ABSTRACT BOOK



2nd WORKSHOP ON

RECENT ADVANCES IN BROAD-BAND SOLID-STATE NMR OF CORRELATED ELECTRONIC SYSTEMS

September 4-9 2011, Trogir, Croatia



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GENERAL INFORMATION

The Second international workshop on "Recent advances in broad-band solid-state NMR of correlated electronic systems" is scheduled for 4-9 September 2011, in Trogir, Croatia. The first workshop took place in September 2010, as part of the SOLeNeMaR project (FP7 #229390) of the European Commission and will mark the foundation of the first solid-state NMR facility in Zagreb, established with the support of the SOLeNeMaR project and the Croatian Government.

The conference site and housing are again within the walls of the historic town of Trogir, one of the UNESCO World Heritage Sites, situated close (6 km) to the international airport of Split (SPU).

The second workshop is meant to build on the strong point of the first, namely, a particular focus on the abilities of NMR to provide pertinent insight into the outstanding physical problems of our day. It will cover topical results on: high-Tc superconductors, fullerides and pnictides, quantum magnetism, spin liquids, heavy fermion conductors, actinides and skutterudites, as well as advances in broad-band NMR techniques. The target audience is both experimental and theoretical researchers in the field, as well as post-doctoral students specializing in broad-band NMR. The workshop is open to exploring relations between NMR and other methods, as well as introducing physical problems to which NMR investigations may contribute in the future, so it may be interesting to researchers in other fields as well.

A specific ambition of the workshop is to foster the development of NMR expertise among young researchers, which is one of the formal goals of the above-mentioned SOLeNeMaR project. To this purpose ten grants will be made available from the project to cover all the expenses at the conference for selected young researchers.

VENUE

The ancient town of Trogir on the Croatian coast is closer to Split international airport than Split itself. It is one of only two towns on the Eastern Adriatic to have preserved intact a street plan dating before the Mongol invasion of 1242. The town hall in the main square will host the conference sessions, while coffee breaks will be held at the nearby open-air loggia, which served for solemn civic occasions during the Middle Ages. Both can be seen at http://whc.unesco.org/en/list/810/gallery. All conference hotels are impeccably restored 16th and 17th century town houses within the walls, with modern amenities. Most are appointed with similarly restored late 19th and early 20th century furniture. The total capacity of hotels in the old town is around 150 guests, so that most have been booked full for the purpose of the conference.



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PROGRAMME

	Monday	Tuesday	Wednesday	Thursday	Friday
8:45-9:00	opening				
9:00-9:50	M. Takigawa	V. Kataev	MH. Julien	M. Takigawa	D. Arčon
9:50-10:40	W. Halperin	Y. Furukawa	M. Poggio	F. Bert	N. J. Curro
10:40-11:10	Coffee	Coffee	Coffee	Coffee	Coffee
11:10-12:00	A. Keren	P. Prelovšek	A. Smontara	M.Horvatić	De Renzi
12:00-12:30	F. Hammerath	L. Bossoni	A. Zorko	E. Kermarrec	Closing
12:30-13:30	- Lunch	Lunch	Excursion	Lunch	Board meeting
13:30-16:00					Lunch
16:00-16:50	H. Mukuda	I. Eremin		F. Mila	
16:50-17:20	M. Klanjšek	G. Koutrolakis		I. Heinmaa	
17:20-17:50	Coffee	Coffee		Coffee	
17:50-18:40	K. Ishida	H. H. Klauss			
18:40-19:10	T. Shiroka	B. Perić		Poster session	
19:10-20:00					
20:00				Banquet	

ORAL SESSIONS

Place: The town hall in the main square (Knežev dvor, Trg Ivana Pavla II, Trogir) will host the conference sessions, while coffee breaks will be held at the nearby open-air loggia.

Presentation time:

50 min. (40 min talk + 10 min Q/A)

30 min. (25 min talk + 5 min Q/A)

Speakers should bring their presentation as a single stand-alone file on CD or USB flash drive. The session room is provided with one laptop with LCD projector, and standard presentation software.

Speakers can use their own laptops, but we strongly recommend using the one in the session room, unless a stand-alone presentation file is for some reason impractical. Speakers are welcome to check their presentations well ahead of time.

POSTER SESSION

Place: Cate Dujšin-Ribar gallery **Poster Set-Up:** Thursday morning (Sep 08) Poster Session: Thursday (Sep 08) 17:50-20:00 **Poster Removal:** Thursday evening (Sep 08) Poster Size (max): H 120 x W 90 cm

INVITED LECTURES

Unconventional superconductivity in alkali-doped fullerides close to the Mott boundary

Denis Arčon¹

¹*Faculty of mathematics and physics, University of Ljubljana and Institute*

The superconductivity in A_3C_{60} has been for many years explained by the phonon driven BCS theory with the *s*-wave pairing symmetry. Recent discovery that Cs_3C_{60} has an antiferromagnetic Mott-insulating (AFI) ground state and that the superconductivity appears only after Cs_3C_{60} was exposed to hydrostatic pressure [1,2] implied that the electron correlations are very important in this class of materials.

These findings open an exciting opportunity for understanding the interactions producing superconductivity in correlated electron systems, as it allow us the isolation of the influence of only electronic factors (including orbital degeneracy) without introducing any disorder or causing structural deformations. In this contribution we report on the comprehensive temperature and pressure study of the ¹³C, and ¹³³Cs NMR in Cs₃C₆₀ close to the Mott insulating phase. We show that in this part of the phase diagram $1/T_1T$ shows clear deviations from the simple Korringa relation. In addition, $1/T_1$ below the critical temperature will be analysed and discussed. These results complement our previous measurements under ambient pressure conditions, where NMR was the key experimental technique to reveal the insulating ground state and the antiferromagnetic ordering at low temperatures.

[1] Y. Takabayashi et al., Science **323**, (2009) 1585.

[2] A. Y. Ganin et al., Nature 466, (2010) 221.

Quantum Kagome Antiferromagnets : Herbertsmithite vs Vesignieite

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The frustration of antiferromagnetic interactions on the loosely connected kagome lattice associated to the enhancement of quantum fluctuations for S=1/2 spins was acknowledged long ago as a key combination to stabilize novel ground states of magnetic matter of the spin-liquid type [1]. Only in 2005, a model compound, the Herbersmithite ZnCu₃(OH)₆Cl₂, could be synthesized and has triggered since then a remarkable activity[2]. Among the salient achievements in the study of this material are the absence of any kind of spin freezing down to at leat 50 mK through μ SR experiments and a gapless susceptibility evidenced through ¹⁷O NMR.

