14th Prague Colloquium on *f*-Electron Systems

Prague, 15th - 18th June 2023

Program & Abstracts

Katedra Fyziky Kondenzovaných Látek
Department of Condensed Matter Physics
F K K L

MATHEMATICA PHYSICAQUE
FACULTAS

Welcome to PCFES!

Almost every second year since 1992 we organized the *Prague Colloquium on f-Electron Systems*, an exciting meeting covering topics in physics of actinides and lanthanides. Also this year we keep the tradition having the pleasure to welcome you at 14th PCFES, an informal forum for presentations and discussions on the current issues of magnetism, strongly correlated systems, spectroscopies, materials science, as well as progress in theory. The meeting should also provide ground for close interaction of students and other early-stage researchers with experienced specialists.

Regarding the venue for PCFES, the Faculty of Mathematics and Physics belongs to the youngest faculties of the Charles University, which was founded in 1348 by the Roman Emperor and King of Bohemia, Charles IV. The Faculty itself was founded in 1952, splitting from the Faculty of Science. The building Ke Karlovu 5, where the PCFES sessions will take place, is now over 100 years old. Careful reconstructions succeeded to provide high functionality while meticulously preserving or restoring most of the details, carrying the spirit of the founders in early 1900s as well as following generations of professors and students. Part of the laboratories of the Department of Condensed Matter Physics (technology, X-ray diffraction, high-pressure lab) is located on the ground floor of the building. Neighbour building in the Ke Karlovu street, number 3, is the official and administrative seat of the Faculty. It is followed by the Church of the Virgin Mary and St. Charlemagne, built in the 14th century and known for its unique vaulted central dome without any support. Those who stay till Sunday can attend the Holy Mass at 9:30 a.m. (in Czech) and at 11:00 and 17:00 (in Latin).

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

The 14th Prague Colloquium on f-Electron Systems takes place with the contribution of material and human potential of the Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University.

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

Silvie Mašková-Černá & Štěpán Sechovský
On behalf of the PCFES Organizers

Poster session

Besides the oral sessions, taking place in the lecture room F2, the discussions at posters will be possible on the 1st floor corridor. Presenters are requested to mount the posters as soon as possible and keep them for the whole duration of PCFES to allow informal discussions. One dedicated poster session will take place on Friday evening, during which presenters are expected to be present at their posters.

Refreshment

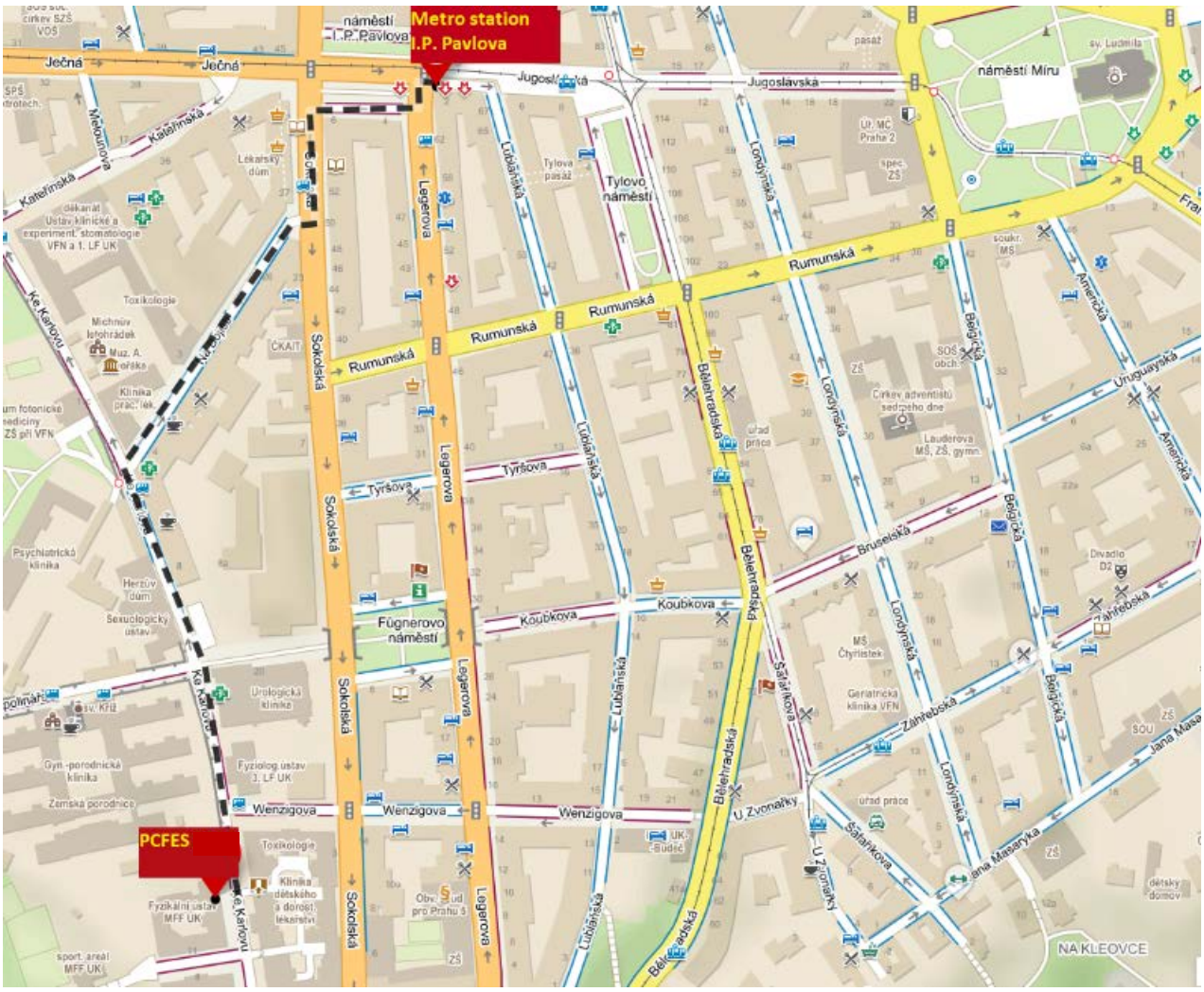
During PCFES, refreshment will be provided during coffee breaks and evenings. Lunches are not provided. You can find numerous small restaurants in the lively part of the town north of the Ke Karlovu street.

On-site connection to internet

It is possible to connect using Wi-Fi via **EDUROAM**.
Or
Special conference wifi access:

SSID: **PCFES2023**
Password: **NiceDay4ever**

Information update on: https://pc-cfes.kfkl.cz/



PROGRAM

Wednesday 14 June

15:00-17:00 **Registration**

Thursday 15 June

8:00-	**Registration**			
8:55	Opening	Silvie Mašková-Černá	Charles U., Prague, CZ	
	Electronic structure - Theory I	*Chair: Ladislav Havela*		
9:00	Systematic analysis of the exchange interactions within Anderson-lattice model: Kondo and superexchange vs Dzyaloshinskii-Moriya interaction	Józef Spałek	Jagiellonian U, Krakow, PL	T1
9:30	Field-induced superconducting and metamagnetic phase transitions in a four-orbital model of UGe_2	Maciej Fidrysiak	Jagiellonian U, Krakow, PL	T2
10:00	Itinerant vs. localized f-electrons behavior in magnetic anisotropic properties of U-based ferromagnets	Dominik Legut	VSB - TU Ostrava, CZ	T3
10:30	*Coffee break*			
	Electronic structure - Theory II	*Chair: Ladislav Havela*		
11:00	The Density Functional theory study of electronic structure and magnetic properties of antiferromagnetic U_2TGa_3 (T = Pd, Pt) intermetallics	Mane Sahakyan	INTiBS PAS, Wroclav, PL	T4
11:30	Spin-orbit interactions - the atomic physics in the solid-state physics	Ryszard Radwanski	Jagiellonian U, Krakow, PL	T5
12:00	*Lunch break*			
	RE-compounds (Ce)	*Chair: Evgenia Chitrova -Tereshina*		
14:00	Investigating the Superconducting State of the Heavy Fermion Compound Ce_3PtIn_{11}	Jeroen Custers	Charles U., Prague, CZ	T6
14:30	Low-temperature antiferromagnetic order in orthorhombic $CePdAl_3$	Vivek Kumar	TU München, Garching, DE	T7
15:00	Magnetism of R_2Cu_2In intermetallic compounds	Petr Král	Charles U., Prague, CZ	T8
15:30	*Coffee break*			
	RE-compounds I	*Chair: Evgenia Chitrova -Tereshina*		
16:00	Structural 130 K phase transition and emergence of a coherent Kondo state in Ce_2Rh_2Ga explored by $^{69,71}Ga$ NQR	Shingo Yamamoto	HZD-R, Dresden, DE	T9
16:30	Optical control of magnetization dynamics in 4f electron systems	Karel Carva	Charles U., Prague, CZ	T10
17:00-19:00	**Welcome Party**			

