase transitions above 20 T.

L40

From multiple-scattering theory to orbitals (NMTOs); applications to magnesiumdiboride and high-temperature superconductors.

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In order to compute and describe the electronic structure and properties of solids, one often starts by solving Schroedinger's equation for a single electron in a potential given by some approximation to density-functional theory. For systems containing d- and in particular f-electrons, pseudopotentials and plane-waves are not useful. LCAO methods are useful, but not intelligible, first of all because the atoms are characterised by a wealth of one, two, and three-centre integrals and, secondly, because accurate basis sets need many atomic orbitals, often with more than one radial quantum number. The tight-binding (TB) method in its two-centre, orthogonal form is intelligible, and it

forms the single-electron part of the Hubbard-type Hamiltonians traditionally used to describe correlated d and f-electron systems. But it is an empirial method. This talk describes progress towards deriving a first-principles tight-binding theory, specifically in deriving low-energy basis sets (Wannier-like functions) from scattering theory.

Since the potential is approximately spherically symmetric near the atoms and flat in between – a muffin-tin (MT) potential – the one-electron problem can be formulated elegantly in partial-wave representation as one of selfconsistent multiple scattering. This was done by Korringa, Kohn and Rostoker more than fifty years ago. This KKR formalism has two-centre form and is expressed solely in terms of the phase-shifts of the individual atoms (the MT-wells) and a structure matrix, both of which are functions of energy, but otherwise independent. Since only channels with non-zero phase shifts enter the formalism, matrix dimensions are small. Moreover, it is a Green's-function formalism, well suited for – and extensively used in – ab initio computations for crystals with localized defects and alloys with coherent-potential type approximations. However, the partial waves – and, hence, the structure matrix – have long range and violent energy dependencies. This, not only makes the formalism un-intelligible, but also prevents applications to extended defects and topologically disordered systems. This was remedied thirty years ago by the atomic spheres approximation (ASA), which simply sets the kinetic energy in the interstitial to zero and substitutes the MT-spheres by "space-filling" atomic spheres. For use in variational calculations, correct to linear order in energy around some chosen energy point, a set of linear muffin-tin orbitals (LMTOs) were derived from the the partials waves and their first energy derivatives. Having zero kinetic energy, the LMTO envelopes behave like multipole potentials, and it was realized that, through screening transformations, one can form superpositions with short range, so-called TB-LMTOs. These have become popular for treating d- and f-electron systems, in particular with SIC, LDA+U, and DMFT-functionals.

Ten years ago, multiple-scattering theory was proved to hold also for overlapping spherically-symmetric potential wells, to first order in the potential overlap. This is important for practical applications because, except for close-packed systems, the MT-approximation is insufficient for the potential. Secondly, screening transformations which work also for positive kinetic energies, below a certain limit, were found. These two results made the ASA unnecessary and screened multiple-scattering theory useful and intelligible, because limiting the range of the partial waves reduces their energy dependence, and because one may "downfold" unwanted partial waves into the tails of the remaining partial waves, by choosing a screening transformation in which the screened phase shifts vanish for the downfolded channels. Thirdly, it was shown how from the partial waves evaluated at a mesh of N+1 energies one can derive a set of orbitals (NMTOs), which spans the exact solutions of Schroedingers equation at the energies of the mesh. This is polynomial approximation generalized to basis sets. The NMTO Hamiltonian and overlap matrices are expressed solely in terms of the KKR matrix (or its inverse, the scattering path matrix) and its first energy derivative evaluated at the mesh points. The size of the basis depends on the degree of downfolding, but not on N. This allows one to construct minimal basis sets for specified regions of energy, e.g. for merely the occupied states of band insulators (Wannier functions) and the conduction-band orbital(s) for metals.

This will be illustrated by applications to two novel superconductors: magnesium diboride and the class of high-temperature superconducting cuprates. That will constitute the main part of the talk.

L41
Unconventional superconductivity in UPd_2Al_3 from realistic selfconsistent calculations

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We report realistic selfconsistent calculations of unconventional superconductivity in the heavy-fermion material UPd_2Al_3. Our calculations for UPd_2Al_3 start from accurate energy band dispersions that are computed within the local spin-density functional theory and that provide Fermi surfaces in agreement with experiment. Using physically motivated, realistic pairing potentials and a simplified version of the multiband gap equation, we find that the superconducting gap has two lines of nodes around the *z*-axis. Thus, the order parameter exhibits *d*-wave symmetry in the A_{1g}-representation of the hexagonal (D_{6h}) group, which is in agreement with experimental observations. Our result suggests that in a superconductor with gap nodes the prevailing symmetry is dictated by the constraint that nodes must be as far as possible from high-density areas.

L42
Role of orbital fluctuations for unconventional superconductivity in f-electron systems

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In order to describe the low-energy excitations for f-electron systems, we construct an orbitally degenerate Hubbard model by combining the band-structure calculation and the tight-binding method. Based on this model, we elucidate the mechanism of superconductivity in $CeTIn_5$ (T=Ir, Rh, and Co), by emphasizing that orbital fluctuations control the appearance of unconventional superconductivity induced by spin fluctuations. We further attempt to discuss superconductivity in uranium compounds from the viewpoint of competition and cooperation among spin and orbital fluctuations.

L43
Effect of paramagnetic fluctuations on superconductivity in $CeCoIn_5$

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The recently discovered and studied family of materials $Ce(Co,Rh,Ir)In_5$ are the layered version of $CeIn_3$, can be made very clean, and show both superconductivity and magnetism of various kinds. For these reasons, they can help us understand the cuprates, but they are interesting in their own right. Of these, $CeCoIn_5$ has the highest superconducting transition temperature Tc of all the heavy-fermion materials to date, 2.3K, which can be raised to 2.6K by applying the hydrostatic pressure of 15kbar. At Tc=2.3, the jump in the specific-heat coefficient is three times bigger than the BCS value of 1.4, and it decreases as Tc is increased. We propose that the big jump is caused by coupling of superconductivity to paramagnetic fluctuations. We model $CeCoIn_5$ by a Ginsburg-Landau functional with superconductivity, magnetization, and coupling between them, all of the simplest possible form. We find that due to this coupling, Tc is suppressed and the jump is increased. Further, quenching the fluctuations monotonically increases Tc, and, for strong enough coupling, decreases the value of the jump.

L44
Phase Diagrams of $CeMIn_5$ heavy-fermion superconductors (M=Rh, Ir and Co)

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We discuss detailed phase diagrams for the new family of heavy fermions superconductors $CeMIn_5$ (M=Rh, Ir and Co) constructed as a function of doping and hydrostatic pressure. Alloying studies in $Ce(Rh,Ir,Co)In_5$ reveal superconductivity(SC) ($T_c \cong 2.3$ K) over a wide range of compositions, which coexists with a magnetically ordered state with $T_N \cong 4$ K for $CeRh_{1-x}(Co, Ir)_xIn_5$ ($0.30 \leq x \leq 0.6$).

For $CeRh_{1-x}Ir_xIn_5$ in high magnetic fields and $CeCoIn_5$ under pressure we find evidence that the unconventional superconductivity in these compounds develops out of a non-Fermi-Liquid normal state in the vicinity of a T = 0 antiferromagnetic transition where quantum critical fluctuations control the physical properties. Further, temperature-pressure phase diagrams for $CeCoIn_5$ and $CeRhIn_5$ reveal remarkable similarity to the phase diagram of the cuprates.

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P1
Neutron experiments under very high pressures and low temperatures Recent developments at LLB

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We review high-pressure facilities installed on the ORPHEE reactor of the Laboratoire Léon Brillouin (LLB). We focus on magnetic neutron diffraction under very high pressures.
Powdered samples with magnetic moments >1 μ_B are routinely studied in the pressure range P<10 GPa and the temperature range 1.4<T<300 K using a specialized high-pressure powder diffractometer G6.1 "MICRO" and pressure cells with sapphire and diamond anvils. Even higher pressures (up to 50 GPa) could be reached on systems having large magnetic moments (>4 μ_B), though these experiments require longer counting time. In the recent future we expect to increase the available pressure range by implementing a new neutron multidetector, now under tests at the LLB.
Single crystal measurements are performed on a lifting-counter diffractometer 6T2 uder pressures up to 7 GPa. The diffractometer and the pressure cells are compatible with dilution refrigerator and cryomagnet, providing unique range of thermodynamical parameters P=7 GPa, T=0.1 K and H=7.5 T.
The above facilities are available for external research groups. Details about proposal submission could be found on the LLB web-site: www.llb-cea.fr.

P2
High-magnetic-field and neutron-diffraction studies on strongly-correlated-electron systems under multi-extreme conditions

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Driving thermodynamical parameters, like temperature, external pressure and applied magnetic field, to extreme values can induce unusual magnetic properties in systems with strong electron correlations. At the Pulse Field Facility, NHMFL, Los Alamos, and at the Los Alamos Neutron Science Center, we are developing a complementary program for doing high-magnetic-field and neutron-scattering studies under multi-extreme sample-environment conditions, which will provide further insight into the nature of magnetism in strongly-correlated-electron systems. For example, the configuration of magnetic moments can be perturbed by the application of sufficiently high pressures or high magnetic fields, where different dependencies allows separating direct and indirect exchange interactions as well as contributions due to coherence, Zeeman and crystal-field terms. I will discuss some of the technological challenges and the scientific opportunities for studying such systems under multi-extreme conditions.