Vesignieite [3], BaCu₃V₂O₈(OH)₂, is one of the very few new recent candidate materials for this physics. In high quality powder samples[4], neutron diffraction measurements evidence that the kagome lattice is close to the perfect and indeed the susceptibility measured through ⁵¹V NMR closely resemble that of Herbert-smithite [5]. However the low *T* behaviour of Vesignieite surprisingly contrasts with the one of Herbertsmithite. A kink in the susceptibility below T = 9 K is matched to a slowing of the spin dynamics observed by μ SR and NMR. Our results point to an exotic quantum ground state with small frozen moments coexisting with slowly fluctuating ones. While Dzyaloshinskii-Moriya interaction is relevant in both compounds, we propose that it is large enough in Vesignieite to drive the system through a quantum critical point and towards a magnetic phase.

[1] Introduction to frustrated magnetism. C. Lacroix, P. Mendels and F. Mila, Springer (2011)

[2] For a review see : P. Mendels and F.Bert, J. Phys. Soc. Jpn 1, 011001 (2010)

[3] Y. Okamoto and H. Yoshida and Z. Hiroi, J. Phys. Soc. Jpn 78, 033701 (2009)

[4] R. Colman, F. Bert, D. Boldrin, A.D. Hillier, P. Mendels, and A.S. Wills, Phys. Rev. B 83, 180416 (2011)

[5] J. A. Quilliam, F. Bert, R. H. Colman, D. Boldrin, A. S. Wills and P. Mendels, arXiv:1105.4338

Nuclear Magnetic Resonance Studies of Domain Walls in Antiferromagnetic CaFe₂As₂

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Resistivity, magnetization and microscopic ⁷⁵As nuclear magnetic resonance (NMR) measurements in the antiferromagnetically ordered state of the iron-based superconductor parent material CaFe₂As₂ exhibit anomalous features that are consistent with the collective freezing of domain walls. Below $T^* \approx 10$ K, the resistivity exhibits a peak and downturn, the bulk magnetization exhibits a sharp increase, and ⁷⁵As NMR measurements reveal the presence of slow fluctuations of the hyperfine field. These features in both the charge and spin response are strongly field dependent, are fully suppressed by $H^* \approx 15$ T, and suggest the presence of filamentary superconductivity nucleated at the antiphase domain walls in this material.

Co NMR in *Ca*₃*Co*₂*O*₈**: an intriguing frustrated Ising chain system**

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 $Ca_3Co_2O_6$ is a geometrically frustrated, Ising-spin-chain system, with alternate stacking of a high-spin (S = 2) Co^{3+} trigonal (T) site and a non-magnetic Co^{2+} octahedral (O) site along the *c* axis, arranged in a triangular lattice. Exchange coupling is ferromagnetic (FM) and stronger between neighboring T ions along the chains, whereas it is antiferromagnetic (AF) and much weaker between chains.

For 5K $< T < T_c \approx 25$ K. a long wavelength incommensurate spin density wave correctly describes the magnetic structure, whose average local justifies the name of modulated partially disordered antiferromagnet (MPDA). Magnetic field along \hat{c} leads to successive transitions to a ferrimagnetic (FI), and a FM phase. The mean field picture of these three phases is however questioned by the appearance of magnetization steps, hysteretic behaviour and metastability at lower tempertures.

In a single crystal the quadrupole split spectra of O ⁵⁹Co from FM chains, at high field, are distinguished from the minority FI chains and majority FI chains, at lower fields.[1] The thermally activated nuclear spin-lattice relaxation of T ⁵⁹Co in the three distinct local configurations provide slightly different energy gaps that fit the Glauber model for the spin susceptibility of an Ising spin system. The intraand inter-chain exchange constants $J_1, J_2 + J_3$ are the variational parameters, whose best-fit values yield the correct critical temperature T_c and the magnetic wavevector at T = 0. This simple mean field model and its pitfalls will be discussed in relation with the stability of the zero-field ground state, which has been recently identified by neutron scattering [2] as the commensurate antiferromagnetic structure, surprisingly taking over the incommensurate spin-density wave at low temperature (below 5K).

[1] G. Allodi et al., Phys. Rev. B 83, 104408 (2011).

[2] S. Agrestini et al., Phys. Rev. Lett. 106, 197204 (2011).

Itinerant magnetic excitations in iron-based superconductors: from SDW metal to the superconductor

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Recent discovery of superconductivity in the iron-based layered pnictides with T_c ranging between 26 and 56 K generated enormous interest in the physics of these materials. In my talk I will analyze current experimental and theoretical evidences in favor of extended s-wave superconductivity. I will further discuss the selection of the stripe magnetic order in the unfolded BZ within itinerant description. Selecting one hole and two electron pockets we find that SDW order is highly degenerate if electron pockets are circular and interactions involved are between holes and electrons only. Repulsive charge interactions between two electrons as well as ellipticity of the electron pockets break the degeneracy and select metallic $(0,\pi)$ $[(\pi,0)]$ SDW state in the unfolded BZ — the same order as seen in the experiments. Next we analyze the evolution of the spin excitations from the parent antiferromagnetic phase to the superconducting phase and address in particular the coexistence phase of antiferromagnetism and superconductivity. Finally, we address the salient experimental features of the magnetic excitations in the spindensity-wave phase of iron-based superconductors. We show that ellipticity of the electron bands accounts for the anisotropy of the spin waves along different crystallographic directions and the spectral gap at the momentum conjugated to the ordering one.

[1] A. Akbari, J. Knolle, I. Eremin, and R. Moessner, Phys. Rev. B 82 (2010) 224506; Phys. Rev. Lett. 104 (2010) 257001.

[2] A.V. Chubukov, and I. Eremin, Phys. Rev. B 82, (2010) 060504(R)

[3] I. Eremin and A.V. Chubukov, Phys. Rev. B 81, (2010) 024511

[4] A.V. Chubukov, D. Efremov, and I. Eremin, Phys. Rev. B 78, (2008) 134512

NMR studies of nanoscale molecular magnets

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Recently there have been intense experimental and theoretical efforts in synthesis and investigation of nanoscale molecular magnetic systems which are composed of a controllable number of transition-metal ions with spins. A shell of organic ligands shields the individual molecular magnets from each other so that the magnetic interaction between neighboring molecular magnets is very small and the observed magnetic properties of the bulk samples are considered to originate from intramolecular magnetic properties only. The discovery of quantum phenomena like quantum tunneling of the magnetization (QTM) observed in single molecular magnets such as Mn12 and Fe8 has triggered further interest in the investigation of magnetic properties of other nanoscale molecular magnets which have different structures such as coplanar ring, triangular, spherical shapes and so on. We have been carried out NMR and magnetization measurements to investigate the magnetic properties of these nanoscale molecular magnets.