Friday 16 June

	U-compounds (UTe2)	*Chair: Józef Spałek*		
9:00	Recent Updates on the High Field Phase Diagram of UTe_2	Peter Czajka	NIST, Gaithersburg, USA	T11
9:30	Structural Phase Transition and Appearance of a New Superconducting Phase in UTe_2 under high pressure	Fuminori Honda	Kyushu U, Fukuoka, JP	T12
10:00	Anisotropic signatures of electronic correlations in the electrical resistivity of UTe_2	Tristan Thebault	CNRS, Toulouse, FR	T13
10:30	*Coffee break*			
	U-compounds (U-Te)	*Chair: Józef Spałek*		
11:00	Structure of the Normal State in UTe_2 and its analogy to URu_2Si_2.	Sergii Khmelvskyi	TU Wien, AT	T14
11:30	Electronic structure of the U-Te thin films studied by photoelectron spectroscopy	Evgenia Tereshina-Chitrova	IOP ASCR, Prague, CZ	T15
12:00	*Lunch break*			
	U-compounds I	*Chair: Fuminori Honda*		
14:00	Magnetism and superconductivity in Hg-based *f*-electron compounds	Mitja Krnel	CPFS MPI, Dresden, DE	T16
14:30	Searching for new uranium-based arsenides	Nazar Zaremba	CPFS MPI, Dresden, DE	T17
15:00	Heat capacity of the Zintl phase UCu_2P_2	Ladislav Havela	Charles U., Prague, CZ	T18
15:30	*Coffee break*			
	Other materials	*Chair: Fuminori Honda*		
16:00	The enhanced role of orbital moment in van der Waals ferromagnet VI_3	Dávid Hovančík	Charles U., Prague, CZ	T19
16:30	Streamlining Sample Preparation by Means of Automation	Petr Čermák	Charles U., Prague, CZ	T20
17:00-19:00	**Poster session + refreshment**			
P01	Pseudogap and fluctuation conductivity of $YBa_2Cu_3O_{7-\delta}$ single crystals in the course of long-term aging	Liudmyla Bludova	B. Verkin ILTPE, Kharkow, UA	P01
P02	Field-Dependent Magnetic Ordering Dome and Quantum Spin Fluctuations in the Natural Mineral Henmilite	Ankit Labh	Charles U., Prague, CZ	P02
P03	Electronic Structures of RTe_3 (R=Pr, Er) Rare-Earth CDW Systems via Angle-Resolved Photoemission Spectroscopy	Jeongsoo Kang	Catholic U., Bucheon, Korea	P03
P04	Discovery of the kagome superconductor in the Half-Heusler "NbRhSb"	Mir Ali	ST, Relizane, Algeria	P04
P05	Structure and Magnetic Properties of $GdFe_2$-H Hydrides	Evgeniya Tereshina-Chitrova	IOP ASCR, Prague, CZ	P05
P06	Investigating the spin dynamics of Mn_5Si_3 and Mn_5Ge_3	Nikolaos Biniskos	Charles U., Prague, CZ	P06
P07	Physical properties of Uranium-Hafnium alloys and their hydrides	Shanmukh VV Devanaboina	Charles U., Prague, CZ	P07
P08	Understanding phonon-crystal field coupling, insights from polarized inelastic neutron scattering measurements on $CeAuAl_3$ and new theoretical framework	Michal Stekiel	FZ Juelich, Garching, DE	P08
P09	Structural studies of UCu_2P_2 under pressure	Oleksandr Kolomiyets	Lviv PN U., UA	P09
P10	Uranium hydride thin films: stabilization of thermodynamically unstable phases	Alexandra Koloskova	Charles U., Prague, CZ	P10

Saturday 17 June

	RE-compounds II	*Chair: Jeroen Custers*		
9:00	Magneto-elastic coupling and new phases in the Shastry-Sutherland compound RB_4 (R = Nd, Er, Ho)	Rüdiger Klingeler	Heidelberg U., DE	T21
9:30	Kagome spin ice in HoAgGe	Philipp Gegenwart	Augsburg U., DE	T22
10:00	Ambient and high-pressure electrical transport and structural investigations of magnetic Weyl semimetal PrAlGe	Utpal Dutta	IOP ASCR, Prague, CZ	T23
10:30	*Coffee break*			
	RE-compounds III	*Chair: Jeroen Custers*		
11:00	Spin Waves to Spin Excitons: using Weak β-Decay as a Probe	Sarah Dunsiger	TRIUMF, Vancouver, CA	T24
11:30	Heavy quasiparticles and electronic instabilities in $CeRh_2As_2$	Mitja Krnel Gertrud Zwicknagl	TU Braunschweig, DE	T25
12:00	*Lunch break*			
	***f*-electron compounds**	*Chair: Gertrud Zwicknagl*		
14:00	On valence-band photoemission from Am metal	Jindřich Kolorenč	IOP ASCR, Prague, CZ	T26
14:30	Hidden orders and magnetic excitations in spin-orbit correlated insulators	Leonid Pourovskii	CPHT, CNRS, Paris, FR	T27
15:00	Scaling down in order to reveal intrinsic properties of solid-state materials	Eteri Svanidze	MPI CPfS, Dresden, DE	T28
15:30	*Coffee break*			
	Applications	*Chair: Gertrud Zwicknagl*		
16:00	Simulation Tools for Improvement of the Fission Track Analysis Method for Nuclear Forensics	Itzhak Halevy	Ben Gurion U., Beer Sheva, IL	T29
16:30	Additive Manufacturing in Biomedical Applications	Galit Katarivas-Levy	Ben Gurion U., Beer Sheva, IL	T30
17:00	Summary			
19:00-22:00	Conference grill party			

Sunday 18 June

9:00 - 12:00	**Non-structured discussion and excursions to the laboratories**

TALKS

T01

Systematic analysis of the exchange interactions within Anderson-lattice model: Kondo and superexchange vs Dzyaloshinskii-Moriya interaction

Józef Spałek, Ewa Kądzielawa-Major, Maciej Fidrysiak, Maciej Hendzel

Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland

The Anderson-lattice model is regarded as the appropriate for description of the heavy-fermion systems, which reduces to the Kondo-lattice model in the case of strictly localized *f*-electrons. In the Kondo-lattice limit one can expect some sort of *f-f* exchange interaction which is intermediate between the superexchange and RKKY interaction.

In this paper we discuss results of a systematic expansion in the hybridization magnitude of the periodic Anderson model in the heavy-fermion limit for strongly-correlated *f*-electrons. We obtain the values of both Kondo exchange and superexchange integrals in that order, as well as that of the Dzyaloshinskii-Moriya interaction, in which three-spin interaction represents the coupling of conduction and lattice spins. Also, a residual hybridization is still present and leads to heavy effective masses of *f*-electrons.

If time allows, we present briefly our results in the limit of entirely localized *f*-electrons, when the Dzyaloshinskii-Moriya interaction is absent. Our results may form a basis of a systematic analysis of the Ce ($4f^1$) systems.

This work was supported by Grant OPUS No. UMO-2021/41/B/ST3/04070 from Narodowe Centrum Nauki. Funding by „Laboratories of the Young" as part of the „Excellence Initiative – Research University" program at the Jagiellonian University in Kraków is also acknowledged.

T02

Field-induced superconducting and metamagnetic phase transitions in a four-orbital model of UGe_2

Maciej Fidrysiak, Ewa Kądzielawa-Major, Danuta Goc-Jagło, Józef Spałek

Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland

The class of uranium-based compounds, encompassing UGe_2, UCoGe, URhGe and UIr, exhibits coexistent superconductivity and ferromagnetism, calling for identification of the underlying microscopic pairing mechanism [1]. Given substantial variation of ordered magnetic moments among those materials, both fluctuation- and local-correlation-driven scenarios have to be considered as candidates.

Here we extend our previous study [2] of UGe_2 and explore local-correlation induced paired states, with primary focus on magnetic and superconducting transitions induced by applied magnetic field. A four-orbital degenerate Anderson-lattice model is employed, encompassing two strongly correlated 5*f* orbitals, hybridized with conduction bands. Correlations in the *f*-electron sector are incorporated by means of intra- and inter-orbital Coulomb repulsion, as well as ferromagnetic (Hund's rule) interaction. The ferromagnetic exchange supports formation of local triplet Cooper pairs. The model is analyzed within the framework of Statistically-Consistent Gutzwiller wave-function method (SGA).

The reference SGA zero-field phase diagram encompasses high- and low-moment ferromagnetic orders, FM2 and FM1, respectively, as well as the paramagnetic phase. The transitions between magnetic states are controlled by the hybridization magnitude between *f*- and conduction-electrons, and are all of the first order at low temperature. Spin-triplet superconductivity of A_1 and A_2 types (in analogy to the notation used for superfluid ^{3}He) emerges in between the FM2 and FM1 states, qualitatively reproducing the structure of experimental pressure-temperature phase diagram of UGe_2. We subsequently demonstrate that external magnetic field is capable of driving the system through an analogous series of joint metamagnetic and superconducting transitions [3] (from FM1+A_1 to FM2+A_2 state), resulting in a physically sound overall phase diagram for a single set of microscopic model parameters. The field-dependence of orbital-resolved magnetic moments, superconducting order parameters, and their symmetries will be also discussed.

Finally, we remark on the complementary character of fluctuation- and correlation-driven pairing schemes, as well as outline the possibility of their unification within recently developed variational wave function approach combined with field-theoretical 1/*N* expansion [4].

This work was supported by Grant OPUS No. UMO-2021/41/B/ST3/04070 from Narodowe Centrum Nauki. Funding by „Laboratories of the Young" as part of the „Excellence Initiative – Research University" program at the Jagiellonian University in Kraków is also acknowledged.

[1] D. Aoki, K. Ishida, and J. Flouquet, J. Phys. Soc. Jpn. **88**, 022001 (2019).
[2] E. Kądzielawa-Major, M. Fidrysiak, P. Kubiczek, and J. Spałek, Phys. Rev. B **97**, 224519 (2018).
[3] M. Fidrysiak, D. Goc-Jagło, E. Kądzielawa-Major, P. Kubiczek, and J. Spałek Phys. Rev. B **99**, 205106 (2019).
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T03

Itinerant vs. localized *f*-electrons behavior in magnetic anisotropic properties of U-based ferromagnets

Alexandr Shick[1,2,3], Itzhak Halevy[4], Maxim Tchaplianka[1], Dominik Legut[3,5]

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[3]*VSB - Technical University of Ostrava, Ostrava, Czech Republic.*

[4]*Ben Gurion University of the Negev, Negev, Israel.*

[5]*Charles University, Prague, Czech Republic.*

Exploration of the electronic and magnetic character of quantum matter is one of the most fundamental fields of modern condensed matter physics. Traditionally, two competing itinerant and localized characteristics distinguish magnetic and heavy Fermi-liquid behaviour. Only a handful of quantum materials that show this itinerant-localized dichotomy are the uranium-based compounds UGe_2, UTe_2, URhGe, and UCoGe, where ferromagnetism coexists with unconventional superconductivity.

In this work, we examine the itinerant-localized dichotomy in selected U-based ferromagnets using the correlated band theory implemented in a local-spin-density plus Coulomb-U approach (LSDA+U). At first, we demonstrate that the LSDA+U with exact atomic limit LSDA+U(HIA) which combines the relativistic density functional theory with the Anderson impurity model provides a good quantitative description for spectroscopic and magnetic properties, including the magnetic anisotropy energy (MAE), of UGa_2. These results are compared with previous experimental and theoretical works and additional features are pointed out.
Next, the method is applied to UFe_{12} and $UFe_{10}Si_2$ ferromagnets. We estimate the thermodynamic stability for these materials in terms of the enthalpy of formation, and illustrate that the Si atom substitution into UFe_{12} stabilizes the $ThMn_{12}$-type crystal structure. Furthermore, the LSDA+U(HIA) calculations yield the uniaxial MAE of $UFe_{10}Si_2$ in agreement with available experimental data, and suggest $UFe_{10}Si_2$ ferromagnet as a candidate for magnetically hard material.