P3
HMI - present and future research possibilities

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The Hahn-Meitner Institute (HMI) is a scientific research institute, which focuses on two main areas of work: structural and solar energy research. Around 40% of the 800 employees are scientists, mostly physicists and chemists.

The research reactor BER II is a source of neutron beams for structural and materials research. The experiments with the reactor are co-ordinated by the Berlin Centre for Neutron Scattering, BENSC, in the HMI. Around 400 visiting scientists use approximately 70% of the measuring time on the reactor every year. The NAA-Laboratory is available for the analysis of chemical elements with neutrons. BENSC is the most modern running neutron research facility in Germany and it is the world leader in neutron scattering work in magnetic fields - it offers continuous high magnetic field environments of up to 17 Tesla. Recently, the HMI has put a proposal forward to expand its capabilities by constructing a dedicated Neutron Magnetic Field Laboratory providing 30-40 Tesla for the neutron scattering .
The accelerators in the Ion Beam Laboratory, ISL, generate high energy ion beams. The surfaces and internal structures of solid matter can be analysed and changed in a targeted manner using ion beams. Furthermore, there is a radiation therapy unit for the treatment of eye tumors with fast protons. The solar energy research of the Institute focuses on the principles of innovative solar cells and electrochemical energy accumulators. In this field the Institute works within the German Solar Energy Research Alliance (FVS) with seven German scientific institutions. The HMI is also making increased use of the synchrotron radiation of the electron storage ring BESSY in Berlin-Adlershof. The combination of neutron and ion radiation with the synchrotron radiation of BESSY offers unique opportunities for the analysis of the structure of solid matter.

P4
The Actinide User Laboratory at ITU-Karlsruhe

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The interest in actinide materials arises mainly from their fundamental physics and chemistry and the complexity of their behaviour as illustrated through numerous papers of this conference. Such research also impacts on nuclear fuel technology and the problem of nuclear waste and long-term storage.
Despite the great interest in the actinides the number of Laboratories equipped to handle these materials is steadily decreasing due to heavy and costly security requirements. The Institute for Transuranium Elements (ITU) is a Laboratory of the Joint Research Centre of the European Commission which addresses a large number of questions related to actinides, both basic and applied and is the *only* non-classified Laboratory in Europe where research on appreciable quantities of transuranium materials is conducted across a wide range of chemistry and physics.
In order to keep alive an essential and exciting field of research in physic and chemistry, we have decided to offer access to our facilities to external users through an Actinide User Laboratory [1]. Materials preparation facilities and a suite of instruments, together with expert technical assistance, are available for conducting basic or applied research studies.
The Actinide User Laboratory is selected as a user facility to participate in the **European Community-Access to Research Infrastructures action** of the **Improving Human Potential Programme (IHP)** [2] which supports access to our actinide facility for the selected users teams, travel and subsistence fees of visiting scientists. The programme is opened to EC users and to scientists of the associated states.
Further information on this programme can be found on our website [1] or contacting the authors at actuslab@itu.fzk.de
References:
[1] Website at http://itu.jrc.cec.eu.int
[2] see http://www.cordis.lu/improving/infrastructure/home.htm

P5
Calculated structural stabilities of U, Np, Pu and Am; new high-pressure phases for Am and Pu

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The high pressure phase of americium Am IV recently found experimentally, which is a primitive-orthorhombic structure with four atoms in the unit cell, is also found to be stable theoretically at high

pressure in Am by a calculation using the full potential linearized augmented plane wave (FPLAPW) method. The possibility of the Am IV structure being a stable high-pressure phase of U, Np or Pu, like in the case of Am, is examined using the FPLAPW method by comparing the total energy as a function of volume with ten other crystal structures. The results indicate that the Am IV structure is not a high pressure phase for U and Np but it is for Pu, for which it is proposed that the sequence under pressure is •-Pu • Am IV • body-centred cubic. Our calculations are reliable because they give theoretically the stability of the crystal •-phases of U, Np, Pu under ambient conditions. The normal pressure phase of Am is modeled by our fully relativistic muffin-tin orbital method with unhybridized 5f electron states.

P6
Computer calculations of the fine electronic structure and properties of 4*f*/5*f* -electron compounds

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We would like to demonstrate the abilities of our calculation package BIREC 1.5 (Basic Interactions in Rare Earth Compounds), that has been developed in Center for Solid State Physics. This program allows to calculate many of magnetic and electronic properties of compounds containing rare-earth atoms. The main assumption of the used approach is the fundamental role of the local symmetry of the environment of the paramagnetic ion in the crystal, taken into account by using the Crystal Electric Field (CEF) formalism. The package allows to obtain the discrete (fine) electronic structure of RE-ions which determines magnetic and electronic properties of the whole compound e.g. the specific heat and the magnetic entropy, the magnetic moment and its behavior in external magnetic fields, the magnetic susceptibility and its anisotropy, the probability of inelastic-neutron-scattering transitions, the spin and orbital moments of the RE ions and many more.
Program BIREC allows calculations of magnetic and electronic properties of compounds containing rare-earth atoms, both in inter-metallic and ionic compounds.

P7
Ab initio studies of actinide species

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1. Theoretical evidence for substantial π bonding in UF_6 molecule is found. Short U-F distances, shape of molecular orbitals and calculated natural bond orbital populations suggest that bond order in UF_6 is 1.5 and also explains well-known stability of the U-F bond in uranium species.
2. The bonding trends among the naked, triatomic $[OAnO]^{q+}$ groups or the oxyfluorides $[AnO_n F_m]^q$ with f^0 configurations are studied by fully relativistic Dirac-Fock and quasirelativistic pseudopotential methods. The triatomic f^0 series is suggested to range from the bent ThO_2 via the linear $OPaO^+$ to at least NpO_2^{3+}, a possible new gas-phase species [1]. Several novel actinide oxyuoride species are predicted. The neutral ones include the experimentally so far unknown NpO_2F_3 and PuO_2F_4 [1]. Some experimentally known species such as NpO_3F and Pu(VI) oxyfluoride species are characterized for the first time by means of the calculated structure and vibrational spectra [1]. The participation of $5f\varnothing$ orbital in equatorial bonding of actinyls is studied [1]. For $UO_2F_3^-$, $UO_2F_4^{2-}$, NpO_2F_3, $NpO_2F_4^{2-}$, and $NpO_2F_5^{2-}$ the $5f\varnothing_U$-$2p_F$ overlap populations are 0.11, 0.03, 0.16, 0.24, and 0.21, respectively.
3. Possible candidates for Pu(VIII) species are studied theoretically. The $PuF_8(O_h)$, $PuO_2F_4(D_{4h})$, and $PuO_4(D_{4h})$ gas-phase systems are found to be true minima lying 1243, 514 and 274kJ/mol above the experimentally known gas-phase $PuF_6 + O_2 + F_2$ [1]. The $PuO_4(D_{4h})$ has been claimed experimentally [2].
4. The high-energy UO_6 system is studied as a possible candidate for the exotic U(XII) oxidation state [3].
5. The theoretically predicted π-electron-rich N_n rings such as N_7^{3-} [4], N_6^{4-} and N_3^{3-} [5] show strong multiple $\bullet^n$ bonding to actinide elements. The predicted Th($\bullet^6$-N_6) (C_{6v}) system is a true minimum and lies 73kcal/mol above Th U($\bullet^3$-N_3)$_2$ sandwich lies at about 80kcal/mol above the known NUN and $2N_2$

molecules and is D_{3h} system at minimum.

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P8
Ga NMR/NQR Study of $UTGa_5$ (T = Pt, Ni)

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$UPtGa_5$ and $UNiGa_5$ are 5*f*- itinerant antiferromagnets with Neel temperatures T_N = 26 K (Pt), 86 K (Ni) and electronic specific heat coefficients γ = 57 mJ/mol K^2 (Pt), 30 mJ/mol K^2 (Ni). Remarkably, recent neutron scattering experiments reveal that $UPtGa_5$ and $UNiGa_5$ have rather different magnetic structures below T_N. From the viewpoint of electronic structure, the difference in magnetic structure is somewhat surprising, since the two compounds show almost identical Fermi surface properties in the paramagnetic state. To elucidate the magnetism of $UTGa_5$, we have performed ^{69,71}Ga-NMR/NQR studies on $UPtGa_5$.
From the NMR spectrum in the paramagnetic temperature region, the hyperfine coupling constants $A_{hf,para}$ in the paramagnetic state have been evaluated for Ga(1) and Ga(2). The zero-applied-field NMR spectrum in the antiferromagnetic temperature region can be satisfactorily explained as ^{69,71}Ga nuclear resonances for the Ga(1) and Ga(2) sites which reflect an internal Zeeman interaction along with the electric quadrupole interaction. For Ga(2), the magnitude of the transferred field has been evaluated from the spectrum, yielding a value for the hyperfine coupling constant $A_{hf,AF}$ in the antiferromagnetic state. The estimated value of $A_{hf,AF}$ is an order of magnitude larger than that of $A_{hf,para}$. This implies either the existence of a strong hyperfine interaction path through the $PtGa_2$ layer or a major change in the hyperfine couplings at T_N. The mechanism of the hyperfine interaction will be discussed in terms of RKKY interactions.