This work was done in collaboration with K. Kumagai, P. Kogerler, G. A. Timco, R. E. P. Winpenny, and D. Gatteshci.

Vortex Induced Spin-Density Wave and Core Charge in Bi₂Sr₂CaCu₂O_{8+v}

William Halperin¹

¹Northwestern University

Competition with magnetism is at the heart of high temperature superconductivity, intensely felt near a vortex core. To investigate vortex magnetism we use a spatially resolved probe based upon NMR spin-lattice-relaxation spectroscopy in Bi₂Sr₂CaCu₂O_{8+y}. These experiments indicate a spin-density wave associated with a vortex,¹ consistent with results from elastic neutron scattering in other cuprates. In magnetic fields up to H = 30 T, we have determined the spin-modulation amplitude, found the decay length from the vortex core to be twice the coherence length, and that the period is ~ 8a₀.

At low fields H < 10 T, but still at magnetic fields much greater than that of the decoupling transition, we have observed a narrowing in the distribution of local fields with increasing applied field,² and interpret this observation as a vortex lattice structural instability associated with charge trapped on the core. Our calculation of the latter, to be consistent with the experiment, requires a charge of magnitude $\sim 2x10^{-3}e$ per vortex pancake, decreasing with increased doping.

This work was performed with A.M. Mounce, S. Oh, S. Mukhopadhyay, A.P. Reyes, P.L. Kuhns, K. Fujita, M. Ishikado, and S. Uchida, supported by the Department of Energy, contract DE-FG02-05ER46248 and the National High Magnetic Field Laboratory, the National Science Foundation, and the State of Florida.

[1] A.M. Mounce, et al. Phys. Rev. Lett. 106, 057003 (2011).

[2] A.M. Mounce, et al. Nature Physics 7, 125 (2011)

NMR studies of BEC-type quantum spin systems close to quantum critical points

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In antiferromagnetic quantum spin systems a magnetic field can induce a phase transition from a gapped into a gapless state, which at low temperature turns into a 3D ordered state that can be described as Bose-Einstein condensation (BEC). However, the true nature of real compounds is often more complicated and/or incompatible with the canonical BEC. NMR T_1^{-1} measurements, reflecting the low-energy excitations, are particularly suitable to monitor the critical behaviour around the corresponding critical field H_c , and to reveal whether the expected gapless behaviour is perturbed by some residual gap. Along these lines, we present results in two quasi-1D model systems, the spin-1/2 ladder compound CuBr₄(C₅H₁₂N)₂ (BPCB) [1] and the compound NiCl₂-4SC(NH₂)₂ (DTN) containing chains of S = 1 spins subject to a single-ion anisotropy. Both compounds exhibit the same scalable critical behaviour, not yet described theoretically [2]. In DTN we discuss the relevance of the observed residual gap. We also briefly report the latest results from the 2D dimer compound BaCuSi₂O₆ (Han purple), in which a special, layered BEC state is observed [3].

- [1] M. Klanjšek et al., Phys. Rev. Lett. 101 (2008) 137207
- [2] S. Mukhopadhyay et al., unpublished
- [3] N. Laflorencie, F. Mila, Phys. Rev. Lett. 102 (2009) 060602; arXiv:1009.5978

NMR Studies on Iron-Based Superconductors

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In my presentation, we review NMR results obtained in various Fe-based superconductors, mainly focus on the relationship between antiferromagnetic (AFM) fluctuations with the stripe correlations and superconductivity.

First, we introduce our NMR results on BaFe₂(As_{1-x}P_x)₂ with the "122" structure. BaFe₂(As_{1-x}P_x)₂ is one of the best systems in the Fe-based superconductors, since high-quality single crystals are available and isovalent P-substitution does not change carrier content essentially. $1/T_1T$ in BaFe₂(As_{0.67}P_{0.33})₂ with a maximum $T_c \sim 31$ K in BaFe₂(As_{1-x}P_x)₂ continues to increase down to T_c , indicating the development of the AFM fluctuations, and sharply decreases below T_c due to opening of the SC gap. The AFM fluctuations are suppressed and T_c also decreases systematically with increasing P content. From the analyses of $1/T_1T$ in the normal state, it is shown that the maximum T_c sample is located in the vicinity of the quantum critical point of the AFM instability, and that the AFM fluctuations are intimately related to the superconductivity[1]. The similar results have also reported in Ba(Fe_{1-x}Co_x)₂As₂ with the same "122" structure[2].These NMR results are compared with those obtained in other Fe-based systems such as "1111", "111" and "11" compounds.

I also discuss relationship between magnetic ordering and superconductivity observed in compounds located near the boundary between magnetic and superconducting phases.

Our NMR studies have been done in collaboration with Y. Nakai, S. Kitagawa, T. Iye for NMR measurements, S. Kasahara, T. Shibauchi, Y. Matsuda, and T. Terashima for $BaFe_2(As_{1-x}P_x)_2$ samples, and Y. Kamihara, M. Hirano, and H. Hosono for $LaFeAs(O_{1-x}F_x)$ samples.

[1] Y. Nakai, T. Iye, S. Kitagawa, K. Ishida, S. Kasahara, T. Shibauchi, Y. Matsuda, and T. Terashima, Phys. Rev. Lett. 105, 107003 (2010).

[2] F. L. Ning, K. Ahilan, T. Imai, A. S. Sefat, M. A. McGuire, B. C. Sales, D. Mandrus, P.Cheng, B. Shen and H.-H Wen, Phys. Rev. Lett. 104, 037001 (2010).

Magnetic-field-induced charge-stripe order in YBa2Cu3Oy

Marc-Henri Julien¹, Tao Wu¹, Hadrien Mayaffre¹, Steffen Krämer¹, Mladen Horvatić¹, Claude Berthier¹, Walter Hardy², Ruixing Liang², Doug Bonn²

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In the search of the broken-symmetry state inferred from quantum oscillation and other transport measurements [1], we undertook high magnetic field NMR experiments in ultra clean, oxygen-ordered, untwined single crystals of YBa2Cu3Oy. We find that the translational symmetry breaking does not arise from the magnetic order anticipated by most of us, but from a unidirectional charge-ordered state. Because it occurs only in strong magnetic fields oriented along the crystalline c-axis, this charge order appears to compete with superconductivity. While two (orthogonal) ordered patterns are compatible with the NMR spectra, we argue that the charge ordered state is most likely the 4a-periodic stripe phase "à la Tranquada". Nevertheless, we provide evidence that the stripe order remains partly fluctuating down to low temperatures. While the charge order is visibly pinned here by CuO chains, its occurrence at doping levels near 1/8 hole/Cu in a noticeably cleaner cuprate than e.g. La2-xBaxCuO4, strengthens the idea that charges have an intrinsic, and most likely generic, propensity to order in the CuO2 planes of hole-doped cuprates.