In recent years there is extensive research targeting new permanent magnets with a reduced amount of rare-earth elements. A good permanent magnet ought to have a reasonably high Curie temperature, a large magnetization for a high-energy product, and a substantial uniaxial MAE to resist demagnetization. Our results suggest that replacing a part of U atoms by some rare-earth like Sm in $UFe_{10}Si_2$ will further enhance the magnetization and MAE. This can facilitate the development of new rare-earth-lean permanent magnets.

We acknowledge partial support provided by EU OPVV project SOLID21-CZ.02.1.01/0.0/0.0/16_019/0000760, and the Czech Science Foundation (GACR) Grant No. 22-22322S. DL acknowledges the project e-INFRA CZ (ID:90140) by the Ministry of Education, Youth and Sports of the Czech Republic. ABS acknowledges financial support from the Israeli Ministry of Aliyah and Integration Grant 140636.

T04

The Density Functional theory study of electronic structure and magnetic properties of antiferromagnetic U_2TGa_3 (T = Pd, Pt) intermetallics

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Theoretical analysis of the electronic and magnetic characteristics of a series of light actinide compounds U_2TGa_3 (T = Pd, Pt) crystallizing in an orthorhombic $CeCu_2$-type structure (space group Imma) is presented in this research. The U-based compounds are ordered antiferromagnetically based on data of electrical resistivity, magnetism, and magnetic susceptibility measurements [1, 2]. According on neutron-diffraction patterns, the ordered uranium magnetic moments are estimated to be 0.32(5) μ_B/U and 0.38(5) μ_B/U for U_2PdGa_3 and U_2PtGa_3, respectively, being significantly lower than the moments of free uranium ions (U^{3+} (3.6 μ_B/U) and U^{4+} (3.58 μ_B/U)). This fact, along with the specific heat and electrical resistivity measurements, demonstrates that the Kondo effect may be present in an antiferromagnetically ordered state. Using density functional theory (DFT), we show considerable changes in the magnetic moments and electronic structural characteristics of these compounds. Using Full-Potential Linearized Augmented Plane-Wave (FP-LAPW) method [3], the electronic structure properties are discussed in terms of Hubbard U and J parameters. While taking into account the importance of orbital magnetism in uranium-based compounds the Orbital Polarization Correction (OPC) was used to model the magnetic properties by the Full-potential local-orbital (FPLO) method [4]. The reduced magnetic moments in comparison to the theoretical magnetic moment of U^{3+} ion support the previously obtained experimental findings. However, better convergence to the experimental data is in the case of GGA+OPC. In particular, the reduction in magnetic moments and DOS enhancement at the Fermi energy are in good agreement with the Kondo lattice characteristics. Moreover, the frequency-dependent dielectric functions for U_2TGa_3 (T = Pd, Pt) were also estimated using the dynamical model that was employed in time-dependent DFT computations (TDDFT) [5].

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T05

Spin-orbit interactions - the atomic physics in the solid-state physics

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Spin-orbit interactions, well known in the atomic physics, are rather weak interactions - only recently their importance have been revealed in theoretical description of oxides with open-shell d atoms. The first effect of s-o interactions have been observed for iridates due to their much stronger interactions in heavy ions. In Sr_2IrO_4 a localized state at 0.6 eV has been interpreted as originated from crystal-field + s-o interactions of the Ir^{4+} ion. This interpretation proves the importance of s-o interactions, as well as postulated earlier the existence of ions with the integer valency. At present more and more experiments reveal the existence of the discrete low-energy electronic structure also in 3*d*-ion oxides.

The experiments confirm the author's 35-years scientific project "From the atomic physics to solid-state physics" which one could call as Quantum Atomistic Solid-State Theory (QUASST). QUASST starts theoretical description of a solid containing open *d*/*f* shell atoms from analysis of the charge and low-energy electronic structure of the involved 3*d*/4*f*/5*f*/4*d*/5*d* ions. This low-energy electronic structure is determined by crystal-field and spin-orbit interactions. Crystal-field interactions are related to the charge distribution with the crystallographic lattice. Crystal field effect is a multipolar Stark effect known in the atomic physics. Similarly, in the magnetically-ordered state one deal with the Zeemann effect.

Recently also in so profound heavy-fermion intermetallics like $CeRh_2Si_2$, $YbRh_2Si_2$, $CeCu_2Si_2$, known as Kondo-lattice intermetallics, practically all Ce and Yb atoms turn out to be in the well-defined trivalent state exhibiting low energy crystal-field localized states.

Results for $CeRh_2Si_2$, K_2CoF_4, $FeBr_2$, $LaCoO_3$, Sr_2VO_4, Ba_2IrO_4 , Sr_2RuO_4 will be shown. Sr_2RuO_4, exhibiting superconductivity below 1.5 K, will be discussed pointing out its persistent nonmagnetic state as due to the nonmagnetic singlet ground state of the Ru^{4+}-ion produced by intra-atomic spin-orbit interactions . It is somehow realization of the Jahn-Teller effect.

We claim that

i) the conventional crystal-field interactions should be evaluated the first for any meaningful description of magnetic and electronic properties of any 3*d*/4*d*/5*d*/4*f*/5*f* compound,

ii) in such compounds there exists the discrete electronic structure, giving effects close to the Fermi surface at the energy scale even below 1 meV,

iii) the 3*d* electrons exhibit a substantial localized character forming strongly-correlated 3dn configurations, and

iv) the standard band structure calculations, in the eV-energy scale, should be complemented with this discrete low-energy atomic-scale electronic structure.

T06

Investigating the Superconducting State of the Heavy Fermion Compound Ce_3PtIn_{11}

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The heavy fermion compound Ce_3PtIn_{11} shows various unusual properties. The compound belongs to the $Ce_nT_mIn_{3n+2m}$ class of materials which comprises a numerous number of interesting compounds including $CeCoIn_5$, $CeRhIn_5$, and Ce_2RhIn_8. The crystal structure is tetragonal *P4/mmm* with lattice parameters a = 4.6874(4)Å and c = 16.8422(12)Å. Interestingly, the a-lattice parameter is close to the one of $CeIn_3$ yielding 4.6907Å.

At ambient pressure, the compound displays two consecutive magnetic transitions into antiferromagnetic (AFM) states at T_{N1} = 2.2K and T_N = 2.0K, respectively. Below T_c = 0.32K superconductivity (SC) is found [1]. It has been speculated that the coexistence of AFM and SC results from the presence of two inequivalent Ce sites. The surrounding of the Ce1-ion is identical to Ce-atoms in Ce_2TIn_8 with T being a transition element and is believed to be largely Kondo screened and responsible for SC. The Ce2-ion experiences a $CeIn_3$-like environment and hence, is assumed to order magnetically. Entropy analysis indeed conjectured this idea [1] and further support comes from ^{115}In NQR experiments [2] revealing that the magnetic moment of Ce2 has to be 20 to 40 times larger than the moment of Ce1 [2,3]. More intriguing, in the NQR experiment a sudden drop of spin-relaxation rate $1/T_1$ emerges upon entering the superconducting state suggesting a first order type of transition from the AFM state into the SC one [4]. Such would indicate a breaking of symmetry implying that magnetic order and superconductivity compete. Here we discuss recent results on low-temperature specific heat and magnetization measurements. In addition, we conducted zero-field and longitudinal field muon spin resonant experiments in the paramagnetic state and the SC state. We found evidence for the presence of a static or quasi-static internal field for $T < T_c$ corroborating the co-existence of magnetic order and superconductivity.

*Samples have been grown in MGML (mgml.eu), which is supported within the program of Czech Research Infrastructures (project no. LM2023065)

T07

Low-temperature antiferromagnetic order in orthorhombic $CePdAl_3$

Vivek Kumar[1], Andreas Bauer[1], Christian Franz[1,2], Jan Spallek[1], Michal Stekiel[1,2], Astrid Schneidewind[2], Marc Wilde[1], Christian Pfleiderer[1]

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Recently, Ce-based intermetallic compounds with the structure formula $CeTAl_3$ (with *T* being a transition metal) [1] attracted considerable scientific attention due to the observation of vibronic bound states and magneto-elastic hybrid excitations in $CeCuAl_3$ [2] and $CeAuAl_3$ [3]. Here, we report a study of the magnetic and thermodynamic properties of single-crystal $CePdAl_3$ grown by means of the optical floating zone technique. Depending on the growth conditions, either a tetragonal (space group *I*4*mm*) or an orthorhombic (space group *Cmcm*) modification crystallizes. Twinning occurs in the orthorhombic crystals with twins differing in their orientation in the basal plane, while sharing a common hard axis. While the tetragonal compound remains nonmagnetic down to the lowest temperatures studied, the orthorhombic compound develops antiferromagnetic order below a Néel temperature of 5.6 K. In this state, the localized cerium moments align antiparallel along the magnetically easy axes. The magnetic properties exhibit a pronounced anisotropy, with magnetic fields along the easy axes inducing a spin-flop transition. The electronic contribution to the specific heat is described by a Sommerfeld coefficient of 121 mJ K^{-2} mol^{-1}, characteristic of moderate heavy-fermion behavior. Magnetic phase diagrams are inferred, providing a solid point of reference for further studies of this compound [4].

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T08

Magnetism of R_2Cu_2In intermetallic compounds

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Family of R_2T_2X compounds crystallizing in the tetragonal Mo_2FeB_2-type structure (*P*4/*mbm*) represents a playground for investigation of magnetism in the broader context. The reason is that these systems are formed both by lanthanides and actinides allowing to compare the localized magnetism of regular rare-earths with the delocalized 5*f* states, e.g. in U-compounds, through potentially unstable magnetism in systems based on anomalous rare earth elements. Although the main attention is dedicated to compounds with anomalous 4*f* and 5*f* elements, the physics of localized systems is interesting as well and important for understanding of the behavior throughout the given R_2T_2X family.

Anisotropic properties of R_2T_2X are often related to the details of crystal structure with specific layout of R-atoms in the *aa*-planes, forming the motif equivalent to the potentially frustrated 2D Shastry-Sutherland lattice. Competition of magnetic interactions on potentially frustrated anisotropic lattice, together with their typically oscillating RKKY character, may result in the complex magnetic structures and rich magnetic phase diagrams. Another structural aspect is given by the fact that *P*4/*mbm* structure is realized rather in compounds with larger unit cell volume $V_{u.c.}$, while the systems with lower $V_{u.c.}$ adopt different structure.