P9
LDA+U calculations of the electronic structure of UPd_3 and URh_3

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A modified version of the LDA+U method which takes into account that in the presence of strong spin-orbit coupling the occupation matrix of localized electrons is not diagonal in spin indexes is used to study the electronic structure of UPd_3. In agreement with the experimental data LDA+U calculations result in a solution with two localised U 5f electrons which are placed at about 1 eV below the Fermi level which seems to be consistent with the recent ARPES measurements. The LDA+U band structure is compared to the band structure of $ThPd_3$ and it is found that the main features of the angular dependence of the dHvA frequency in UPd_3 can be reproduced using the bands calculated for $ThPd_3$. In order to check the ability of the LDA+U to correctly predict the localisation of U 5f electrons we also performed calculations for URh_3 in which 5f electrons are known to be delocalised and found no solution with localized f electrons.

P10
Magnetism in URhSi

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A single crystal of URhSi has been grown and subsequently investigated by magnetization, electrical resistivity, specific heat and neutron-diffraction measurements. The neutron-diffraction experiment confirms

that URhSi crystallizes in the orthorhombic TiNiSi-type of structure. All low-temperature experimental data point to ferromagnetic order in URhSi below 10.5 K. Similar to previous powder neutron-diffraction experiments, our single-crystal data are consistent with a collinear ferromagnetic ordering of U moments of 0.6 ± 0.1 μ_B/U oriented along the crystallographic *c*-axis. No superconductivity has been detected at temperatures down to 50 mK. However, high magnetoresistance effect is found around the magnetic phase transition.

P11
Magnetization densities in UPtAl studied by polarized neutron diffraction

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UPtAl orders ferromagnetically below 43 K. We present results of a polarised neutron diffraction experiment. The data were analyzed by two different approaches, which both try to fit the experimental flipping ratios. The maximum entropy method assumes nothing on the magnetization distribution whereas the other is based on the atomic model and on the assumption that magnetic moments are carried by certain atomic sites. Our results reveal that the ratio between the orbital and spin uranium moment ($\mu_L \approx 2.7\ \mu_B$, $\mu_S \approx 1.5\ \mu_B$, $-\mu_L/\mu_S \approx 1.80$) is reduced compared to the U^{3+} free-ion value of 2.57, indicating delocalisation of the *5f* - electron states. In adition to the main uranium moments, we observe magnetic moments induced on the Pt sites and in the interstitial region.

P12
Effect of magnetic field and pressure on $U(Ni_{1-x}Pd_x)_2Si_2$ single crystals

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Single crystals of $U(Ni_{1-x}Pd_x)_2Si_2$ for $x = 0.05$, 0.10 and 0.15 have been grown. Magnetization and electrical resistivity measurements were performed in a wide range of temperatures, magnetic fields and high pressures in order to study stability of magnetic phases in the solid solutions between UNi_2Si_2 and UPd_2Si_2 with a special emphasis on the type of ground state. In UPd_2Si_2 the simple AFI-type antiferromagnetic structure of U moments is observed at low temperatures. UNi_2Si_2 adopts the uncompensated AF structure (UAF) with the $++-$ stacking of U moments along the *c*-axis and consequently this compound exhibits a spontaneous magnetization corresponding to 1/3 of the U moment.
The substitution of Pd for Ni leads to a rapid decay of the spontaneous magnetization. The evolution of magnetization and electrical resistivity behavior with Pd doping is tentatively attributed to the coexistence of the AF-I and UAF phases in the ground state of $U(Ni_{0.9}Pd_{0.1})_2Si_2$ and $U(Ni_{0.85}Pd_{0.15})_2Si_2$. In this scenario, the volume fraction of the AF-I phase rapidly grows with Pd doping on account of the UAF. At lowest temperatures an irreversible metamagnetic transition to the UAF phase is observed when a sufficiently high magnetic field is applied along the *c*-axis. The electrical resistance of $U(Ni_{1-x}Pd_x)_2Si_2$ (x=0.10) has also been measured under high pressure. At 0.7 GPa, the onset of anomaly in the electrical resistivity has been detected, which is attributed to the increase of the volume fraction of UAF in the ground state phase.

P13
Noncollinear magnetism on the U_2T_2In, T=Ni, Pd series: ab-initio calculations

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The U_2T_2In (T=Ni,Pd,Pt) series form in a tetragonal crystal structure. The symmetry of these compounds permits several magnetic structures; according to neutron diffraction experiments [1], different, noncollinear, magnetic structures have been determined for the Ni, Pd and Pt compounds. In order to clarify the origin of these differences we have performed ab-initio calculations for these three compounds for the different structures involved. We present a comparison of the magnetic moments and energies across the system.

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P14
EXAFS Investigation of structural anomalies in US-LaS system at the U L_3 and at the La K edge.

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We report EXAFS measurements performed at the La K-edge and the U L_3 edge of eleven powder samples in the system $U_xLa_{1-x}S$. Our experiments revealed a complex local variation of the first neighbours distances, with the La-S distances d_{LaS} systematically longer than the U-S distances d_{US} and almost concentration independent for $x \leq 0.5$. Around this concentration d_{LaS} starts to decrease linearly with x.
It is worth noticing that around this critical concentration, well above the percolatice threshold, the ferromagnetic long-range ordering collapses abruptly. From the study of the second neighbour distances we confirm a non Vegard behavior of the lattice parameter. A strong reduction of the amplitudes of the signals coming from the chains X-S-Y where X and Y are (U or La) is also reported, this is to be related to an increase of the static disorder with approaching $x \bullet 0.5$.

P15
Structural behavior of UO_2 and THO_2 under high pressure

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Samples of ThO_2 and UO_2 were reinvestigated in order to establish the high pressure phases of these compounds [1](Pnma or Cmcm space group) and to obtain accurate data for determining the compressibility.
We have studied the structural high-pressure properties under pressure of ThO_2 and UO_2 in a diamond anvil cell using angle dispersive x-ray powder diffraction. The synchrotron experiments were performed up to a maximum pressure of 65 GPa on the beamline ID30 at the ESRF.
Both compounds exist in the fluorite (C1) type structure (Space group Fm3m, Z=4) at ambient pressure, as do most actinide dioxides (AnO_2). Our experiments have shown that these two dioxides, ThO_2 and UO_2, undergo a first order phase transition starting above 36 GPa to an orthorhombic ($PbCl_2$) type structure (Space group Pnma, Z=4) accompanied by a 6 and 7 % volume collapse respectively. The high pressure structures obtained were determined from Rietveld refinements. The pressure dependencies of the lattice parameters were obtained and the relative volume (V/V_0) was fitted to the Birch-Murnaghan equation of state. From these fits obtained with the low-pressure phase data, we determined a bulk modulus of B_0=198(1) GPa with a pressure derivative of B'_0=4.6(1) for ThO_2 and B_0=210(1) GPa with B'_0=3.9(1) for the uranium dioxide.
These new results show that thorium and uranium dioxides exhibit an identical structural behaviour under pressure; both transform rather sluggishly to the Pnma high pressure structure. At the highest pressure of 65 GPa, we still observed some of the initial cubic phase, which is in contradiction with earlier measurements [2,3]. With regards to these new results, and re-calculations performed on other actinide dioxides PuO_2 and AmO_2 we obtain a different evolution of the bulk moduli through the actinide dioxides series[1].

P16
Preparation and study of U/Co multilayers

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The behaviour of uranium multilayers has been so far almost unexplored. Most of the work done is still restricted to the pioneering study at the IBM, more than ten years ago, of some uranium amorphous films and multilayers in search for possible magneto-optic effects.[1-3]. With the aim of expanding the studies on this type of materials, U/Co multilayers were recently prepared by dc magnetron sputtering. Here we report on the preparation of U/Co multilayers and their magnetic characterization.
The depositions were performed onto glass at room temperature, using two different current values, the thickness of each layer ranging from 50–200 Å. Rutherford backscattering spectrometry (RBS) was used to check the thickness and the interfacial roughness of the deposited layers. The magnetic properties were measured using a SQUID magnetometer.
RBS measurements indicate that the layers have a roughness or mixing depth of a few tens of Å that increases with the increasing thickness. The multilayers have a ferromagnetic behaviour bellow 300K, with a saturation magnetization increasing with the layer thickness. The easy magnetic direction is on the plane of the films and the anisotropy field increases with the thickness of the layers.