Key words : stripes, NMR, high fields, quantum oscillations, competing order

[1] Mike Norman, Fermi-surface reconstruction and the origin of high-temperature superconductivity, Physics 3, **86** (2010)

High magnetic field ESR spectroscopy on FeAs-based superconductors

Vladislav Kataev¹

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In the introductory part of the talk possibilities and challenges of the sub-THz tunable ESR spectroscopy in strong magnetic fields for studies of strongly correlated electron spin systems will be briefly discussed.

Further in the talk, we will specifically address an intensively discussed issue of a possible interplay between magnetism and superconductivity in the iron pnictide high temperature superconductors. Recent systematic high field ESR studies at the IFW Dresden of the $GdO_{1-x}F_xFeAs$ and $(Eu,Ba)[Fe_{1-x}Co_x]_2As_2$ compounds will be presented. Interplay between the rare-earth and the Fe magnetic subsystems as revealed by Gd^{3+} and Eu^{2+} ESR will be discussed. The ESR data give evidence that though the long range magnetic order in the FeAs planes is suppressed upon doping, short range static on the ESR time scale magnetic correlations between Fe spins remain even up to the doping level optimal for superconductivity. This suggests that the studied compounds may feature coexistence of quasi-static magnetism and superconductivity on a large doping range which emerges as a generic property of iron pnictide superconductors.

Critical-doping universality for cuprate superconductors: Oxygen nuclear-magnetic-resonance investigation of $(Ca_xLa_{1-x})(Ba_{1.75-x}La_{0.25+x})Cu_3O_y$

Amit Keren¹

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The critical oxygen levels in cuprates, where the ground state changes its nature from an antiferromagnet, to a spin glass, to superconductor, to metal, are not universal. We investigate the origin of these critical level variations by measuring the in-plane oxygen p_{σ} hole density in the CuO₂ layers as a function of the oxygen density y in (Ca_xLa_{1-x})(Ba_{1.75-x}La_{0.25+x})Cu₃O_y [CLBLCO]. This is done using the oxygen-17 nuclear quadrupole resonance parameter v_Q. We compare compounds with x = 0.1 and 0.4 which have significant critical y variations and find that these variations can be explained by a change in the efficiency of hole injection into the p_{σ} orbital. Our finding allows us to generate a unified phase diagram for the CLBLCO system across the entire doping range, with no adjustable parameters.

Competing order in Fe-based superconductors

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We have examined the magnetic and superconducting order parameters and electronic phase diagrams in several classes of iron pnictide superconductors by μ SR and Mössbauer spectroscopy [1,2,3,4]. The results prove the competition between SDW magnetism – often combined with an orthorhombic lattice distortion – and superconducting order. The temperature dependence of the superconducting order parameter reveals two gap multiband superconductivity. We examined the interplay of iron and rare earth magnetic order in ReO_{1-x}F_xFeAs [5]. The undoped compounds show different magnetic coupling strength of the rare earth ion to the antiferromagnetic iron layers ranging from independent order to strong polarization of the 4f electron with states at the Fermi energy leads to a rich phase diagram in CeO_{1-x}F_xFeAs and CeOFFeAs_{1-x}P_x. Finally, we present recent studies on Cs0.8Fe2Te2 based chalcogenide superconductors where high temperature magnetic order (T_N 500K) may coexist with superconductivity below 30 K [6].

[1] H. Luetkens et al., Nature Materials 8, 305 (2009)

[2] H. R. Khasanov et al., Phys. Rev. Lett. 102, 187005 (2009)

[3] R. Khasanov et al., Phys. Rev. B 80, 140511 (2009)

[4] Z. Shermadini et al., Phys. Rev. B 82, 144527 (2010)

[5] H. Maeter et al., Phys. Rev B 80, 094524 (2009)

[6] Z. Shermadini et al., Phys. Rev. Lett. 106, 117602 (2011)

NMR investigation of frustrated quantum magnets

Frederic Mila¹

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Frustrated quantum magnets are antiferromagnets in which the competition between different interaction channels prevents simple ordering and often leads to exotic phases. Over the years, NMR has proven to be an invaluable tool to identify the nature of the ground state of several frustrated magnets. In this talk, I will review the theoretical interpretation of the NMR spectra of two quasi-two dimensional frustrated magnets, $SrCu_2(BO_3)_2$ and $BaCuSi_2O_6$, and I will show how it has allowed to identify the nature of the remarkable high field phases realized in these systems.

Antiferromagnetism and high-*T_c* superconductivity in cuprates and Fe-pnictides

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In the first part, we review extensive studies on multilayered copper oxides by means of site-selective NMR, which have uncovered the intrinsic phase diagram of antiferromagnetism(AFM) and high-Tc superconductivity(HTSC) for a emergence disorder-free CuO₂ plane with hole carriers. We present the existence of AFM metallic state, the uniformly mixed phase of AFM and HTSC, and the dwave SC with a maximum of T_c just outside a critical carrier density, at which the AFM moment disappears. These results can be accounted for by the *Mott physics* based on the t-J model. The large superexchange interaction J_{in} plays the vital role as the glue for the Cooper pairs, which is the main reason for raising the T_c in cuprates.[1] In second topics, we present ⁷⁵As-nuclear quadrupole resonance (NQR) studies on $(Ca_4Al_2O_{6-\nu})(Fe_2As_2)$ with $T_c = 27$ K. Measurement of $1/T_1$ has revealed a significant development of AFM spin fluctuations down to T_c . Below T_c , the temperature dependence of $1/T_1$ without any trace of the coherence peak is well accounted for by an s_{\pm} -wave multiple gaps model. From the fact that T_c is comparable to T_c =28 K in the optimally-doped LaFeAsO_{1-v} in which AFM spin fluctuations are not dominant, we remark that AFM spin fluctuations are not a unique factor to enhance T_c among existing Fe-based superconductors, but a condition for optimizing SC should be addressed from the lattice structure point of view. [2]

[1] H. Mukuda et al, Special topics in J. Phys. Soc. Jpn (2012)

[2] H.Kinouchi et al., Phys. Rev. Lett, in press.