The border of *P*4/*mbm* structure stability is almost copied by the unit cell volumes of compounds from R_2Cu_2In series making these systems of particular interest. Here we present the magnetic studies on Ce_2Cu_2In, Dy_2Cu_2In and Tm_2Cu_2In. Kondo-lattice system Ce_2Cu_2In is known to exhibit two successive antiferromagnetic phase transitions at 5.5 K and 4.8 K [1], while the character of magnetic ordering in Dy_2Cu_2In is not fully clear [2,3]. Ferromagnetic Tm_2Cu_2In as the system with almost lowest $V_{u.c.}$ among *P*4/*mbm* compounds was found to exhibit the glassy features [4,5].

We report on the resistivity, magnetization and specific heat measurements, however the special focus is given to the neutron diffraction experiment providing the important insight into the microscopic details of R_2Cu_2In magnetism [6]. Due to the strong relation of magnetic properties and crystal lattice, the results are discussed in context of lattice changes in various conditions. The non-magnetic analogue Lu_2Cu_2In allowing to estimate the lattice contribution to observed behavior was prepared and investigated as well. In addition, the experimentally obtained results are compared to supportive DFT calculations.

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T09

Structural 130 K phase transition and emergence of a coherent Kondo state in Ce_2Rh_2Ga explored by $^{69,71}Ga$ NQR

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Objectives and methods:

The recently synthesized compound Ce_2Rh_2Ga [1] exhibits a structural phase transition at T_t ~ 130 K [2] that is accompanied by a slight increase of the Ce valence beyond 3+ [3]. The symmetry reduction below T_t results in two inequivalent Ce and Ga sites. To obtain microscopic information on the nature of the 130 K phase transition as well as on the formation of the correlated ground state, we used $^{69,71}Ga$ NQR as a site-selective microscopic probe of Ce_2Rh_2Ga [4].

Results:

A structural phase transition at T_t is revealed by a splitting of the high-temperature single NQR line into two well-resolved NQR lines, providing evidence for two crystallographically inequivalent Ga sites. The NQR frequencies are in good agreement with fully relativistic calculations of the band structure. Our NQR results indicate the absence of magnetic or charge order down to 0.3 K. The temperature dependence of the spin-lattice relaxation rate $1/T_1$ shows three distinct regimes, with onset temperatures at T_t and 2 K. The temperature-independent $1/T_1$, observed between T_t and 2 K, crosses over to a Korringa process, $1/T_1 \propto T$, below $\sim$ 2 K, which evidences a dense Kondo coherent state. For the two different Ga sites, the Korringa process sets in at different temperatures, 2.0 and 0.8 K.

Conclusions:

The NQR spectral variations with temperature across T_t provide evidence for the absence of magnetic or charge order. The temperature dependence of the spin-lattice relaxation rate at the two Ga sites clearly indicates the formation of a heavy-fermion state, but the transition to this state occurs at two different temperatures. Ce_2Rh_2Ga is thus a rather unusual 4*f* system that can serve as a platform to study the two-ion Kondo physics.

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T10

Optical control of magnetization dynamics in 4*f* electron systems

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All-optical magnetization switching is emerging as a novel magnetic recording technology. A complete reversal of magnetization due to a fs laser pump has been observed in specific rare-earth basedintermetallics with ferrimagnetically ordered sublattices. We use first-principles methods to calculate exchange interactions between atomic moments, as well as the intra-atomic exchange between Gd 4*f* and 5*d* orbitals to allow mapping of the problem onto an effective orbital-resolved Heisenberg Hamiltonian. A subsequent simulation based on the LLG equation has shown distinct magnetization dynamics of 4*f* and 5*d* orbitals, and reproduced the switching behavior [1]. We will discuss why Gd and Tb exhibit significantly different magnetization dynamics on ultrafast timescale, and complications associated with the ab initio description of Tb [2].

We also show that with ultrashort laser pulses the magneto-crystalline anisotropy (MCA) can be manipulated via excitations of the orbital state. In high-density magnetic recording media large MCA stabilizes the stored information against decay through thermal fluctuations and allows for higher information density. However, it also renders the change of magnetization state more difficult. Therefore an effect allowing to control efficiently a high-anisotropy magnet is of high importance. In Tb metal the magnetic moment and high MCA both source in the 4*f* electronic shell. Electron-electron scattering processes following IR-laser pumping lead to selective excitations from the 4*f* ground-state. These orbital excitations allow us to alter the MCA. This cannot be achieved by heating: The material would rather be damaged than the 4*f* configuration changed. Besides their technological potential, MCA-changing excitations have implications for the understanding of magnetic dynamics processes on ultrashort time scales, where the orbital state affects the angular momentum transfer between spin system and lattice.

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T11

Recent Updates on the High Field Phase Diagram of UTe_2

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UTe_2 has attracted an enormous amount of interest in recent years as a likely spin triplet superconductor. The material displays a complex phase diagram, which includes reentrant superconductivity and metamagnetism. The unique interplay between these effects is highlighted by the surprising emergence of an additional high field superconducting phase for fields oriented 20 to 40 degrees from the b towards the c axis. The underlying mechanism and order parameter(s) for the various superconducting phases are still unclear. A guiding focus of our group has been the investigation of how the superconducting phase diagram responds to a variety of perturbations such as pressure, sample composition, and field orientation. Here, I will discuss some recent high field experiments and how our results fit into the ongoing debate over the system's precise superconducting phenomenology.

T12

Structural Phase Transition and Appearance of a New Superconducting Phase in UTe_2 under high pressure

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UTe_2 is one of the hottest topics in condensed matter physics, because of its unusual superconducting properties, such as topological superconductivity, field-reentrant superconductivity, and multiple superconducting phases in a magnetic field as well as under high pressure [1,2]. Indeed, the huge field-reentrant superconductivity detected in the hard-magnetization axis in UCoGe and URhGe [3] resembles that observed in UTe_2 for H || b-axis. On the other hand, no magnetic ordering was found down to low temperatures, revealing a paramagnetic ground state in UTe_2, which is quite in contrast to the above-mentioned ferromagnetic superconductors.

The pressure response of UTe_2 is very sensitive, displaying different superconducting and magnetic states. Applying the pressure, the superconducting transition temperature splits above 0.3 GPa, revealing multiple superconducting phases. Above the critical pressure of 1.5 GPa, superconductivity is suppressed and the magnetically ordered phase, most likely antiferromagnetism, appears under higher pressure. Surprisingly, UTe_2 reveals such rich and unexpected phase diagrams under pressure and magnetic field. This is most likely due to a unique crystal structure and its instability. It is important to elucidate the pressure response of the crystallography and the electronic state at high pressures. In order to clarify these points, X-ray diffraction and electrical resistivity measurements up to 10GPa have been carried out [4].

The X-ray diffraction measurements under high pressure using a synchrotron light source reveal anisotropic linear compressibility of the unit cell up to 3.5 GPa, while a pressure-induced structural phase transition is observed above $P_{O\text{-}T}$ ~ 3.5-4 GPa at room temperature, and around 5.5 GPa at 29 K, where the body-centered orthorhombic crystal structure with the space group Immm changes into a body-centered tetragonal structure with the space group I4/mmm. The molar volume drops abruptly at $P_{O\text{-}T}$, while the distance between the first-nearest neighbor of U atoms, $d_{U\text{-}U}$, increases, implying a switch from the heavy electronic states to the weakly correlated electronic states. We have also discovered a new superconducting phase at pressures higher than 7 GPa with T_{sc} > 2 K with an upper-critical field, $H_{c2}(0)$ ~ 3 T. The resistivity above 3.5 GPa, thus, in the high-pressure tetragonal phase, shows another anomaly around 230 K.

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T13

Anisotropic signatures of electronic correlations in the electrical resistivity of UTe_2

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Following the discovery of unconventional superconductivity in UTe_2 in 2019, multiple superconducting phases were found in this system under magnetic field and pressure, in relation with a complex competition of electronic correlations. Here, we studied the anisotropy of the magnetoresistivity to have some insight on the correlations leading to superconductivity. By changing the current direction from **a** to **c**, we evidenced the magnetic field evolution of two temperature scales at 15 K and 35 K, under a field up to 70 T along the three crystallographic directions. We extracted an anisotropic Fermi-liquid-like coefficient A at low temperature from the T^2 dependence of the resistivity. We observed differences in the field-variations of A for **I** || **a** and **I** || **c** near the metamagnetic transition induced at $\mu_0 H_m$ = 35 T for **H** || **b**. Our findings will be discussed in relation to the high-field stabilization of superconductivity near Hm in this material.

T14

Structure of the Normal State in UTe_2 and its analogy to URu_2Si_2.

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The newly discovered UTe_2 superconductor is regarded as a heavy fermion mixed-valence system with very peculiar properties within the normal and superconducting states. It shows no signs of magnetic order but strong anisotropy of a magnetic susceptibility and a superconducting critical field. In addition to the heavy fermion-like behavior in the normal state, it exhibits also a distinctive Schottky-type anomaly at about 12 K and a characteristic excitations gap ~35-40 K. Here we show, by virtue of dynamical mean-field theory calculations with a quasi-atomic treatment of electron correlations, that ab-initio derived crystal-field splitting of the $5f^2$ ionic configuration yields an agreement with these experimental observations. A close analogy of the normal paramagnetic state of UTe_2 to that of URu_2Si_2 in the Kondo arrest scenario is revealed. We consider the impact of the anisotropic super-exchange interactions within the U-U structural dimer on magnetization and development of strong orbital and magnetic moment fluctuations in UTe_2. We calculate on an ab-initio level the crystal filed splitting of the ground state multiplet of the U ion by employing a charge self-consistent DFT+DMFT methodology, based on the assumption of a full localization of the $5f^2$ configuration. We show that this assumption and derived ab-initio results are fully consistent with the observed macroscopic measurements of magnetization and specific heat. The present results may add to the better understanding of the nature of the mixed valence state in UTe_2, which is a the subject of heated discussion in current literature.

T15

Electronic structure of the U-Te thin films studied by photoelectron spectroscopy

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Uranium tellurides have a range of bulk compositions, including UTe, U_3Te_4, U_2Te_3, U_3Te_5, U_7Te_{12}, UTe_2, U_2Te_5, UTe_3, and UTe_5, and have been the subject of previous research focusing on their magnetic properties [1-3]. The discovery of unconventional superconductivity in UTe_2 [4] has rekindled interest in the electronic structure of these materials, prompting the need for more detailed studies.