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P17
Electron – magnon interaction in heavy fermion $CePd_2Al_2Ga$ compound

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Recent works have shown that heavy fermion (HF) compounds $CePd_2Al_3$ and $CePd_2Ga_3$ are distinguished by the kind of arrangement of Ce magnetic moments, being AF for $CePd_2Al_3$ and FM for $CePd_2Ga_3$, without any change in the crystalline structure.
At first glance, the influence of high pressure on both types of magnetic order in these ternary compounds can be described in the usual picture of Doniach's phase diagram. In $CePd_2Ga_3$, there is an evidence for the breakdown of ferromagnetism under pressure near 23 kbar, but there are indications that some kind of unidentified magnetic order exists beyond that pressure. In the same system with the hexagonal $PrNi_2Al_3$ structure there exists an intermediate compound $CePd_2Al_2Ga$ which displays FM order at T_C = 1.8 K. This compound can be very important to understand the difference between $CePd_2Al_3$ and $CePd_2Ga_3$.
Here we report about electrical resistance measurements under hydrostatic as well as quasihydrostatic pressure (0 – 50 Kbar) in the $CePd_2Al_2Ga$ compound and discuss the results obtained in a large temperature range. Due to the low temperature of the magnetic ordering transition a He^3-He^4 dilution system (diluette), which can reach temperatures around 50 mK, was used. Our results show that bellow T_C the temperature dependence of the resistivity is determined by the scattering of the conduction electron by elementary excitations (spin waves) of the correspondent magnetic order. Moreover the values of the gap in the magnon spectra were derived. These evaluations suggest a change in the magnon spectrum around ~ 5 kbar. It is concluded that the ferromagnetic order breaks down at this pressure, but similar to $CePd_2Ga_3$ there is another magnetically ordered phase - presumably AF - before the expected transition into the paramagnetic state takes place at higher pressures.

P18
Quantum criticality in a magnetic field: a study of $CeCu_{5.8}Au_{0.2}$

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The heavy-fermion alloy $CeCu_{6-x}Au_x$ exhibits a quantum critical point (QCP) at a Au concentration $x_c = 0.1$ above which long-range antiferromagnetic order occurs. For $x > 0.1$ the magnetic order can be suppressed and the quantum critical point can be reached by applying hydrostatic pressure or a magnetic field. The behavior of the low temperature properties in a magnetic field is in marked contrast to the concentration or pressure tuned QCP. Near the critical pressure or the critical Au concentration the specific heat C and the electrical resistivity ρ vary as $C/T = a \ln(T_0/T)$ and $\rho = \rho_0 + A' T$, while close to the critical magnetic field one finds $C/T = \gamma_0 - a' T^{0.5}$ and $\rho = \rho_0 + A'' T^{1.5}$. Inelastic neutron scattering was performed on $CeCu_{5.8}Au_{0.2}$ in a magnetic field in order to investigate the low-lying magnetic fluctuations near these quantum phase transitions. At the critical magnetic field the magnetic response is quasielastic with a linewidth $\Gamma \propto T$ and a Lorentzian lineshape. This is in marked contrast to the concentration tuned QCP for $x = 0.1$ where the lineshape is a modified Lorentzian. The different behavior reflects itself also in a scaling analysis which yields a scaling exponent $\alpha \approx 0.8$ for $x = 0.1$ while one finds $\alpha \approx 1.0$ for the field tuned $CeCu_{5.8}Au_{0.2}$. Therefore we conclude that the nature of the fluctuations driving the field tuned QCP is qualitatively different from the critical fluctuations observed in concentration or pressure tuning.

P19
Substitution and pressure effects on magnetism in $CeFe_2$ with competition between ferromagnetism and antiferromagnetic spin correlation

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Itinerant electron system $CeFe_2$ shows quite unique magnetism in which an antiferromagnetic spin fluctuation with a propagation vector $\boldsymbol{q}$ = (1/2, 1/2, 1/2) competes with ferromagnetic interaction. Therefore, $CeFe_2$ has the lowest Curie temperature T_C = 230 K and the smallest saturation moment M_s = 2.3 μ_B/f.u. at 4.2 K among the C15 cubic Laves phase RFe_2 family. The purpose of this study is to clarify how $CeFe_2$ does behave near an instability of ferromagnetism by substitution and pressure effects. Firstly, we carried out the magnetization measurements of $Ce(Fe_{1-x}Co_x)_2$ and $(Ce_{1-x}Sc_x)Fe_2$ to investigate the substituted effect on magnetism in $CeFe_2$. The lattice parameters in each system monotonically decrease with increasing Co and Sc contents, respectively. However, the small amount of Co substitution for Fe makes a stable AF order at low temperature, while ferromagnetism is stabilized in Sc substitution for Ce system. It can be understood that an enhancement of Ce4f-Fe3d hybridization due to significant decrease of interatomic distance leads to stable antiferromagnetism in $Ce(Fe_{1-x}Co_x)_2$, while the enhancement of ferromagnetism in $Ce_{1-x}Sc_xFe_2$ is induced by suppression of the f-d hybridization due to the decrease in the number of Ce atoms. Accordingly, we believe the antiferromagnetic spin fluctuation must develop in $CeFe_2$ under high pressure, because the 4f-3d hybridization is enhanced. Thus, we performed magnetization measurements on single crystal $CeFe_2$ under high pressures up to 8kbar. The results indicated that the magnetization along the each principal axis was quite anisotropically suppressed at 5 K even in the cubic symmetry by applying the hydrostatic pressure. Furthermore, it was found from neutron scattering experiments on single crystal $CeFe_2$ under 15kbar that the Fe magnetic moment was smaller than that under ambient pressure below $T \sim 100$ K and the antiferromagnetic spin fluctuation with a propagation vector $\boldsymbol{q}$ = (1/2, 1/2, 1/2) was enhanced by applying the hydrostatic pressure.

P20

What about the crystal field effects in the $CeFe_4Sb_{12}$ resistivity behavior?

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The thermal variation of the resistivity of $CeFe_4Sb_{12}$ shows a drop below 150 K when the temperature decreases. Up to now, this behaviour has been explained by the onset of the coherent scattering of the charge carriers by the cerium sublattice. Another explanation is the crystal electric field (CEF) effect. We have performed resistivity experiments on the solid solution $Ce_{1-x}La_xFe_4Sb_{12}$ in order to confirm one of these two hypothesis. The cerium resistivity ($\rho(Ce_{1-x}La_xFe_4Sb_{12}) - \rho(LaFe_4Sb_{12})$) shows a maximum around 150 K for all cerium concentration. So that the CEF effect hypothesis seems the best one. Also, inelastic neutron scattering experiments have been performed on $CeFe_4Sb_{12}$ and $LaFe_4Sb_{12}$.

P21

Metal-insulator transition of filled skutterudites $PrRu_4P_{12}$ and $SmRu_4P_{12}$

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The filled skutterudite-type compounds $PrRu_4P_{12}$ and $SmRu_4P_{12}$ show a metal-insulator (M-I) transition around 60K and 16K, respectively. The M-I transition in $PrRu_4P_{12}$ is a non-magnetic one of second order and is caused by a structural phase transition and a perfect three-dimensional nesting of Fermi surface. On the other hand, the M-I transition of $SmRu_4P_{12}$ has magnetic origin and occurs in two successive steps. This M-I transition seems to be caused by two successive transitions of antiferro-quadrupolar ordering and antiferro-magnetic ordering. Furthermore, nesting of Fermi surface may be also important for this transition.
The dissimilarity is due to the difference between non-Kramers ions (Pr^{3+}) and Kramers ions (Sm^{3+}). The crystal electric field (CEF) ground state of $PrRu_4P_{12}$ is Γ_{23} doublet in T_h symmetry (the same as Γ_3 in O_h). While in $SmRu_4P_{12}$, the CEF ground state is Γ_{67} quartet (the same as Γ_8). We report our recent experimental results and the mechanisms of these anomalous M-I transitions are discussed.

P22

Ultrasonic measurements on the filled skutterudiite compounds

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Elastic properties of the ternary iron phosphides with general formula *Re*-Fe_4P_{12} (*Re*=La, Pr, Nd) were investigated by means of ultrasonic measurements. For Pr- and Nd- cases, elastic softening towards low temperature was observed reflecting on their 4*f* ground state split by crystalline electric field (CEF) effect. Our results indicate that Γ_8-quartet, Γ_3 non-Klammers doublet are realized as 4*f*-CEF-ground-state in $NdFe_4P_{12}$ and $PrFe_4P_{12}$, respectively. Especially, the field-induced elastic softening appeared in $(C_{11}-C_{12})/2$ for Pr-case. No softening was observed in the C_{44}. On the other hand, $(C_{11}-C_{12})/2$ as a function of temperature exhibits a slight softening in the absence of any applied field. However, the softening towards low temperature becomes gradually larger with increasing the applied field. A ratio of the softening reaches about 15 % under the magnetic fields of 8 T. We will discuss the results in terms of quadrupolar Kondo effect, that is, nature of the non Krammers doublet and its magnetic field dependence.

P23
Anomalous magnetism of $PrCu_2Ge_2$

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The ternary compound $PrCu_2Ge_2$, crystallizing in the tetragonal $ThCr_2Si_2$-type structure, orders antiferromagneticallly and has an anomalous high Neel temperature [1]. To make clear this anomalous behavior, measurements of magnetization and magnetic susceptibility have been carried out on a $PrCu_2Ge_2$ single crystal compound. An irreversible magnetization process is found along the *c*-axis, the easy magnetization direction below 3 K. The temperature dependence of magnetic susceptibility along the *c*-axis is different from the initial state and the state after magnetization saturated below 3 K. This fact suggests a field-induced state change. The details will be given in the presentation.

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P24
X-Ray Magnetic Circular Dichroism Studies of Transition Metals/ Rare-Earth Magnetic Compounds.