Recent progress in force-detected MRI

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Over the last 20 years, researchers have been making steady progress improving the sensitivity of force-detected magnetic resonance. Sensitivity has doubled roughly every 8 months and presently surpasses the sensitivity of conventional, inductive nuclear magnetic resonance detectors by 8 orders of magnitude. In 2009, IBM researchers demonstrated the promise of these developments by using magnetic resonance force microscopy (MRFM) to capture 3D images of individual virus particles with a resolution better than 10 nm. I will describe new efforts to apply this technique to the small ensembles of nuclear spins contained in semiconductor nanostructures such as quantum wells, nanowires, and quantum dots.

Transport in clean and disordered spin chains

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Spin chains represent interesting quantum many-body systems, well realized in several novel materials. In spite of long history, there remain theoretical questions, in particular regarding the finite-temperature transport in such systems, also in relation to recent experiments on thermal conduction in such materials revealing long mean free paths and impurity dominated transport at low T. Theoretical understanding of transport in clean and disordered spin chains will be reviewed in the talk. T > 0 spin stiffness will be discussed in connection with the integrability of the model. In particular, the interplay of electron correlations and random static disorder will be analysed with respect to possible many-body Anderson localization. It will be shown that a single static impurity as well as coupled impurity spins at T > 0 lead to the incoherent transport with a well defined current relaxation rate, allowing also for either cutting or healing effect.

Decagonal Quasicrystals and Approximants - 2D or 3D Solids

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Decagonal quasicrystals (d-QCs) and their periodic approximants are traditionally described as a periodic stacking of atomic planes with either quasiperiodic atomic order in one plane in the case of d-QCs, or translationally periodic order in three directions in the case of the approximants. Consequently, d-OCs are considered to be two-dimensional (2D) quasicrystals, whereas they are periodic crystals in the third dimension. Examples of the stacked-layers d-QC structures are d-Al-Ni-Co with two atomic layers within the periodicity length of about 0.4 nm along the stacking tenfold direction, d-Al-Ni, and d-Al-Si-Cu-Co with four layers within the periodicity length of about 0.8 nm, d-Al-Mn, and d-Al-Mn-Pd with six layers within the periodicity length of about 1.2 nm and d-Al-Pd and d-Al-Cu-Fe with eight layers within the periodicity length of 1.6 nm. Decagonal approximant phases are characterized by large unit cells but preserve the stacked-layer structure with the periodicity lengths along the stacking direction almost identical to those of the d-QCs. Decagonal approximant, known as the Y phase of Al-Ni-Co, comprises two atomic layers within one periodic unit. The other $Al_{13}TM_4$ (TM=transition metal) family with TM = Co, Fe, ..., represents four-layer approximant phases, whereas the Al_4TM phases, and Taylor-phase T- Al_3Mn represent six-layer approximant. In order to see whether this pseudo-2D description is justified also from the chemical bonding scheme, or the compounds are true 3D solids, we performed transport and a ²⁷Al NMR spectroscopic studies of single crystals the members of the $Al_{13}TM_4$ family. From the structural and the physical-property points of view, the $Al_{13}TM_4$ decagonal approximants are true 3D solids. Their description in terms of 2D atomic layers stacked along the pseudotenfold direction is a convenient geometrical approach to describe and visualize their complex structures but is not appropriate for the description of their physical properties, which should be analyzed by taking into account the full 3D nature of the chemical bonding framework.

Novel Magnetic Structures on Strongly Frustrated Lattices

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Both localized moments and itinerant electrons on frustrated lattices provide promising playground to look for exotic ordering and fluctuation phenomena. In this talk I will discuss two frustrated systems, in which NMR has played powerful role for unambiguous determination of the magnetic structure. The first example is $SrCu_2(BO_3)_2$, a quasi-two dimensional magnetic insulator on the Shastry-Sutherland (orthogonal dimer) lattice. It shows a sequence of magnetization plateaus, which has been a subject of intense research since 1999. We have used a combination of torque and NMR measurements in high magnetic fields up to 34 tesla produced in LNCMI, Grenoble to determine the complete sequence of magnetic phases. Moreover, we have developed a systematic method to analyze the 11B-NMR spectra to determine the spin structure. We found a stripe order of triplets in all plateau phases. The sequence of plateaus and incommensurate phases combined with the evolution of spin structure allowed us to identify the magnetization process of $SrCu_2(BO_3)_2$ as an "incomplete devil's staircase". This work was done in collaboration with M. Horvatić, F. Mila, T. Waki, C. Berthier, S. Krämer, F. Levy, I. Sheikin, H. Kageyama, and Y. Ueda. The second example is the pyrochlore oxide $Cd_2Os_2O_7$. This material has been known for the continuous metal-insulator transition at 226 K since 1974, for which a Slater mechanism (opening of a band gap due to SDW order) was invoked. Recently, 5d pyrochlore oxides attract renewed interest because of the possibility of novel topological effects. We have performed ¹⁷O-NMR measurements on a single crystal of $Cd_2Os_2O_7$ and found that the M-I transition is accompanied by an antiferromagnetic order with the all-in/all-out spin structure. Since this spin order does not break space group symmetry including the periodicity of the lattice, Slater mechanism should be irrelevant. We also discuss unusual thermodynamic and critical behavior. This work was done in collaboration with I. Yamauchi, J. Yamaura, and Z. Hiroi.

Application of NMR to Strongly Correlated Electron Systems

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The purpose of this pedagogical talk is to illustrate in a systematic way how one can use NMR to detect phase transitions, structure of various ordered phases, and dynamics of strongly correlated electron systems. In the first part, I will start with simple symmetry principles which relate NMR spectra to the local site symmetry. Then I will describe how the change of NMR spectra (line splitting or broadening) across the phase transition can be analyzed to identify the broken symmetry and the structure of the order parameter. The examples include not only the ordinary magnetic ordering but ordering of charge, quadrupole, and even higher order electronic multipoles. This methodology based on the local symmetry is complementary and contrasting to the diffraction technique and particularly powerful when a single crystal is available.

In the second part, I will explain what one can learn about dynamics from the measurements of spin-lattice relaxation rate and spin-echo decay rate, taking examples from quantum spin systems and superconductors with strongly anharmonic phonons.