In the present work, we investigated the electronic structure of the sputter-deposited U-Te thin films using in-situ X-ray Photoelectron Spectroscopy (XPS). The films were prepared in the home-built [5] ultra-high vacuum equipment using separate U and Te targets, with Te evaporated simultaneously with plasma sputtering of the U target (natural uranium, 99.9 wt.% purity). The non-equilibrium process of sample preparation allowed for the stabilization of a variety of compositions, both stable and non-existent in bulk. We followed evolution of the U-5*f* core level lines and of the valence band spectra, addressing the problem of localization of the 5*f* electrons in films with various U-Te compositions. Electrical resistivity and magnetization measurements were also conducted, with the results matching those of bulk compositions.

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T16

Magnetism and superconductivity in Hg-based *f*-electron compounds

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Crystallographically complex compounds containing 4*f* and 5*f* electrons often have peculiar chemical and physical properties. Among Hg-based lanthanides and actinides, such an example is the antifferomagnetic heavy fermion $U_{23}Hg_{88}$ [1]. The toxicity and air- and moisture sensitivity of some Hg-based *f*-compounds makes synthesis and characterization of these compounds challenging. Therefore the properties for some Hg-based *f*-compounds have not been explored in detail so far.

By using the existing phase diagram of La-Hg, we tried to resynthesize the $LaHg_{6\sim}$ compound and explore its properties. We were able to synthesize single crystals of this compound by using self-flux method, identify its chemical composition by single crystal XRD as $LaHg_{6.4}$ and do a complete characterization of its chemical and physical properties. In a similar way we were able to synthesize single crystals of the isostructural $UHg_{6.4}$.

The $LaHg_{6.4}$ [2] and $UHg_{6.4}$ [3] crystallize in a new structure type that can be represented by La/U centered polyhedra with coordination numbers 13 and 14. Despite the $LaHg_{6.4}$ is strongly crystallographically disordered in one dimension, superconductivity was observed. The measurements of specific heat, magnetization and electrical resistivity reveal that $LaHg_{6.4}$ enters the superconducting state below T_c = 2.4 K, being a conventional type II superconductor. The same kind of disorder as in $LaHg_{6.4}$ is found in $UHg_{6.4}$, which orders antiferromagnetically below T_{N1} = 35.5 K and displays another transition at T_{N2} = 47.3 K, which is also likely antiferromagnetic.

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T17

Searching for new uranium-based arsenides

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As new classes of superconducting materials emerge, puzzles of high-temperature superconductivity continue to be one of the pressing issues in condensed matter physics and solid-state chemistry. In particular, iron pnictide superconductors still pose many open questions. Surprisingly, very few actinide-based analogs of iron pnictide high-temperature superconductors have been reported so far, perhaps as a result of synthesis complications imposed by toxicity, reactivity, and high vapor pressure of constituent elements. In this work, we revisit the U-Fe-As ternary, in which only one compound has been reported to exist so far – $UFeAs_2$ (*P*4/*nmm* space group) [1]. By implementing flux synthesis, we were able to grow large single crystals of UFe_5As_3 compound, which adopts UCr_5P_3 structure type [2] ($P2_1/m$, *mP*18) with lattice parameters a = 7.0501(17) Å, b = 3.8582(9) Å and c = 9.6342(13) Å, β = 100.2(8)° [3]. The refined composition agrees well with the elemental ratio established by the EDX analysis – $U_{9.9(2)}Fe_{58.7(2)}As_{31.4(2)}$. The magnetic behavior of UFe_5As_3 was studied by magnetic susceptibility measurements in the temperature range 1.8 - 600 K and an antiferromagnetic ordering below T_N = 56 K was established. The Sommerfeld coefficient γ = 138 mJ/mol K^2 indicates enhanced effective electron mass. More in-depth investigations of this and other U-Fe-As ternary compounds are currently underway.

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T18

Heat capacity of the Zintl phase UCu_2P_2

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The highest T_C in a purely 5*f* ferromagnet was found in UCu_2P_2. Its T_C = 216 K [1] can be still dramatically enhanced under pressure. It belongs to the layered Zintl phases with the trigonal structure of the $CaAl_2Si_2$ type (*P*-3*m*), formed by alternating cationic (Ca) and anionic (Al-Si) layers. Computations show that the polar character of the bonding is a vital ingredient in reaching such high T_C. One of important results is that it is a half-metal. Spin polarization of the 5*f* states is imprinted also on the light electronic states, leaving only a low density of spin-up states at the Fermi level. Spin-down states form a gap.

U moments are aligned along the *c*-axis. The Ising character of magnetism was, however, difficult to reconcile with heat capacity measurements. An optimum Debye model used to describe the phonon contribution was leaving lot of magnetic entropy at low temperatures. Therefore we performed ab-initio calculation of phonons using harmonic and quasi-harmonic approximations, which give an excellent match to experimental data. They indicate that the lattice is strongly non-Debye like and there is no magnetic entropy up to ≈ 100 K. Analysis shows that the soft transversal acoustic mode (0,0,*q*) related to the U atoms is the culprit. The magnetic entropy can be described by an exponential function of *T* assuming a magnon gap of ≈ 500 K. The total entropy is however still high, pointing to local-moment character of 5*f* magnetism.

The soft phonon mode also describes entirely the low-*T* non-linearity of $C/T(T^2)$, which helps to identify that the Sommerfeld coefficient is only 0.5 mJ/mol K^2.

This work was supported by the Grant Agency of the Czech Republic under the grant No. 21-09766S.

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T19

The enhanced role of orbital moment in van der Waals ferromagnet VI_3

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Van der Waals (vdW) materials based on 3*d*-transition metals showing long-range magnetic order down to monolayer limit are an ideal platform for studying two-dimensional (2D) magnetism with vast application potential in the field of spintronics. The magnetic anisotropy plays a key role in forming 2D magnetic order in these materials which rises an importance of understanding its microscopic origin. We used the X-ray magnetic circular dichroism (XMCD) effect to address the electronic and magnetic properties of vdW ferromagnet VI_3. Our results provide direct evidence of large unquenched out-of-plane orbital moment of the V^{3+} ion explaining the strong magnetocrystalline anisotropy[1]. We signify the effect of spin-orbit coupling on the electronic ground state[2]. The simulations of the XMCD spectra using ligand field multiplet approach with the synergy of DFT calculations suggest the existence of two inequivalent V^{3+} ion structural positions with different orbital configuration.

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T20

Streamlining Sample Preparation by Means of Automation

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We are currently on the cusp of the fourth industrial revolution, which could revolutionize not only industrial production but also scientific research. By leveraging the power of big data and artificial intelligence, the fourth industrial revolution will usher in an era of smart laboratories and automation that has never before been possible. This will be a game-changer for scientific fields such as the physics of *f*-electron systems, where sample preparation relies heavily on manual work by scientists.

The field of inelastic neutron scattering has long faced the persistent problem of needing large sample sizes for analysis. Traditional methods of co-aligning single crystals to achieve the necessary sample size are time-consuming and imprecise [1]. However, the newly constructed Automatic Laue Sample Aligner (ALSA) represents a significant breakthrough in the field. ALSA utilizes state-of-the-art technology, including an X-Ray Laue diffractometer, robotized manipulators, real-time computer vision, a Bayesian optimization engine, and bespoke neural network software for crystal placement and Laue pattern solving. This innovative device will automate the crystal co-alignment process, drastically reducing sample preparation time and improving precision.

The same robotic system can be used for precise positioning of the samples to the holders, sample preparation, cutting, and polishing of the bulk crystals. The implications of these techniques for the future of condensed matter physics are significant and will be discussed in detail during the talk.

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T21

Magneto-elastic coupling and new phases in the Shastry-Sutherland compound RB_4 (R = Nd, Er, Ho)

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The family of tetraborides RB_4 exhibits magnetic frustration of the rare earth moments which are arranged on a frustrated Shastry-Sutherland lattice. The materials enable one to study frustrated magnetism in a quasi-classical limit of large magnetic moments and with the evolvement of orbital degrees of freedom. We report high-resolution dilatometry studies on single crystals of RB_4 in DC magnetic fields up to 35 T. The dilatometry studies are supported by specific heat and magnetization data. In all RB4 under study, evolution of various magnetically ordered phases is associated with lattice changes thereby evidencing significant magneto-elastic coupling and enabling us to quantify uniaxial pressure dependencies. In NdB4, commensurate antiferromagnetic order appears at T_N = 17.2 K while incommensurate order and an additional low-temperature phase appear at T_{IT} = 6.8 K and T_{LT} = 4.8 K, respectively. We attribute the later to a structural transition. From the observed anomalies the magnetic phase diagrams for $B \| c$ up to 15 T and for $B \| [110]$ up to 35 T are constructed. New in-field phases are discovered for both field directions and already known phases are confirmed. In particular, phase boundaries are unambiguously shown by sign changes of observed anomalies and corresponding changes in uniaxial pressure effects. In ErB_4, we find magnetization plateaus at 1/3, 1/2, and 2/3 for $B||a$ in addition to a previously reported ½ plateau for $B||b$, all of which associated with magnetostriction anomalies. For ErB_4 and HoB_4 the magnetic phase diagrams are constructed too and uniaxial pressure effects are evaluated.

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T22

Kagome spin ice in HoAgGe

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Spin ice denotes a novel state of matter, arising in certain geometrically frustrated magnets that do not have a single minimal-energy state but rather fulfill an ice constraint, leading to highly degenerate local spin configurations. While three-dimensional pyrochlore spin ice is well established, its two-dimensional counter-part "Kagome spin ice", with 2 in-1 out or 1 in-2-out ice rule, leading to a honeycomb lattice of positive/negative magnetic monopoles, was only studied on artificial nanorods of ferromagnet films. The rare-earth intermetallic HoAgGe has non-Kramers $4f^{10}$ moments on a distorted kagome lattice with the four lowest crystal electric field modes contributing to magnetism at low temperatures. Remarkably the in-plane magnetization at low temperatures reveals a series of metamagnetic transitions separating fractional magnetization plateaus. Refinement of single crystal neutron diffraction reveals that all these states fulfill the kagome ice rule, establishing HoAgGe as first crystalline kagome spin ice [1]. Magnetotransport and anomalous Hall effect (AHE) show pronounced signatures related to the transitions between the fractional magnetization plateaus. They allow to distinguish domains with opposite toroidal orders and differing AHE yet similar magnetization, implying a hidden time-reversal-like degeneracy, related to the non-trivial distortion of the kagome lattice in HoAgGe [2]. We also discuss emergent quantum magnetism in the low-T c-axis magnetization.