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Many current and anticipated applications for magnetic materials involve heterostructures or alloys containing magnetic and "non-magnetic" components. The experimental technique that allows one to study the induced magnetism in "non magnetic" elements is X-Ray Magnetic Circular Dichroism (XMCD). XMCD is defined as the difference in X-ray absorption spectra for right and left circularly polarized x-rays. It provides accurate quantitative information on spin and orbital magnetic moments of atoms in both amplitude and direction. Since X-ray absorption spectra are related to the density of unoccupied states at the absorbing atom for a given angular momentum, the XMCD is an appropriate tool to study hybridization effects and inter-atomic magnetic interactions. In the case of 3*d*/5*d* compounds, X-ray magnetic circular dichroism (XMCD) studies at the $L_{3,2}$-edges of the *5d* TM element have revealed a strong polarization of the 5*d* band induced by a large 3d/5d hybridisation. Surprisingly enough the shape of the XMCD signal at the L-edges of 5*d* elements was found to be practically not sensitive to the nature of 3*d* elements. However, magnetic systems involving both a Rare-Earth (e.g. Gd) and a non-magnetic 5*d* metal (e.g. Ir, Pt) have received very little attention. Despite the strongly localized character of the 4*f* shells one might expect that they could nevertheless induce a sizeable magnetization at the Pt atom. It can be seen as a result of *5d-5d* ferro (antiferro)-magnetic interaction where the RE 5*d* electrons are polarized via strong ferromagnetic interatomic 4*f*-5*d* interactions. These systems have been measured on the beamline ID12 at the ESRF. In such metallic systems we will demonstrate via theoretical support that the 4*f*-electrons play the most important role and therefore also induce some magnetic moment and that the shape of the XMCD signal at the L-edges of 5*d* elements are directly related to the nature of 4*f* elements.

P25
Resistivity of ferromagnetic compounds and alloys in terms of the reduced s-d model

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The magnetic contribution to the resistivity of a system described by the *M*-impurity s-d Hamiltonian is calculated. The calculation proceeds according to the idea of reduction of s-d model proposed by

Mackowiak (1993) and treating the reduced s-d Hamiltonian as a basis for second order perturbation theory. This procedure proves to be particularly effective for systems which exhibit ferromagnetic order at low temperatures. The proposed method allows to reproduce the dependence of resistivity on temperature not only for $T > T_c$ but also for $T \in [0, T_c]$. Different results are obtained for compounds and alloys due to respective periodic and random arrangement of magnetic ions. Theoretical predictions are compared with experimental data on resistivity of various ferromagnetic compounds and alloys exhibiting Kondo behaviour above T_c.

P26
The effect of the coupling between the internal and the external vibrations in the observed spectral intensities in the elpasolite type systems

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In this paper, we report explicit calculations for the spectral intensities of the seventy-five emissions $\left|\left({}^4I_{13/2}\right)\Gamma_k\right\rangle \rightarrow \left|\left({}^4I_{15/2}\right)\Gamma_l\right\rangle + \nu_m ; m = 3,4,6$, where the irreducible representations labels are chosen as: $\left(\Gamma_k;\Gamma_l\right) = \left(\Gamma_6, 2\Gamma_7, 2\Gamma_8; \Gamma_6, \Gamma_7, 3\Gamma_8\right)$, of the $ErCl_6^{3-}$ clusters in the $Cs_2NaErCl_6$ crystal. The details of the spectrum suggest that in an energy range of about $400 cm^{-1}$, a substantial number of transitions [25 magnetic dipole (MD) and 75 vibronic electric dipole (VED) excitations] may be observed and also that a number of super positions of these transitions is most likely to occur. This experimental evidence is rather complicated to analyze and there is a need for more theoretical backup to gain understanding in both radiative and non-radiative processes in these materials. In this paper, we have taken a broader view of the intensity mechanisms associated with vibronically allowed electronic transitions and have decided to further test our current calculation models (VCF-LP) with reference to the $\left|\left({}^4I_{13/2}\right)\Gamma_k\right\rangle \rightarrow \left|\left({}^4I_{15/2}\right)\Gamma_l\right\rangle + \nu_m$, emissions for this crystal. It is interesting to realize that, although the intrinsic limitations of our models and methods to estimate spectral intensities, the final output (calculated oscillator strengths) indicate a fair and sensible agreement between our theoretical predictions and experimental data. As a further test of our vibronic intensity model, in a forthcoming paper, we will examine the rather unexpected intensity associated with the $\left|\left({}^4S_{3/2}\right)\Gamma_l\right\rangle \rightarrow \left|\left({}^4I_{15/2}\right)\Gamma_k\right\rangle$ emissions for this elpasolite. We analyze the effect of the coupling among the internal and the external vibrational modes in this system and generalization of this model are suggested to include both the short-range and the long-range interaction terms in the dynamic matrix.

P27
The magnetic properties of the Tb_xLa_{1-x} Mn Si intermetallic compounds

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The magnetic properties of the Tb_xLa_{1-x} Mn Si intermetallic compounds have been investigated by magnetization measurements. The Tb_xLa_{1-x} Mn Si alloys were prepared by arc-melting from commercially available high purity elements. The X-ray phase analysis and the metallographic analysis were employed in the research of crystal structure of these compounds. It was found that crystal transition is observed in these compounds: from orthorhombic TiNiSi-type structure for TbMnSi to tetragonal CeFeSi- type structure for LaMnSi. The La substitution for Tb in Tb_xLa_{1-x} Mn Si samples leads to change on the character of the magnetic ordering in these compounds. LaMnSi .is antiferromagnetic and TbMnSi-demonstrates a complex temperature magnetic behavior (antiferromagnetic, noncollinear antiferromagnetic). These magnetic

transition can be connected with peculiarities of the crystalline structures and with the exchange interaction character of the Tb_xLa_{1-x} Mn Si compounds. The work was supported by RFFR Grant 00-02-17862.

P28
About hydrogen and nitrogen insertions in R_2Fe_{17} and $RFe_{11}Ti$ single crystals

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The discovery that nitrogen absorption drastically improves the magnetic properties of Sm_2Fe_{17} has sparked interest in the gas-phase interstitial modification of rare-earth intermetallics. In present work we investigated the effect of the hydrogen and nitrogen on the fundamental properties (structure, Curie temperature, magnetization, magnetic anisotropy, spin-reorientation transitions, magnetostriction, etc) of $RFe_{11}Ti$ and R_2Fe_{17} single crystals using several techniques (x-ray scattering, torque and capacitive magnetometer, Mössbauer measurements, etc). In many cases the magnetic characteristics are shown to be dramatically changed, especially magnetocrystalline anisotropy (MCA). Magnetic phase diagram for hydrides and nitrides have been obtained. The effect of interstitials on the magnetic anisotropy constants and SR transitions is determined by the following three factors: (i) the type of the interstitial atoms (it is an established fact that the interstitial effects are of different signs for nitrogen and hydrogen); (ii) the local surrounding of the R ions (in R_2Fe_{17} and $RFe_{11}Ti$ crystals the positions of interstitial atoms are different with respect to the R ion – either in a plane perpendicular to *c*-axis (R_2Fe_{17}) or along the tetragonal *c*-axis ($RFe_{11}Ti$)); (iii) the orientation of the quadrupole moment q of the asymmetric 4*f* shell with respect to the direction of the resulting magnetic moment of 4*f* electrons μ_R (for $\alpha_J > 0$ μ_R is oriented along the elongation direction of the space charge distribution of 4*f* electrons, and is perpendicular to it when $\alpha_J < 0$).

Concluding, interstitial elements in the $RFe_{11}Ti$ and R_2Fe_{17} crystal lattices provide effective means for the controlling of both magnitude value and sign of magnetic anisotropy constants.

P29
Importance of the Lanthanide Site in the Magnetic Ordering in FM La4Ba2Cu2O10 and AFM $Nd_4Ba_2Cu_2O_{10}$

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The occurrence of ferromagnetism in La4Ba2Cu2O10 was surprising and has been difficult to explain [1]. The fact that isostructural Nd4Ba2Cu2O10 orders in the more common antiferromagnetic fashion deepens the mystery, and implies that the lanthanide site -- which is rather far removed from the Cu spins -- is somehow involved in the mechanism of ordering. By calculating Cu d(x^2-y^2) Wannier functions (all electron, full potential using the LAPW method), and using them to calculate (not fit) the tight-binding effective hopping amplitudes and also to calculate the direct exchange integral between these Wannier functions, the FM ordering in $La_4Ba_2Cu_2O_{10}$ and the difference between it and AFM $Nd_4Ba_2Cu_2O_{10}$ become readily evident. The Wannier function extend through the oxygen ions neighboring the Cu spin, and extends onto the lanthanide site; it will be shown that it is this chemical difference between La and Nd accounts for the difference in ordering of these two compounds. Calculations for $La_4Ba_2Cu_2O_{10}$ under pressure predict a FM → AFM transition.