ORAL CONTRIBUTIONS

⁷⁵As NMR study of the Flux Lines Lattice dynamics in 122 iron-based superconductors

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Since the discovery of high temperature superconductivity in iron pnictides, much attention has been addressed to the comprehension of the microscopic mechanisms leading to superconductivity, while not so many works dealing with the Flux Lines Lattice (FLL) of these type II superconductors have been published. The 122 family of pnictides superconductors offers the possibility to investigate the FLL properties in large single crystals which allow to perform broadband NMR experiments.

We performed ⁷⁵As NMR on an Ba(Fe_{1-x}Rh_x)₂As₂ single crystal with x~0.07 by measuring spin-lattice and spin-spin relaxation rates both in the normal and in the superconducting state, at different applied magnetic fields (7 T and 3 T) with $\mathbf{H}_0 \parallel c$. The high temperature behavior of $1/T_1$ can be related to Korringa's law, typical of a metal, while just below T_c we found a peak in $1/T_1$ and $1/T_2$ which is tentatively ascribed to the FLL motion. From a simple model we were able to estimate the effective correlation time τ_e of the FLL motion, as previously done for the cuprate YBa₂Cu₄O₈. This model allowed us to decribe also the dimensionality of the FLL, and to derive an energy barrier, related to the applied magnitude of the magnetic field.

[1] D.C Johnston, Advances in Physics 59, 803-1061 (2010);

[2] M. Corti et al. Phys. Rev. B 54, 13 (1996).

Spin Gap in the Zigzag S=1/2 Spin Chain Compound Sr_{0.9}Ca_{0.1}CuO₂

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We present ⁶³Cu Nuclear Magnetic Resonance (NMR) measurements on undoped SrCuO₂ and Ca-doped Sr_{0.9}Ca_{0.1}CuO₂ single crystals. The crystal structure contains one-dimensional CuO₂ double chains that are magnetically decoupled due to frustration. For SrCuO₂ the spin lattice relaxation rate, T_1^{-1} , is temperature independent as it is expected for a one-dimensional S=1/2 Heisenberg spin chain. Doping with nonmagnetic, isovalent Ca takes place on the Sr sites outside the spin chains, and should not affect the magnetic properties of the compound. It is therefore very surprising that we do observe a decrease of T_1^{-1} in Ca-doped Sr_{0.9}Ca_{0.1}CuO₂ for temperatures below 90K that clearly evidences the opening of a gap in the spin excitation spectrum. Density Matrix Renormalization Group (DMRG) calculations of the J_1 - J_2 Heisenberg model are presented to discuss the origin of this spin gap.

[1] F. Hammerath et al., Phys. Rev. Lett. 107, 017203 (2011).

CryoMAS NMR - an efficient research tool for correlated electronic systems

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We have developed a magic angle spinning (MAS) technique which allows recording of high resolution MAS-NMR spectra in a wide temperature region (10K < T < 300K) including cryogenic temperatures. Reasonably high sample spinning speeds (50 kHz at 300 K and 20 kHz at 20 K) make the technique suitable to study temperature dependencies and small structural changes in correlated electronic systems. We will present the description of the CryoMAS probe and the results of studies on various structural changes and phase transitions in magnetic systems such as $Na_5RbCu_4(AsO_4)_4Cl_2$, in $Sr_2Cu(BO_3)_2$ and spin-Peierls compound $TiPO_4$; and on the temperature dependence of the Knight shift in superconducting MgB_2 .

³⁵Cl NMR and μSR investigation of Kapellasite, a new S=1/2 *kagome* system

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Quantum fluctuations and a frustrated geometry are major ingredients to destabilize Néel ordering in antiferromagnets. The materials with a 2D triangular corner-sharing *kagome* network and S=1/2 spins can even turn into a quantum spin liquid state at low T. The first structurally perfect S=1/2 *kagome* material synthesized was Herbertsmithite $Cu_3Zn(OH)_6Cl_2$. Recently, other related compounds have become available like Kapellasite, a polymorph of Herbertsmithite. There, the 2D character is more pronounced since the *kagome* planes are only weakly coupled via hydrogen bonds.

We present ³⁵Cl NMR and μ SR experiments, as well as magnetization (SQU-ID, VSM) and heat capacity measurements. ³⁵Cl NMR investigation reveals a multiplicity of magnetic sites which can be related to intersite mixing between Zn and Cu, in agreement with ICP and neutron diffraction analysis. This disorder does not induce any magnetic transition down to 20 mK as probed by the zero field μ SR experiment. We have measured the ³⁵Cl NMR Knight shift which yields an intrinsic local susceptibility which differs from Herbertsmithite. These results are completed by low-T heat capacity experiments and interpreted within a J1-J2 model on the *kagome* lattice.

[1] R.H. Colman, C. Ritter and A.S. Wills. Chem. of Mat., 2008, 20 (22), 6897

Magnetic field controlled frustration in a system of coupled spin chains

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In a certain range of applied magnetic fields, the ground state of an antiferromagnetic spin-1/2 chain is critical. Known as a Luttinger liquid, this state exhibits gapless excitations at a few points in the reciprocal space, where the dynamical spin susceptibility diverges on lowering temperature. Consequently, when weakly coupled, the spin chains magnetically order at low enough temperature. In simple coupling geometries, the chain mean-field theory (CMFT) proved to successfully capture the nature of such magnetic ordering, in particular, the transition temperature and the zero-temperature order parameter [1]. Geometric frustration of interchain couplings brings novelty and increases the number of possible ordered states, already when treated within CMFT. Using nuclear magnetic resonance, we demonstrate that $BaCo_2V_2O_8$ [2] provides an excellent experimental example of a system of weakly coupled spin chains with interplay of quantum criticality and geometric frustration. A unique combination of both allows to tune the effective strenght of interchain couplings by an applied magnetic field over a wide range. Consequently, the system can be brought over a novel zero-temperature phase transition separating two ground states with different phase arrangement of ordered spin density waves in the chains.

[1] M. Klanjšek et al., Phys. Rev. Lett. 101, 137207 (2008).

[2] P. Lejay, E. Canevet, S. K. Srivastava, B. Grenier, M. Klanjšek, and C. Berthier, J. Cryst. Growth **317**, 128 (2011).

Low-Temperature Properties of the Candidate Quantum Spin Liquid in EtMe₃Sb[Pd(dmit)₂]₂ as Revealed by NMR.