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T23

Ambient and high-pressure electrical transport and structural investigations of magnetic Weyl semimetal PrAlGe

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We present a comprehensive study of the ambient and high-pressure electrical transport and structural properties of PrAlGe, a recently discovered magnetic Weyl semimetal. At ambient pressure, we observe an anomaly related to the Curie temperature at T_C = 15.1 K in the temperature dependence of electrical resistivity, accompanied by the presence of the anomalous Hall effect (AHE) at temperatures below T_C. Under high-pressure conditions, we find that the Curie temperature increases with pressure at a rate of 1.4 K/GPa, resulting in $T_C \approx 47$ K at 23.0 GPa. Furthermore, we identify a strong competition between the Lorentz force mechanism and spin scattering mechanism, which is suppressed by a magnetic field, as deduced from magnetoresistance measurements under pressure. Surprisingly, the AHE persists even at the highest applied pressures, indicating its robustness in the high-pressure regime. We also observe a clear anomaly in the pressure dependence of T_C, magnetoresistance, and Hall effect at 12.5 GPa, suggesting a pressure-induced electronic transition. High-pressure XRD measurements reveal that this transition is an isostructural electronic transition, as the $I4_1md$ structure remains stable up to ~19.6 GPa. Our findings provide important insights into the interplay between electronic and structural properties in PrAlGe, shedding light on the unique behavior of this material as a magnetic Weyl semimetal under both ambient and high-pressure conditions.

T24

Spin Waves to Spin Excitons: using Weak β-Decay as a Probe

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Variants of conventional nuclear magnetic resonance (NMR), μSR and β-detected NMR techniques offer a sensitive probe of the local magnetic environment in condensed matter. I will describe examples of how radioactive species like muons or ^{8}Li nuclei may be used to probe the nature of the magnetic excitations, ranging from spin waves through to those in topological Kondo insulator candidates:

Europium chalcogenides have long been recognised as experimental realisations of classic 3D Heisenberg spin systems, with simple rock salt crystalline structures. The compounds EuO and EuS are also rare examples of ferromagnetic semiconductors, where strong indirect exchange interactions between the localised Eu^{2+} ions are mediated by charge carriers rather than superexchange. More recently, artificial magnetic semiconducting heterostructures have generated tremendous interest, due to their potential for spintronics applications. One candidate, EuO_{1-x}/ n-Si:As combines a model ferromagnet with the dominant semiconductor used for practical devices. The low frequency spin dynamics may be investigated locally both within the film and also in a proximal manner using depth resolved low energy μSR. Complementary β-NMR measurements, sensitive to spin fluctuations on much longer millisecond timescales, enable the investigation of the dynamical response within the underlying substrate.

The mixed-valence compound SmB_6 is a well-known Kondo insulator, in which the hybridisation of itinerant 5d electrons with localized 4f electrons leads to a transition from metallic to insulating behavior at low temperatures. Recent studies suggest that SmB_6 is also a topological insulator, with topological metallic surface states emerging from a fully insulating hybridized bulk band structure. Yet there are several puzzling and unexplained physical properties of the insulating bulk. It has been proposed that bulk spin excitons may be the source of these anomalies and may also adversely affect the topologically protected metallic surface states. Muon spin rotation measurements of SmB_6 that show thermally activated behavior for the temperature dependence of the transverse-field relaxation rate below 20 K and a decreasing contact hyperfine field contribution to the positive muon Knight shift below 5–6 K.

It is also possible to disentangle extrinsic and intrinsic sources of low-temperature bulk magnetism in the candidate topological Kondo insulator (TKI) SmB_6 using μSR. Results on Al-flux-grown SmB_6 single crystals are compared to those on a large floating-zone-grown $^{154}Sm^{11}B_6$ single crystal in which a 14 meV bulk spin exciton has been detected by inelastic neutron scattering. Below ∼10 K, we detect the gradual development of quasistatic magnetism due to rare-earth impurities and Sm vacancies. Our measurements also reveal two additional forms of intrinsic magnetism: (1) underlying low-energy (∼100 μeV) weak magnetic moment ($\sim 10^{-2}$ μ_B) fluctuations similar to those detected in the related candidate TKI YbB_{12} which persist down to millikelvin temperatures, and (2) magnetic fluctuations consistent with a 2.6 meV bulk magnetic excitation at zero magnetic field which appears to hinder surface conductivity above ∼4.5 K. Potential origins of the magnetic response are discussed.

T25

Heavy quasiparticles and electronic instabilities in $CeRh_2As_2$

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The heavy-fermion superconductor $CeRh_2As_2$ exhibits a rich phase diagram at low temperatures. The observation of multi-phase superconductivity has been of particular interest [1]. The present contribution deals with the low-temperature normal state out of which the superconducting phases are forming. The central focus are the narrow quasiparticle bands and the electronic instabilities of the Fermi liquid state. We present calculations of the heavy quasiparticles in the heavy-fermion compound $CeRh_2As_2$. The narrow quasiparticle bands that are derived from the Ce-4*f* degrees of freedom are calculated by means of the Renormalized Band (RB) method. The RB scheme provides a framework for a realistic description of the coherent low-energy excitations in a Fermi liquid which combines material-specific ab-initio methods and phenomenological considerations in the spirit of the Landau theory of Fermi liquids. The central focus of the present study is the role played by the non-symmorphic lattice structure and the consequences of the Crystalline Electric Field (CEF) which removes the orbital degeneracy of the Ce 4f states. We conjecture that the quasi-quartet CEF ground state in combination with pronounced nesting features of the Fermi surface may give rise to a quadrupole density wave [2].

*This work is supported by the ANR-DFG program Fermi-NESt.

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T26

On valence-band photoemission from Am metal

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The 5f states in americium metal are generally agreed to be localized, similar to 4*f* states in lanthanides, being in a well-defined $5f^6$ configuration (Am^{3+}). In the same time, the valence-band photoemission spectrum [1,2] cannot be interpreted as a single set of multiplet transitions ($5f^6 \rightarrow 5f^5$) like in lanthanides [3], and a second set of transitions ($5f^7 \rightarrow 5f^6$) has to be introduced [4]. Two mechanisms were suggested as a possible origin of these additional transitions: (i) Am^{2+} layer forming at the surface of the sample or (ii) a second screening channel for the 5*f* hole created during the photoemission process, with the second mechanism later determined as the more likely [2]. Up to now, there does not seem to be a quantitative theory that ould substantiate these empirical ideas. The best attempt to date [5] combined the DFT+DMFT method with a generalized Hubbard-I impurity solver, which reproduced the $5f^7 \rightarrow 5f^6$ part of the spectrum well, but it also generated a spurious 5*f* intensity at the Fermi level. Here I report a DFT+DMFT study employing a more accurate impurity solver (exact diagonalization) and demonstrate the mechanism leading to the $5f^6$ final-state multiplets in the Am PES spectra.

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T27

Hidden orders and magnetic excitations in spin-orbit correlated insulators

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A large spin-orbit (SO) coupling in heavy transition-metal (TM) and actinide ions often induces spin-orbit-entangled atomic ground states on their partially filled *d* and *f* shells. This SO entanglement is at the origin of unusual low-temperature orders and peculiar magnetic excitation spectra in correlated insulators of these elements. In these systems, inter-site interactions between high-rank multipole moments may strongly affect the nature of magnetic order or even induce purely multipolar "hidden"-order phases. We calculate multipolar intersite exchange interactions in several TM and actinide systems of this kind by means of a many-body ab initio force theorem [1]. Their ordered states are evaluated from the calculated effective Hamiltonians within mean-field; their theoretical inelastic neutron scattering (INS) spectra are subsequently calculated using the random phase approximation in conjunction with a realistic treatment for the neutron scattering form-factors. We first discuss the actinide dioxides UO_2 and NpO_2. Our calculations predict a 3***k*** magnetic order stabilized by quadrupolar superexchange in the former [2] and a non-collinear purely multipolar rank-5 (triakontadipolar) order in the latter [3]. The approach is then applied to the double perovskites (DP) Ba_2BOsO_6 (*B*=Ca, Mg, Zn), where a "hidden"-order phase transition was recently detected [4]. In this case, the SO entangled Os d^2 ground state has an effective angular momentum *J*=2 and a rich space of possible order parameters. Our calculations predict the ground state of ferro-ordered "*xyz*" octupoles coupled by superexchange interactions [5]. Miniscule distortions of the parent cubic structure are shown to qualitatively modify the structure of gaped magnetic excitations. In d^3 DP, the Hund's rule coupling induces a spin-3/2 orbital-singlet ground state. The SO interaction is not expected to qualitatively impact low-energy degrees of freedom in such systems. Indeed, d^3 DP of heavy TM exhibit conventional magnetic orders. However, their INS spectra feature large gaps of unclear origin [6,7]. We calculate first-principles low-energy Hamiltonians for the cubic DP $Ba_2YB'O_6$ (*B'*= Os, Ru) finding unexpectedly significant magnitudes for some multipolar – dipole-octupolar – intersite exchange terms [8]. These terms stabilize a non-collinear 2***k*** antiferromagnetic order. Moreover, they break the continuous symmetry of the spin-3/2 Hamiltonian suppressing the Goldstone modes and opening an excitation gap that scales proportionally to the SO coupling strength.

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T28

Scaling down in order to reveal intrinsic properties of solid-state materials

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Synthesis optimization is a rather lengthy and costly process, during which many obstacles are encountered and, rather frequently, cannot be overcome. This is particularly true when it comes to the discovery and characterization of new materials with yet unknown properties. In this talk, I will discuss a new approach to study solid-state materials on the micro-scale. In particular, this new method allows to examine the electrical resistivity of polycrystalline material by extracting micro-scale sized domains using focused-ion-beam structuring [1]. This technique has been previously applied to Be_5Pt [2] and TaIrGe [3]: for both materials, transport measurements on the micro-scale have confirmed the semiconducting ground state predicted by band structure calculations and thus could resolve the discrepancy between the latter and bulk electrical resistivity measurements indicating metallic behavior, likely caused by secondary phases. This approach is now used to study intrinsic properties of UBe_{13} – an unconventional superconductor with a fragile ground state [4].

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T29

Simulation Tools for Improvement of the Fission Track Analysis Method for Nuclear Forensics

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To answer the nuclear forensics questions, we are developing new techniques and new approaches to make this analysis more reliable and more accurate. Till now the images from the microscope were analyses by a trained researcher. Since the analysis is done by human skills, it is clear that different researchers will give a bit different result. The Certification to a new worker is long and must cover a lot of examples that were measured before and even some that we can only predict.