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P30
Thermal expansion of single-crystalline $LaSrNiO_4$ with high resolution dilatometer

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We constructed a high-resolution dilatometer with a parallel plate capacitance cell. High-quality quartz is used for the cell to reduce the background since thermal expansion coefficient α for quartz is extremely small ($\alpha \approx 4.8 \times 10^{-7}$ K^{-1} at room temperature) comparing that for Cu ($\alpha \approx 1.7 \times 10^{-5}$ K^{-1} at room temperature), which is widely used for the capacitive dilatometer. It is also possible to measure small size of sample, such as, $2 \times 2 \times 2$ mm^3.
Anomalies are observed at $T \approx$ 180 K and 260 K in both thermal expansion and magnetic susceptibility measurements for a single crystal $LaSrNiO_4$. These may be related to the spin-ordering and charge-ordering, respectively. The results will be discussed with the neutron scattering data.

P31
Antiferroquadrupolar Ordering in the Tetragonal RB_2C_2 Compounds (R = Tb, Dy and Ho)

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We provide experimental works on the tetragonal RB_2C_2 compounds performed based on our interest in novel magnetic properties strongly affected by multipolar interactions by means of magnetization, specific heat, neutron diffraction and 161Dy Mossbauer experiments. Our finding of an antiferroquadrupolar (AFQ) ordering below 24.7 K in DyB_2C_2 triggered the successive findings as follows. HoB_2C_2, unexpectedly, shows an AFQ transition at 4.5 K below an antiferromagnetic (AFM) transition at 5.9 K. An AFM compound TbB_2C_2 with TN=22.0 K shows an anomalous increase of susceptibility below TN, and the magnetic structure is a peculiar one among the RB_2C_2 compounds. Furthermore, it is confirmed by neutron diffraction of the single crystal that an AFQ ordered phase is induced by magnetic fields.

P32
A phenomenological expression for the susceptibility of the Haldane chain of AF Heisenberg spins S=1

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The phenomenological expression kT c(T) = C1(n) exp(-W1(n)/T) + C2(n)exp(-W2(n)/T) describes very accurately the temperature dependence of the magnetic susceptibility computed for antiferromagnetic rings of Heisenberg spins S=1, whose size n is even and ranges from 6 to 20. This expression has been obtained by applying to the results of theoretical calculations a strategy justified by scaling considerations. For n larger than 10, the coefficients of the expression converge towards C1= 0.13, W1= 0.46 J, C2= 0.56, W2= 1.82 J which are appropriate to describe the susceptibility of the Haldane chain. The Curie constant, the paramagnetic Curie-Weiss temperature, the correlation length at T=0 and the Haldane gap are closely related to these coefficients. With this expression, a very good description of the magnetic behavior of Y_2BaNiO_5 and of $Ni(C_2H_8N_2)_2\ NO_2ClO_4$ (NENP), the archetype of the Haldane gap systems, is achieved over the whole temperature range.

P33
Thermodynamics of extended s-d Hamiltonian under varying impurity concentration

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Thermodynamic functions (TF) of the s-d Hamiltonian H_{s-d} supplemented by reduced s-d interaction V_r [1] and AF (antiferromagnetic) interaction between impurities V_{AF} [2] are studied under varying impurity concentration **c**, temperature **T** and magnetic field **B**. V_r is introduced in order to account for the transition to magnetically ordered phase observed in magnetic alloys [3,4] and V_{AF}, which serves as a substitute of the the RKKY interaction, considerably improves dependence of TF on **T** and **B**. Particular emphasis is laid on impurity specific heat c_v and impurity susceptibility • in the vicinity of the transition temperature T_c. The graphs of c_v, • and impurity magnetization m(B,T) are adjusted to fit experimental data on CuCr [3] and $(LaCe)Al_2$ [4].

Two numerical techniques are applied. The first consists in treating the impurity mean field $V_{i(T)}$ thermodynamically equivalent to V_r+V_{AF}, as a field additional to B and solving the single-impurity H_{s-d} with external field $V_{i(T)}+B$ by the method of Andrei et al. [5]. This solution amounts to transforming a system of nonlinear integral equations for functions $•_k$, k=1,2,… determining the impurity free energy, into matrix equations and solving the latter by an iteration procedure. The resulting graph of free energy is differentiated numerically to obtain $c_{v(T)}$. This method proves successful in determining the graph of $c_{v(T)}$ and explaining the presence of a peak in the neighborhood of the Kondo temperature T_K, as well as discontinuity at T_c (e.g. CuCr with $c=51.10^{-6}$, $T_c\approx0.07$ K, [3]), but fails to explain the susceptibility maxima observed in $(LaCe)Al_2$ at T_c [4]. In order to account for these maxima, 2nd order perturbation theory developed in [6], is applied to M - impurity $H_{s-d}+V_r+V_{AF}$. The susceptibility • of the unperturbed system, with Hamiltonian $H_u=H_0+V_r+V_{AF}$ (H_0 standing for the Hamiltonian of the free electron gas), already exhibits 1st order poles at T_c and the 2nd order perturbation theory graphs of •(0,T), m(B,T) are fitted to experimental ones [4] for $V_{AF}=0$, and $V_{AF}•0$. Theoretical •(0,T), m(B,T) exceed experimental values in the former case justifying introduction of $V_{AF}•0$. The transition temperature T_c decreases with c and three distinct graphs of •(0,T) for 6%, 10% and 20% content of Ce in $(La_{1-x}Ce_x)Al_2$ are presented. Felsch et al. [4] found $T_{c20}=0.2$ K, $T_{c10}=0.08$ K. T_{c6} which we evaluate to be 0.037 K was not reached in their experiment. Theoretical values of T_c are exactly fitted to experimental ones.

The perturbation theory approach proved unsuccessful in explaining the full T-dependence of c_v, in particular the presence of a peak near T_K [7]. The maxima of •(0,T) resulting in this approach are also not finite ones, as those detected by Felsch et al. [4], but are resembled by 2nd order poles. The interactions V_r, V_{AF} provide two parameters which, apart from the conduction halfband width D, allow to shape the graphs of •, m as well as c_v in the first method. Both methods yield m(B,T) graphs which agree with the experimental ones for $(LaCe)Al_2$ at $T>T_c$. Our conclusion is therefore that the TF of the $H_{s-d}+V_r+V_{AF}$, studied by the two alternative methods presented, provide the grounds for a complete theory of thermal properties of magnetic alloys.

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P34
Towards ab initio theory of 4f-magnetism at finite temperatures: Gd and Eu

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The contribution reviews a simplified ab initio procedure to investigate basic properties of itinerant magnets containing 4f-electrons. The approach consists in two steps: (i) the selfconsistent electronic structure calculation within the density-functional theory with the 4f-orbitals treated as core orbitals, and (ii) the calculation of parameters of an effective classical Heisenberg Hamiltonian, which are determined using the magnetic force theorem and that are employed in subsequent evaluation of the magnon spectra, the spin-wave stiffness constants and the magnetic transition temperatures. Two elementary metals, namely the hcp Gd and the bcc Eu, are chosen to demonstrate the applicability of the developed scheme to various aspects of the itinerant 4f-magnetism: collinear and non-collinear magnetic ground states, long-ranged exchange interactions, and the resulting Curie/Nèel temperatures.

P35
Calculation of equilibrium lattice parameters of rare-earths (Y, La, Gd, Lu)

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Equilibrium lattice parameters of rare-earth crystals (hcp Y, Gd and Lu, dhcp and fcc La) have been calculated using the full-potential local-orbital minimum-basis band-structure scheme (FPLO). The local density approximation for the exchange-correlation energy funcional within density functional theory has been employed. The theoretical volumes are found roughly 10 % lower than the experimental ones. For the case of dhcp La, we carried out a further calculation with restricted valence basis (no 4f orbitals). The theoretical volume is found much closer to the experimental values, but is off the general trend. In the case of fcc La also the full potential linearized augmented plane wave (FP LAPW) method (WIEN97 code) has been used. The results of both methods are almost identical (V_{theory}(LAPW) / V_{exp} = 87.9 %; V_{theory}(FPLO) / V_{exp} = 87.4 %) using LDA. The generalized gradient approach (LAPW) improves the equilibrium volume for fcc La (V_{theory}(LAPW) / V_{exp} = 99.94 %).

P36
Site susceptibility tensors and local anisotropy axes in f-electron compounds

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Polarized neutron diffraction provides information about the magnetization density of each individual crystallographic site. In the present paper the role of the atomic site susceptibility tensor χ_{ij} accounting for the magnetic response of individual atoms to an external magnetic field is discussed. The symmetry of this tensor is very similar to that of the tensor u_{ij} describing the thermal motion of atoms. By analogy with the atomic displacement parameters (ADPs) atomic suceptibility parameters (ASPs) can be introduced. The six independent atomic susceptibility parameters can be determined from polarised neutron flipping ratio measurements and visualized as *magnetic ellipsoids* which are an alogous to the *thermal ellipsoids* obtained from ADPs. If the local anisotropy is small these magnetic ellipsoids approximate to spheres with diameters proportional to the induced magnetization. In other cases *anomalous* (elongated or flattened) ellipsoids will occur. The ASPs have been determined in the compound Nd_3S_4 which has the Th_3P_4 structure. They correspond to strongly oblate magnetic ellipsoids; in contrast in the isomorphous compound Sm_3Te_4 the

magnetic ellipsoids are found to be prolate. Other examples will be given, which demonstrate that the anomalous elongation of the magnetic ellipsoids can be considered as a precursor of the low temperature magnetic order.