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In recent years, the two-dimensional spin-1/2 triangular lattice of the organic salt EtMe₃Sb[Pd(dmit)₂]₂ has emerged as a candidate for the realization of a quantum spin liquid. Furthermore, thermal conductivity and nuclear magnetic resonance (NMR) experiments unveiled the presence of a low-temperature instability in the spin liquid state, the opening of a spin gap. We performed a detailed ¹³C NMR study on this material at low temperatures (< 1.5 K) and for a wide range of external magnetic field values. In finite fields, a clear break in the temperature derivative of the spin lattice relaxation is observed at a temperature $T_m(H)$, with $T_m \rightarrow 0$ in the limit that $H \rightarrow 0$. We discuss these results in the context of possible instabilities, and existing thermodynamic data.
Magnetic interactions in hexanuclear cluster compounds of niobium and tantalum

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Octahedral hexanuclear clusters of Mo, W, Nb and Ta draw attention in the solid state research due to interesting phenomena they exert such as superconductivity at high critical fields and specific thermoelectric properties. Nb and Ta halide clusters, with the $[M_6L_{12}]^{n+}$ structural unit exist in three different oxidation states (n = 2, 3 or 4). Magnetic interactions between paramagnetic clusters (n = 3) have been noticed experimentally some time ago, whereas the role of bridging atoms (L) has been revealed using ¹⁹F ssNMR spectroscopy only 5 years ago [1]. More recently, a model of Heisenberg antiferromagnet ($\mathcal{H} = -J\sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j$) has been proposed for several Ta₆ halide cluster compounds [2]. Symmetry of the lattice determines the onset of an unusual long-range ordering. Usefulness of broad-band ssNMR and NQR spectroscopies in the investigation of these phase transitions will be discussed.

[1] R. Knoll, J. Sokolovski, Y. BenHaim, A. I. Shames, S. D. Goren, H. Shaked, J.-Y. Thépot, C. Perrin and S. Cordier, Physica B **381** (2006) 47

[2] B. Perić, S. Cordier, J. Cuny, R. Gautier, T. Guizouarn and P. Planinić, Chem. Eur. J. (2011) (DOI: 10.1002/chem.201002332)

Investigating random Heisenberg spin chains via nuclear magnetic resonance

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Exactly solvable theoretical models as well as suitable experimental techniques encouraged recent studies of the fundamental properties of low-dimensional spin systems (consisting of arrays of spins arranged in chains or ladders). According to renormalization group theory, random exchange couplings between spins favour the formation of a random-singlet (RS) state, corresponding to spins coupled at all possible distances and energy scales. However, the scarce availability of suitable random systems has so far prevented a convincing experimental identification of this particular magnetic ground state.

In a recent effort, employing nuclear magnetic resonance (NMR), dc magnetometry and numerical simulations, we found strong evidence for the formation of a random-singlet state in this class of materials. Randomness seems to generate a distribution of local magnetic relaxations, in turn reflected in a stretched exponential NMR relaxation. This distribution exhibits a progressive broadening with decreasing temperature, caused by a growing inequivalence of magnetic sites, as expected from RS theory. Our work suggests that NMR is a very suitable tool for probing the low-energy physics of other disordered magnets, where extended-scale excitations are dominant.

[1] T. Shiroka et al., Phys. Rev. Lett. 106 (2011) 137202.

Unconventional magnetism in CuNCN

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Copper oxides continue to fascinate with a plethora of exotic electronic ground states, including high-temperature superconductivity and cooperative quantum magnetic states. Replacing oxygen with "organic" bridges provides an exciting opportunity to extend this class of materials. Recently, the first nitrogen-based analogue CuNCN of the cupric oxide has been synthesized [1], where the oxygen anion O^{2-} is replaced with isolobal carbodiimide group NCN²⁻. In CuNCN neither susceptibility nor neutron diffraction measurements could detect long-range magnetic ordering (LRO) [2]. Even more surprisingly, the susceptibility of CuNCN is reminiscent of parent cuprates, being heavily suppressed and only weakly temperature dependent, which has triggered lively theoretical activities [3].

We have investigated magnetic properties of CuNCN employing various complementary local-probe techniques, including muon spin relaxation (μ SR), electron spin resonance (ESR) and ¹⁴N nuclear magnetic resonance (NMR) measurements [4]. Our results confirm the absence of LRO down to at least 63 mK. They reveal a highly unusual magnetic behavior. Inhomogeneities are observed below 80 K and partial spin freezing sets in below 20 K. We shall compare two possible unconventional ground states.

[1] X. Liu et al., Z. Natuforsch. B 60 (2005) 593.

[2] X. Liu et al., J. Phys. Chem. C 112 (2008) 11013.

[3] A. A. Tsirlin et al., Phys. Rev. B 81 (2010) 024424; A. L. Tchougréeff et al., arXiv:1008.0182.

[4] A. Zorko et al., preprint.

POSTER CONTRIBUTIONS

⁶³Cu NMR study of detwinned YBa₂Cu₃O_y single crystals (y =6.35, 6.45, and 6.6)

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We report ⁶³Cu NMR investigation in detwinned YBa₂Cu₃O_y single crystals, focusing on the highly oxygen-deficient regime (y = 6.35, 6.45, and 6.6). Both the spectra and the spin-lattice relaxation rates of the ⁶³Cu in the CuO₂ planes uncover the simultaneous presence of two spatially distinct regions in the form of metallic charge and insulating spin domains. From a glassy character of the phase, we interpret this as an evidence of nematic order for which the onset temperature T_0 is well defined. Our phase diagram in the underdoped region of YBa₂Cu₃O_y indicates the existence of a quantum critical hole concentration $p_c \sim 0.1$, below which nematic order emerges. At the same time, the pseudogap is abruptly closed below p_c .

Study of glassy and crystal ethanol by broadband nuclear magnetic resonance

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Deuterated ethanol (C₂D₅OD) was studied by means of broadband nuclear magnetic resonance at fields up to 12 T. Ethanol is used as an ideal model system for properties of glassy states. By varying temperature (30 K - 160K) and thermal history of the sample two stable solid states were achieved - crystalline ethanol and ethanol glass. Difference between these two states was verified by T_1 relaxation measurements, which are at least an order of magnitude longer in crystal than in glass. Relaxation time measurements are in agreement with known results from the literature [1]. In addition, here presented experimental data was measured in broader temperature range and, for the first time, at higher frequencies. Spectrometric measurements do not show any distinction between crystaline and glassy state, however, they do provide insight into the dynamics of methyl groups. Rotations of methyl groups are showed to be suppressed below 120 K and activated above 125 K. Activation of rotational degrees of freedom at relatively high temperatures implies methyl group confinement within ethanol crystal structure in both solid states investigated.

[1] T. Eguchi, G. Soda, and H. Chihara, Molecular Physics 40, 681 (1980).