A good simulation can help in training and can give a tool to grade a new researcher.

The fission tracks were simulated by Monte-Carlo software, GEANT4, which uses all the physics behind the nuclear fission tracks - thermal neutrons flux, fission cross-section, radiation time, particle size, enrichment, etc. The full software is written by MatLab code.

We can simulate an extreme condition and learn new aspect in the fission track technique.

From the simulation we can learn about the proper amount of material to use as a sample in the FTA technique.

The simulation can give as a large database of fission tracks images that are used for artificial analysis (AI).

The simulation can predict and compared to the mini-bulk and the micro-bulk analysis.

New idea of using penetrating fluorescent colors give as the ability to scan our detector in 3D instead of 2D. In this case we used the Dapi marker as a first shoot, this marker is well known for biomedical research.

This new idea to investigate the FT Star more than just by his projection.

Identifying the length of the tracks and their distribution allow us to determine the element source isotope be the shape of “fission products distribution” and the density of the impurities in the source.

The “fission products distribution” in our Lexan detector (wider peek is the high energy products, sharp peek is the low energy products)

Results of the new training software with suggested cutting area and the Training team performance. and the density of the impurities in the source. picture of a star taken with fluorescence microscope activated by Dapi will be presented.

T30

Additive Manufacturing in Biomedical Applications

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Additive manufacturing (AM) processes create three-dimensional structures for additive layering of materials. Those materials are not limited and constantly developing and advancing, ranging from liquid resin to powders to filaments and pellets. AM is also designed to create complex structures that would be extremely difficult or impossible to produce using conventional techniques. Today, AM is becoming a standard manufacturing practice for various biomaterials and biomedical devices and it is expected to revolutionize healthcare. The extensive use of AM in the biomedical field is due to many advantages, such as personalization of medical products, biocompatibility, cost-effectiveness, improved productivity, accessibility, short production time, and simple assembly. The most widely used biomedical applications of AM include the design of patient-specific prosthetics and implants, surgical planning models and tools, local and strategically timed drug delivery, etc. In this talk, I will present three of my group's projects aiming to develop advanced biomaterials for healthcare applications using different AM technologies. The first project focus on fabricating functional bone reconstruction implants with porous lattice architecture using the bound metal deposition AM process in order to improve the implant integration with the bone and tissue and to reduce the prevalence of aseptic loosening and stress shielding. The second project deals with the additive manufacturing of clear dental aligners using stereolithography technology. We aimed to investigate the possibility of printing the aligners directly as opposed to the conventional thermoforming methods. The third project aimed to develop a new printable bioink, based on patient autologous blood, to fabricate vascularized bone tissue constructs using 3D bioprinter.

POSTERS

P01

Pseudogap and fluctuation conductivity of $YBa_2Cu_3O_{7-\delta}$ single crystals in the course of long-term aging

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The temperature dependences of both fluctuation conductivity (FLC) $\sigma'(T)$ and pseudogap (PG) $\Delta^*(T)$ derived from measurements of resistivity $\rho(T)$ of an optimally doped (OD) $YBa_2Cu_3O_{7-\delta}$ single crystal subjected to a long-term storage have been studied. The as-grown sample S1 exibits characteristics typical of OD $YBa_2Cu_3O_{7-\delta}$ single crystals containing twins and twin boundaries (TBs). Analysis of both FLC and PG showed an unexpected improvement in all characteristics of the sample after 6 years of storage (sample S2), indicating that the effect of TBs is somehow limited. After 17 years of storage, all characteristics of the sample changed dramatically, which indicates a strong influence of internal defects formed during the aging process. For the first time, the temperature dependences of both FLC and PG were obtained after 17 years of storage. In contrast to these results, the values of $\sigma'(T)$ and $\Delta^*(T)$ obtained after 17 years of storage (sample S3) changed dramatically. Resistivity $\rho(300K)$, $\rho(100K)$ and their linear slope $\alpha = d\rho/dT$ increased by more than 3, 1.6 and 4 times, respectively. The resistive transition of S3 became very wide ($\Delta T_c \approx 7$ K) and pointed out the appearance of a second low-temperature phase with $T_c(\rho=0) \approx 84$K. Thus, the total $\Delta T_c \approx 16$ K. This form of $\rho(T)$ differs markedly from the "classical" behavior of $\rho(T)$ with a similar slope and $\rho(300K)$, which is obtained by reducing the charge carrier density nf in *YBCO* with a decrease in the oxygen doping level [2]. Correspondingly, the shape of both $\sigma'(T)$ and $\Delta^*(T)$ has also changed greatly. It was found that the fluctuation contribution of 2D-MT is almost completely suppressed. In addition, S3 exhibits the largest scaling factor $C_{3D} = 2.1$ and an unexpectedly increased distance between conducting CuO_2 planes $d_{01} = 6.7$ Å, which is about 1.6 times greater than that estimated for *YBCO*. All this data indicate the presence of a large number of defects leading to significant structural distortions in the crystal. This conclusion is confirmed by the results of the analysis of the pseudogap. A rather peculiar $\Delta^*(T)$ was found in this case, which does not find a direct analogue in our data bank $\Delta^*(T)$.

P02

Field-Dependent Magnetic Ordering Dome and Quantum Spin Fluctuations in the Natural Mineral Henmilite

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Quantum materials have been playing a crucial role in the development of next-generation technologies and devices including quantum computers. Such materials are usually prepared under laboratory conditions. However, some naturally occurring minerals, have also been found to feature complex magnetic ground states, such as Henmilite [2], or Herbertsmithite [1,8]. They possess spin ½ Cu ions which exhibit a magnetic ground state favouring the creation of quantum fluctuations, hinting at a possible quantum spin liquid state [2].

Henmilite $\{Ca_2Cu(OH)_4[B(OH)_4]_2\}$is a bright blue-violet colour mineral, which has been suggested to consist of coupled two-leg ladders, where strong quantum fluctuations suppress (AF) magnetic order at low temperatures [2]. It is an extremely rare mineral only found in the Fuka mines of Japan [6]. In Henmilite, the *B-T* phase diagram has an unusual antiferromagnetic dome [2]. The nuclear crystal structure is complex and contains well-separated sheets of $Cu(OH)_4$ square-planar plaquettes, separated by a network of $Ca(OH)_8$ and $B(OH)_4$ polyhedra. DFT (GGA+U) calculations found interlayer magnetic coupling less than 1% of the dominant intra-plane coupling, confirming the magnetic 2-dimensionality of the material [2].

We will present our experimental results of magnetic susceptibility, heat capacity, and thermal conductivity experiments as well as corresponding theoretical calculations for its magnetic ground structure. A Muon spectroscopy experiment is scheduled at HiFi instrument, ISIS UK, allowing us to study magnetic ground state and spin dynamics in short-range correlation regions above T_N. We will use the newly developed instrument ALSA [7], an AI-controlled robotic arm to co-align smaller crystals into mosaics to use for μSR experiment and later on for neutron spectroscopy.

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P03

Electronic Structures of RTe_3 (R=Pr, Er) Rare-Earth CDW Systems via Angle-Resolved Photoemission Spectroscopy

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Rare-earth (R)–based charge density wave (CDW) systems of RTe_3 exhibit interesting phase transitions, such as two-step CDW transitions for heavy R elements and single-step CDW transitions for light R elements [1]. By employing angle-resolved photoemission spectroscopy (ARPES) and the density functional theory (DFT) band calculations, the electronic structures of $PrTe_3$ and $ErTe_3$ have been investigated, which reveal single-step and two-step CDW transitions, respectively. According to the R 4*d*→4*f* resonant photoemission spectroscopy, R 4*f* electrons do not contribute directly to the CDW formation. The shadow Fermi surfaces (FSs) arising from the interlayer-interaction-induced band folding are observed for both R=Pr and Er. The measured FS in the CDW phase of $PrTe_3$ is explained by the 7×1 CDW supercell formation in Te sheets. In contrast, the measured FS in the non-CDW phase of $ErTe_3$ is described well by the DFT calculations, implying a partial CDW-induced FS reconstruction in $ErTe_3$. This work reveals the different CDW reconstructions in the electronic structures of $PrTe_3$ and $ErTe_3$.

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P04

Discovery of the kagome superconductor in the Half-Heusler "NbRhSb"

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In this work, we present a study of new Kagome superconductor metal discovered for the first time in Half Heusler NbRhSb. We followed a method based on density functional theory (DFT) combined with another method based on weak binding called Tight-Binding to determine his topological indices. This method is very efficient and widely used in ab-initio studies to extract Chern number "C" and the topological number "Z2".The application of SOC generates an opening between the bands equal to 160meV due to the point of contact between the flat bands and the Dirac cone.The results show that NbRhSb has a non zero number topological with cone Dirac and flat bands near Fermi level. All indices indicate that NbRhSb intermetallic has the possibility to be superconductivity non-trivial.

P05

STRUCTURE AND MAGNETIC PROPERTIES OF $GdFe_2$-H HYDRIDES

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In R-Fe intermetallic compounds containing heavy lanthanides (R = Gd^{3+}-Tm^{3+}), the spins of the R and Fe sublattices are oriented in opposite directions. When a sufficiently strong magnetic field is applied, the antiparallel spin configurations can be disrupted. The resulting field-induced transitions provide critical information on the strength of intersublattice coupling. Despite being extensively discussed in the literature, the fundamental problem of estimating the strength of intersublattice exchange interaction using high magnetic fields for R-Fe intermetallic compounds is still not fully resolved for the case of compounds doped with light interstitial elements [1]. The objective of this study is to examine the magnetization processes in the $GdFe_2$-H system under high magnetic fields to elucidate the effect of hydrogenation on the R-Fe exchange interaction.

X-ray diffraction analysis demonstrate that in $GdFe_2H_x$ ($0 < x \leq 5.5$) hydrides the content of the main phase (the cubic $MgCu_2$ - type structure) is not less than 93-95%. The hydrogenation of $GdFe_2$ has been shown to result in a significant expansion of the unit cell volume, reaching 29% for the hydrogen content x = 5.5 at.H/f.u. As a result, the Curie temperature decreases from T_C = 790 K in the parent $GdFe_2$ compound to T_C = 65 K in the $GdFe_2H_{5.5}$ hydride. While the magnetization of the ferrimagnetic $GdFe_2$ saturates quickly, hydrogenation leads to a substantial increase in magnetization. The highest stable (for performing high-field measurements) hydride, $GdFe_2H_{3.7}$, exhibits a critical transition at a field of 33 T at T = 2 K. We analyze the temperature dependence of the first critical field of the $GdFe_2H_{3.7}$ composition and obtain information on the molecular field parameter.