P37
Antiferroquadrupolar order in the magnetic semiconductor TmTe

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In the magnetic semiconductor TmTe long-range antiferroquadrupolar (AFQ) ordering occurs below $T_Q \approx$ 1.8 K [1], far enough above the Néel temperature of about 0.5 K [2,]. Neutrons can probe AFQ order only indirectly by detecting a staggered antiferromagnetic (AFM) component of the magnetic dipole moments induced by a uniform external field. From the magnetic intensities measured for different directions of the applied field [3] one can deduce the symmetry of the quadrupole order parameter through a group theoretical analysis [4].
In the present compound, it was further found that the propagation vector is the same [$\boldsymbol{k}$ = (1/2, 1/2, 1/2)] for both the AFQ and AFM structures This raises the question of the nature of the transition at T_N, especially in the presence of an external field. Experiments have been performed down to 100 mK and an additional ferromagnetic component, implying a small canting of the structure, was clearly observed, in agreement with the prediction of Ref. [4]. The effects of a high magnetic field $H \parallel$ <110> on the AFQ and AFM phases will also be reported.
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P38
Staggered-field effect on the one-dimensional quantum antiferromagnet Yb_4As_3

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Inelastic and polarized neutron scattering experiments have been performed to study the one-dimensional (1D) magnetic property in the chrge-ordered phase of Yb_4As_3. In contrast to the magnetic exictation at zero magnetic field explained by the model of spin-1/2 1D Heisenberg antiferromagnet (HAF), a sharp inelastic responce and excitation gap at the AF zone center for the 1D Yb-ion chain were observed under the magnetic field perpendicular to the chain. The magnitude of gap obeys a power law function of magnetic field with an exponent of 2/3. The polarized neutron measurement revealed a pronounced increase of field-induced magnetic moment of the Yb ions on the 1D chain below about 10 K under magnetic field perpendicular to the chain, although the magnetic moment under the parallel field is reproduced by the model of spin-1/2 1D HAF. These phenomena under magnetic field are explained well by the theory of the staggered field due to the Dzyaloshinsky-Moriya interaction within the chain.

P39
Rare earth titanates under high pressure: a neutron study

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In $R_2Ti_2O_7$ compounds, rare earth R ions with well localized 4f moments occupy a pyrochlore lattice with corner sharing tetrahedra. This lattice is highly frustrated for antiferromagnetic interactions, and for ferromagnetic interactions between ions with a strong local Ising anisotropy. The high frustration leads to exotic magnetic states, such as spin liquid or spin ice states, whose stability is governed by a delicate balance between exchange, anisotropy and dipolar interactions. At ambient pressure, $Ho_2Ti_2O_7$ behaves as a "dipolar spin ice", with a magnetic state mapping that of the ice lattice [1]. In contrast, $Tb_2Ti_2O_7$ behaves as a "spin liquid", retaining short range liquid-like spin correlations down to at least 70 mK, despite a Curie Weiss temperature of -19 K [2]. The energy balance is modified by pressure, since magnetic interactions depend on interatomic distances in different ways.

We have studied the inuence of an applied pressure for the first time, up to 9 GPa, in the temperature range 1.4 K<T< 300 K, by high pressure neutron difraction. In $Ho_2Ti_2O_7$, the spin ice state remains stable up to at least 5 GPa. In $Tb_2Ti_2O_7$, the spin liquid state also remains stable up to 5 GPa, but under higher pressures novel features appear in the neutron spectra, pointing out drastic changes in the microscopic spin arrangement. From our first results, high pressure shows as a new and essential tool to investigate the magnetic interactions responsible for the novel magnetic states observed in highly frustrated magnets. This study was performed using a technique recently developed in Laboratoire Lèon Brillouin[3], which allows one to determine magnetic order up to much higher pressures than in conventional neutron measurements.

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P40
Physical properties of $YbInCu_4$ up to 4GPa

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We have measured the electrical resistivity of single crystal $YbInCu_4$ under hydrostatic pressure up to 3.76 GPa at temperatures down to 33 mK. At ambient pressure, $YbInCu_4$ undergoes a valence transition at 40 K. The transition temperature T_v decreases linearly with increasing pressure: dT_v/dP = -19.5 K/GPa below 1 GPa. Above 3 GPa, a hysteresis due to valence transition disappeared and the transition can't be confirmed clearly. The resistivity of $YbInCu_4$ at low temperature varies as $\rho(T) = \rho_0 + A\,T^2$. The resistivity coefficient A and the residual resistivity ρ_0 increase gradually with increasing pressure. These value increase rapidly just before a transition disappears and take maximum around 3 GPa. In this pressure region, the A-value is extremely large: 2.25 $\mu\Omega cm/K^2$ at 3.39 GPa.

P41
Effect of pressure on the martensitic transition in GdCu intermetallic compound

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The Rcu (R=rare earth) compounds crystallize either in orthorhombic FeB phase for the light rare earth or in the cubic CsCl structures for heavy rare earths. Some of these compounds (R=Ge, Tb and Y) undergo a martensitic transition (MS) evolving from the CsCl structure at room temperature to the FeB structure as decreasing temperature. In the present work, we report the thermal expansion of GdCu in the temperature range from 77 K to 300 K under high pressure up to 1.2 Gpa.
A large anomaly at 239 K, indicating Ms, is observed in the thermal expansion at ambient pressure. The transition temperature Ms rapidly decreases by applying pressure at a rate of *d*Ms/*d*P • 160 K/Gpa, and becomes below 77 K at 0.9Gpa. The discontinuous in the value of •L_{MS}/L_O at the transition also decreases but transition becomes sharp with increasing pressure.

P42
Fermi surface and magnetic structure in Rare earth-Ga_3 compounds

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The measurement of the 2-dimensional angular correlation of the positron annihilation radiation (2D-ACAR), providing a 2D projection of the two-photon electron-positron momentum density, •(p), is a powerful tool to investigate the electronic structure of intermetallic compounds. Utilising tomographic reconstruction techniques, the experiment has the unique ability to sample the Brillouin Zone of truly 3-dimensional systems in a cartesian mesh, thus determining their Fermi surface (FS).
Our studies have addressed the commensurate and incommensurate antiferromagnetic structures of $TmGa_3$ and $ErGa_3$, respectively. For both compounds the FSs resulting from the 2D-ACAR experiments are in fair agreement with de Haas van Alphen measurements and with band structure calculations in local density approximation (LDA) which constrain the 4f electrons to retain a local atomic character [2,3]. Nevertheless, we discover different nesting features along the [110] directions which can account for the magnetic structures of the two compounds. Moreover, we propose methods to estimate the density of states at the Fermi energy (E_F) and the electronic contribution to the specific heat, • [we obtain $N(E_F)$=17 states/(Ryd cell), •=2.8 mJ/moleK^2 and $N(E_F)$=16 states/(Ryd cell), •=2.7 mJ/moleK^2 for $TmGa_3$ and $ErGa_3$, respectively.
We show preliminary results of our measurements on the heavy fermion antiferromagnet UGa_3, performed across the antiferromagnetic transition. Confirming previous discrepancies between experiments and theory [4], the experimental data cannot clearly be interpreted by standard band structure calculations where the f-degree of freedom is either treated as itinerant or localized. Therefore, our results do not fully confirm the standard assumption of UGa_3 as the itinerant antiferromagnet.
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P43
Single-ion anisotropy in compounds of rare earths other than Sm: importance of J-mixing in the room-temperature range.

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Contrary to the established view, J-mixing is found to strongly affect the magnetic anisotropy of compounds of all light rare earths and also of terbium. The fractional contribution of J-mixing to second-order anisotropy constants in the room-temperature range is proportional to absolute temperature and depends on the rare earth element involved but not on the characteristics of the specific solid. For the light rare earths this contribution is given by 12 $(2J-1)^{-1}$~kT/Δ_{so}, where Δ_{so} is the spin-orbit splitting between the centers of gravity of the ground and first excited multiplets, and amounts to 22% for Pr and Nd and to as much as 83% for Sm at T=400 K. For the heavy rare earths the corresponding expression is 12 $(2J+3)^{-1}$~kT/Δ_{so}, that is 11% for Tb at T=400 K and significantly less for the rest of the rare earth series. Analytical expressions are obtained which allow for the J-mixing and are accurate in the room-temperature range for all rare earths with the exception of, perhaps, Sm.

P44
Unexpected high-order anisotropy contributions in magnetic RE-TM compounds (RE=Rare Earth, TM=Transition Metal)

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In a large number of studies of magnetic anisotropy in intermetallic compounds, the high-order contributions to the magnetic free energy are neglected, and only the lowest (second) order term is taken into account. Sometimes, this choice is justified by simple models or by the physical consideration that high-order anisotropy constants vanish at high temperatures. Nevertheless, there are particular cases where the presence of these unexpected high-order contributions can explain physical behaviours which cannot be accounted for otherwise. Two of these situations are examined: the basal-plane anisotropy of Sm_2Co_{17}, which is entirely due to the sixth-order term in the crystal-field Hamiltonian and has zero value if calculated within the ground J multiplet of the rare-earth ion, and the various types of magnetic field-induced transitions detected up to room temperature in the $Pr_2(Co,Fe)_{17}$ class of compounds, whose variety could be explained in the frame of a rigidly coupled model only by considering unphysically large values of terms of eight-order or higher. Two different mechanisms are proposed to account for the experimental data: for Sm_2Co_{17}, the nonzero value of the basal-plane anisotropy is reproduced by taking into account the mixing of small fractions of excited states in the ground J multiplet of the RE ion, while the opening of a canting angle between magnetic sublattices can explain the peculiar behaviour of the magnetic transition in the $Pr_2(Co,Fe)_{17}$ system.