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P06

Investigating the spin dynamics of Mn_5Si_3 and Mn_5Ge_3

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Materials displaying anomalous physical properties have recently attracted scientific interest because they could be potentially used in future spintronic and electronic devices. In this context Mn_5Si_3 and Mn_5Ge_3 are promising candidate materials for applications since they exhibit significant anomalous Hall and Nerst effects [1-3]. Although the crystal structure, the magnetic structure, and the macroscopic properties of these materials were extensively investigated in the past their spin excitation spectrum remained unexplored. In the poster I will present recent results of inelastic neutron scattering measurements and density functional theory calculations [4-7]. The studies indicate that the non-collinear magnetic ground state of Mn_5Si_3 and its modification via external magnetic field is associated with the anomalous transport properties and the interesting thermodynamic phenomena that occur in this material [5,6]. Regarding the ferromagnetic Mn_5Ge_3 the results demonstrate that this compound is the first realization of a gapped Dirac magnon material in three dimensions [7]. Its tunability by chemical doping or by thin film nanostructuring could define an exciting new platform to explore and design topological magnons for applications.

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P07

Physical properties of Uranium-Hafnium alloys and their hydrides

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Uranium hydride (UH_3) is the first known 5*f* ferromagnetic material with magnetic ordering. Uranium metal can form a hydride that exhibits two structural modifications: a stable β-UH_3 phase (complex cubic with a = 664 pm) and a metastable α-UH_3 (*bcc* cubic with a = 414-416 pm). Our prime motivation is to investigate whether Hafnium (Hf) supports the stabilization of *bcc* α-UH_3 phase similar to Zr and to study the reaction of crystal lattice and variations of magnetic and electric properties.

Hydrogenation plays a role of a negative pressure effect that acts as a small perturbation into the system, expanding the crystal lattice. Volume expansion leads to an increase in the lattice parameters and U-U spacing in the hydrides. The reduction of the 5*f*-5*f* overlap leads to a 5*f*-band narrowing [1], which is crucial for fulfilling the Stoner criterion for itinerant ferromagnetism.

Hydrogenation of γ-U phases alloyed by Zr leads to the formation of a single stable phase of α-UH_3 type of hydride with 20% of Zr concentration [2]. This is contrasting with other transition-metal dopants (such as Nb, Mo, V), which yield nanocrystalline β-UH_3 type hydrides. Is Hf playing a similar role as Zr, or is the Zr case unique? Hf is chemically very close to Zr, the atomic radii of Zr and Hf are 160 pm and 159 pm, respectively.

In the present work, the alloys $U_{1-x}Hf_x$ with x = 0.10, 0.15, 0.30, 0.40 were synthesized by arc-melting of pure elements (natural U-2N8, Hf-3N) in an Ar atmosphere. The alloys were hydrogenated by exposure to high pressure of H_2 gas (p = 100 bar) for 100 hours at ambient temperature. XRD analysis revealed that β-UH_3 is the dominant phase for 10 at.% Hf, but it is gradually reduced with increasing Hf concentration up to 40 at%. At this limit, we obtained α-UH_3 as a majority phase, while one can still identify a small peak of β-UH_3 at around 2ϑ = 33.1°. The lattice parameter a of the *bcc* α-UH_3 phase stays invariable and is consistent with the literature [2]. We expect a similar expansion of the *bcc* structure with respect to the *bcc* precursors in the $(UH_3)_{1-x}Hf_x$ alloys, as observed in $(UH_3)_{1-x}Zr_x$.

Magnetization studies of the Hf alloyed hydrides are currently under way. So far we can conclude that the impact of Hf is similar as Zr, favoring the α-UH_3 phase, but the effect is smaller for comparable alloying concentrations. The difference may be seen in the small difference of atomic diameters, which suggests that larger lattice volumes promote the α-UH_3 phase (or impede the α-UH_3 to β-UH_3 transformation). This is contradicting to the α-UH_3 phase promoted by pressure, suggested by one type of ab-initio calculations [3].

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P08

Understanding phonon-crystal field coupling, insights from polarized inelastic neutron scattering measurements on $CeAuAl_3$ and new theoretical framework.

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The magnetoelastic coupling between transitions of *f*-electrons in crystal electric field (CEF) and phonons (CEF-phonon) has been of interest for a long time. Dating back to the 1980s, the observation of unexpected excitations in the neutron scattering spectra of $CeAl_2$ [1] led to the proposal of the formation of magneto-elastic hybrid modes (vibrons) between an optical phonon branch and certain CEF level [2]. However, the effects appeared to be limited to strong CEF-phonon coupling, lacking a full quantitative treatment of the entire spectrum of phonon excitations, notably acoustic phonons, as well as additional coupling phenomena such as anticrossing and damping.

Reaching beyond these seminal studies, inelastic neutron scattering in $CeAuAl_3$ recently revealed an anti-crossing of the CEF excitation with an acoustic phonon at 5 meV and a coupled CEF-phonon excitation around 8 meV, despite weak CEF-phonon coupling [3]. We report polarized inelastic neutron scattering of the magneto-elastic hybrid excitations and phonon-CEF anti-crossing in $CeAuAl_3$.

As our main results we find the same polarization of the CEF excitation at 5 meV and the hybrid mode at 8 meV, unambiguously connecting these phenomena, as well as a transfer of the spectral weight between the magnetic and the nuclear scattering channels around the anti-crossing. Using a generalized coupling scheme between phonons and CEF excitations and utilizing the random phase approximation method [4], the bound hybrid states and anti-crossing with their characteristic transfer of spectral weight may be explained qualitatively and quantitatively based on the implementation of the in McPhase [5]. Our findings promise a comprehensive account of CEF-phonon coupling phenomena in a wide range of materials.

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P09

Structural studies of UCu_2P_2 under pressure

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The work is aimed at the investigation of the crystal structure of UCu_2P_2 under pressure. Both the anisotropy of the compressibility and the evolution of the crystal structure were of interest in the view of the pronounced magnetic anisotropy of the compound. UCu_2P_2 has the Curie temperature of T_C = 216K, the easy magnetization direction along the *c*-axis, and the anisotropy field of about 1MOe (J.Phys.Cond.Mat 2 1990 4185). The external pressure drives the T_C upwards at a rate of +10K/GPa (Solid State Commun. 70 1989 619) till at least 1GPa. Also, the U-U separation within the ab plane is 1.5 times smaller than perpendicular to it (D Kaczorowski, J.Phys.Cond.Mat 2 1990 4185). This naturally brought up the question about the possible bond anisotropy, which could manifest itself via the elastic constants.

The crystal structure of UCu_2P_2 has been studied at pressures as high as 23GPa and the ambient temperature by the X-ray powder diffraction with the Mo radiation in the diamond anvil cell. The patterns contained the contributions from UCu_2P_2 and the steel gasket of the DAC. The peak overlap for these phases was not substantial and allowed for the Rietveld profile analysis.

The results point to the monotonous compression along the *c*-axis and the *a*-axis till about 9GPa. The former compressibility is twice smaller than the latter one: -0.2%/GPa vs. -0.4%/GPa. The estimated bulk modulus of about 100GPa is typical for uranium intermetallics, which we took as the indication of the realistic values obtained from the Rietveld profile analysis. The original hexagonal crystal structure of UCu_2P_2 is likely distorted around 9GPa since the (011) and (101) peaks are no longer at the same 2Θ angle. The next transition comes above 16GPa, after which the structure remains unchanged till at least 23GPa. Judging by the evolution of the peak shapes and positions, further distortion takes place rather than complete reconstruction of the unit cell.

Based on the reported observations we conclude that structural properties of UCu_2P_2, $\Delta a/a < \Delta c/c$, point to the bond anisotropy expected from its magnetic properties. Also, two structural transitions, at 9GPa and 16GPa take place in this compound.

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P10

Uranium hydride thin films: stabilization of thermodynamically unstable phases

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Uranium hydride has been a subject of interest in the field of actinide research for decades. Besides the fundamental importance, it has relevance for nuclear energy and devices [1]. It is known that in the bulk U hydride [2] exists in the trihydride UH_3 form with two allotropes, the transient α-UH_3 phase, which transforms into the stable β-UH_3. Both hydrides have cubic unit cells with the space group *Pm*3*n*, α-UH_3 with a = 416 pm (one U lattice site) and a more complex structure for β-UH_3 (two different U sites, 8 formula units) with a = 664 pm [2,3]. Magnetic properties of allotropes are rather similar, both being ferromagnets with T_C = 170 K [3].

Unlike for other actinides and lanthanides, uranium dihydride was not known so far, thus we implemented a technique of thin film deposition using reactive DC sputtering. The synthesis of materials in the thin film form pushes the system far from the thermodynamic equilibrium, in extreme cases new structure types can be obtained [4]. Our attempt was successful, resulting in the deposition of UH_2 with CaF_2 structure type and a = (535.98 ± 0.14) pm [1]. UH_2 is a ferromagnet, as well, with a lower T_C=120 K.

Besides the stabilization of unstable phases, preparation of thin films provides several advantages. In particular, the stability of obtained samples (contrary to pyrophoric uranium hydride powder, films respond to air exposure by covering up with a protective oxide layer), small amount of radioactive material, sample shape and surface is suitable for XPS studies and resistivity measurements. A deep comparative analysis of the DOS around the Fermi level and magnetic properties for UH_2 and β-UH_3 has been performed [1,5]. Deposition parameters for obtaining UH_2 has been established. However, for the vast majority of combinations for the sputtering parameters (like deposition rate, substrate material, partial pressure of H_2, and temperature), the prepared films exhibit mixed (both UH_2 and UH_3) phase composition.

The next step was the stabilization of α-UH_3 in a film form. Interestingly, in the samples with mixed phase composition and the prevailing UH_2 phase, the residual UH_3 phase was found in the α-UH_3 modification (content not exceeding 10–20%). To prepare pure α-UH_3, we took an inspiration from our bulk studies, where we stabilized α-UH_3 by zirconium alloying. Preliminary conclusion is that despite the absence of α-UH_3 phase in samples with modified composition, we were able to obtain films of pure UH_2 or β-UH_3 structures with lower Curie temperatures compared to clean films. Results of magnetization and resistivity measurements, along with structure analysis will be presented.

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