P45
Sequence of transitions from 2D to 3D superconducting state in $YBa_2Cu_3O_{6+x}$ single crystal

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Using the high-resolution SQUID magnetometer we have observed a sequence of transitions from 2D to 3D superconducting state on $YBa_2Cu_3O_{6+x}$ single-crystals. The transitions reflect the layered structure of material and clearly do not originate in non-homogeneous sample with multiple phases with varying T_c or vortex matter. While both transitions at temperature around 92 K have width only 10 mK and show sudden appearance of phase coherence in 2D CuO_2 planes and CuO_2-Y-CuO_2 sandwiches, the third transition at temperature about 87 K reflects appearance of the weak coupling between sandwiches through the Ba-CuO-Ba barriers. Currently the most accepted is that the superconductivity in the high-T_c cuprates is in the d-wave

channel. There are strong similarities between the doped planes and doped ladders that provide interesting results of strongly correlated electrons.

P46
Rare - earth analogues of Prussian blue - structure and magnetism

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The crystal structure and magnetic properties of $R[Fe(CN)_6]$ nH_2O (R = Pr, Sm, Gd, Dy and Ho) are presented. The crystal structure of the compounds was refined in according to hexagonal model (space group *P* 3/*m*, ICSD 2581). While accuracy of the process for $Pr[Fe(CN)_6]$ $5H_2O$ sample could be considered sufficient, the curves of difference between calculated and measured patterns for the other investigated compounds revealed discrepancies in x-ray intensities. The problem was successfully solved by modification of the structural model when the slightly modified model contains only four molecules of H_2O per formula unit. The removal of the water molecule causes reduction of the symmetry from hexagonal to orthorhombic (space group *Cmcm*, ICSD 203047) and the result of the fitting procedure is significantly improved. Basic magnetic properties of the compounds are mostly determined by trivalent rare-earth ion. On the other hand, it has been found that coordination water can play an active role in low-temperature magnetic properties, where cluster glass – like behaviour was observed and even in basic magnetic properties like the Curie temperature. An example is $Pr[Fe(CN)_6]$ nH_2O where the Curie temperature varies from $T_c \sim 1K$ to $T_c = 14.5$ K.

P47
Luminescent properties of Eu-doped nanocrystallites of barium titanate

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Eu3+ doped BaTiO3 nanocrystalline powders have been obtained by sol-gel method. Their morphology, structure and luminescence properties have been investigated as a function of sintering temperature. The powders sintered at temperatures below 800oC demonstrate luminescence behavior characteristic of the inversed symmetry Eu3+ sites where only the 5Do -> 7F1 transitions are allowed. Above this temperature the system undergoes a phase transition characterized by lack of inversion symmetry what allows the dipole-electric transitions.

P48
Hyperfine fields on actinide impurities in ferromagnetic Fe and Ni hosts

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CBPF - Brazil

In this work, we theoretically discuss the local magnetic moments and magnetic hyperfine fields on actinide impurities diluted in ferromagnetic Fe and Ni hosts. One adopts an Anderson-Moriya model in which a localized 5f level is hybridized with a spin polarized and Koster-Slater perturbed d-conduction band. We use the Hartree-Fock picture to treat electron-electron interaction within the d-band and we include the next neighbor perturbation, due to the d-translational invariance breaking in the hopping, introduced by the 5f impurity. The spin dependent Hartree-Fock potentials are self consistently determined, using an extended Friedel screening condition an d the Hartree-Fock relation between up and down spin potentials. In particular, in some cases the hyperfine fields arising from 5f-orbital contribution are extremely relevant since their orbital magnetic moments are much larger than those arising from the 5f-spin and 6d-spin local

moments. It turns out that our self-consistent numerical calculations for the hyperfine fields at impurity site are in good agreement with the available experimental data.

P49
Local magnetic moment formation at Cd impurity diluted in RNi_2 and RCo_2 intermetallic compounds

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In this work we study the local magnetic moment and hyperfine field of Cd impurity diluted on the R site of the Laves phase intermetallic compounds RNi_2 and RCo_2 (R = Gd, Tb, Dy, Ho, Er). In order to describe the impurity problem in RNi_2 intermetallic compounds we use a Daniel-Friedel-like model in which RNi_2 intermetallic compounds are considered as effective ferromagnetic rare earth hosts. In the case of RCo_2 compounds, the hyperfine field is made up from two contributions. The contribution from the rare earth ions is considered as being the same as in RNi_2 case, whereas the contribution arising from Co sites is described via a Blandin-Campbell two-centre model, in which the Cd site is surrounded by neighbouring Co magnetic moments. The calculated magnetic hyperfine fields are in good agreement with the available experimental data.

P50
Surprising scenario of magnetisation processes in the pure-dipole Ising antiferroamagnet $DyAlO_3$

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Unusual switching of magnetostriction (and magnetisation) in the pure-dipole rare earth Ising antiferromagnet $DyAlO_3$ induced by small sign-variable increments of an external magnetic field was found. Experimental studies of magnetostriction and magnetisation were performed in the temperature range of 1.5-4.2~K and magnetic fields up to 4~T. Along with an expected magnetisation jump of magnetostriction at the metamagnetic phase transition induced by the external magnetic field, unusual behaviour of the field dependence of magnetostriction was observed. The magnetostriction curves measured during "field-up" and "field-down" magnetisation processes were near-symmetric about the H=0 axis and formed a peculiar magnetostriction hysteresis loop. Besides, at any value of the magnetic field (ranging from very small to high fields) small sign-variable increments of the magnetic field resulted in reversible switching of magnetostriction between the "field-up" and "field-down" curves. Such a behaviour is similar to that of the magnetisation curves for "hard" type-II superconductors with strong pinning [1]. Possible mechanisms of these anomalies and the reason for the above-mentioned analogy with "hard" superconductors are discussed.

6th Prague Colloquium on *f*-electron systems

Charles University, Prague, July 5-9, 2002

Because of the large number of participants, who are eager about having a presentation at the Colloquium, we have extended the time for scientific sessions !!!!

The Colloquium begins already on July 5 after lunch – at 13.00 !!!!

Scope:

The ***Prague Colloquium on f-Electron Systems*** (PCFES) is a biennial ***academic meeting*** focused on topics of the current research of electronic structure and material properties of lanthanide and actinide based systems. Nevertheless, few interesting contributions on transition-metal physics are also welcome.

The program of PCFES is traditionally based **on *lectures*** (approx. 30 minutes) given by outstanding specialists and the following discussions with all interested participants. **Besides overhead projectors, a data projector with Powerpoint2000 will be available for oral presentations. In case if you have a doubt about compatibility with your system, send a test file to havela@apollo.karlov.mff.cuni.cz so that it can be checked. It is recommended that your file is copied to the hard disk of the computer before your session starts.**

Because of great interest of participants to present their results, this time also selected ***posters*** will be accepted. **Each poster board is 98 cm wide and 148 cm high).**

Some posters will be devoted to possibilities offered by Large facilities and User laboratories (here the double boards are available = the double width, the same hight).

See the final program

&
Program and Abstract booklet.

No extended printed proceedings are envisaged. An ***abstract booklet*** will, however, be available to each registered participant at the registration desk of PCFES6. Presenting authors are kindly requested to submit an electronic file of their abstract (up to 1/2 page) by e-mail before June 15.

Ample space on the ***Colloquium Web pages*** will be available for extended contributions, lecture files and other materials which may be provided by speakers and poster presenters.

The time of the PCFES is chosen to associate it with some major conference in Europe focused on related subjects. This time the ***PCFES6 is organized from July 5 through 9, 2002 just before SCES'02 (Kraków, July 10 - 13, 2002)***.

Before the PCFES6 the ***Workshop on the Electronic Structure of Solids*** will be held at the ***IFW Dresden (July 3 - 5, 2002)*** and ***The European Conference Physics of Magnetism*** will be organized in ***Poznan (July 1-5, 2002)***.

Accommodation:

Your accommodation will be arranged by the travel agency AR TOUR ONDRACEK in several hotels of various categories from which you can reach the PCFES6 site easily by public transport or even by walk.

Please, download the HOTEL RESERVATION FORM as a WORD, PDF or POSTSCRIPT file, fill in your coordinates and choice of accommodation and book your accommodation by sending the form at your nearest convenience by fax to: +420-2-71743301 or as an attachment of an e-mail to: stgermain@artour.cz.

If you have not send your HOTEL RESERVATION FORM

!!!!!Please, book your accommodation immediately!!!!!

Many tourists are visiting Prague in summer and hotels will be soon overbooked.