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Microscopic theory of the ferromagnetic superconductor UCoGe

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The heavy fermion ferromagnet UCoGe exhibits superconductivity with the transition temperature Tc=0.6 K [1]. A remarkable feature of this systems is that the upper critical field for magnetic fields perpendicular to the easy-axis of the ferromagnetic order is larger than 10 T, in spite of its very low Tc at zero field, while the upper critical field for fields parallel to the easy-axis is much less than 1 T [1]. It is suggested that these mysterious behaviors may be deeply related to the origin of superconductivity of UCoGe. Recently, an important breakthrough for this issue has been achieved by the NMR measurements carried out by Ihara et al. [2]. They found that the ferromagnetic spin fluctuations in this system can be controlled by a magnetic field parallel to the easy-axis, and moreover, the spin fluctuations are intimately correlated with the magnitude of upper critical fields. On the basis of the NMR experimental data, we examine the scenario of spinfluctuation-mediated pairing mechanism for this system theoretically, taking into account the anomalous field-dependence of the correlation length derived from the NMR data. We have calculated upper critical field, and obtained the results which are in good agreement with the experimental data, reproducing the extreme anisotropy of the upper critical fields mentioned above. Our theoretical results establish that UCoGe is a spin-triplet superconductor in which the pairing glue is the exchange of ferromagnetic spin fluctuations.

[1] N. T. Huy et al., Phys. Rev. Lett. 99 (2007) 067006;N. T. Huy et al., Phys. Rev. Lett. 100, 077002 (2008); D. Aoki et al., J. Phys. Soc. Jpn. 78 (2009) 113709

[2] Y. Ihara et al., unpublished; K. Ishida, talk given at ICHE 2010 (Tokyo)

NMR study of pure and Ni and Co doped LiFeAs

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We present Nuclear Magnetic and Nuclear Quadrupole Resonance (NMR/NQR) measurements on pure, Ni and Co doped LiFeAs single crystals. The parent compound LiFeAs exhibits unconventional superconductivity with a transition temperature of about 17 K. Unlike other Fe based superconductors, where superconductivity is induced or stabilized by Co or Ni doping, replacement of Fe by these elements leads to a suppression of the superconducting transition temperature in LiFeAs. In case of Ni doping, a bulk magnetic order is induced below about 160 K. In contrast, for Co doping, the superconducting transition temperature is only reduced, but no magnetic order is observed. We discuss the nature and the origin of this magnetic order and its relation to unconventional superconductivity in pure LiFeAs.

Magnetic anisotropy of low dimensional CuSeO₃

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We present the first study of magnetism of monoclinic CuSeO₃. At high temperatures the system is paramagnetic and at $T_{max} \approx 17$ K the susceptibility has a maximum suggesting a low dimensional magnetic lattice. From consideration of possible Cu-O-Cu paths, we propose a magnetic lattice of spin tetramers. At $T_N = 8$ K the system undergoes a phase transition to long range AFM order. The spin axis direction in the ordered state is determined. Angular dependence of torque was measured in both the PM and the AFM state. A large rotation of the magnetic axes in the PM phase confined to the *ac* plane was detected from torque and confirmed by ESR measurements. The temperature dependence of susceptibility anisotropy and ESR linewidth [1] suggest possible presence of anisotropic exchange. Both symmetric and antisymmetric anisotropic exchange are possible in this system. To address this issue, NMR measurements are planned in the near future.

[1] I. Živković, D. Djokić, D. Pajić, M. Herak et al., manuscript in preparation.

Field tuned critical fluctuations in *YFe*₂*Al*₁₀**:** ²⁷*Al* **NMR/NQR and magnetization investigations**

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Some of the strongly correlated electron (d and f) systems exhibit non Fermi liquid (NFL) behavior near the quantum critical point (QCP) which are manifested by the appearance of unusual scaling laws in bulk properties like magnetization, resistivity, specific heat. The NFL behavior manifested in the local probe NMR usually by the observation of a non-Korringa spin-lattice relaxation rates $(1/T_1)$ in the low T limit for itinerant and local systems. For instance, in YbRh₂Si₂ this NFL behavior is associated with strong ferromagnetic fluctuations. In view of the fascinating features of itinerant ferromagnet and recently discovered aluminides we focused our interest on YFe_2Al_{10} because it is claimed being located close to a Fe-based ferromagnetic instability at very low temperature wherein pronounced NFL phenomena are observed in bulk magnetic properties. The temperature and field dependence of magnetization and magnetic specific heat follows unusual weak power laws over wide temperature and field ranges. This scenario is corroborated on a microscopic scale by NMR and NQR data wherein ²⁷Al NMR/NQR spin lattice relaxation rate follows the same weak power law over wide temperature and field ranges. The divergence in magnetic susceptibility, magnetic specific heat and dynamical spin susceptibility is attributed to the quantum critical fluctuation of Fe moments. These critical fluctuations are suppressed by magnetic field which leads to crossover from NFL to FL behavior of the system presented here. It is interesting to mention that these weak power law divergences in our NMR/NQR and magnetization data possibly suggesting the emergence of quantum Griffith phase close to quantum criticality the origin of which might be associated with lattice disorder due to Fe-Al site exchange. Our investigation is one of the rare examples wherein field tuning FM quantum criticality is studied by the local NMR/NQR probe and shed some light on the critical fluctuations of weak itinerant ferromagnets.

NMR study of La–Sr M–type hexagonal ferrites

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We present ⁵⁷Fe NMR and ab initio study of La–Sr M–ferrites. Substitution of Sr^{2+} by La³⁺ introduces extra electron into the system, hence charge compensation by Fe²⁺ cations is needed. We studied series of single-phase polycrystalline ferrites $Sr_{1-x}La_xFe_{12}O_{19}$, x = 0, 0.25, 0.50, 0.75 and 1 (see [1] for details on samples).

We observed that relative integral intensity in frequency region corresponding to resonance of nuclei of Fe³⁺ ions in $2a + 4f_2$ possitions gradualy decreases with increasing *x*. For x = 0.25 we can ascribe the intensity reduction to 2a resonance, for x = 0.5, 0.75 the 2a and $4f_2$ lines merge into one partly resolved profile and in LaM we observed no 2a resonance. Electronic structure calculations of SrM, charged SrM (one extra electron per unit cell), La_{0.5}Sr_{0.5}M and LaM system indicate tendency towards extra charge being localized on 2a site, which is in agreement with the experimental data and other works [2-3].

Further we analyzed lineshifts and profiles of 2b resonance with respect to La–Sr distribution. We were also able to observe low frequency (9-22 MHz) signal, which we ascribe to ¹³⁹La resonance.

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New NMR insights into modulated BEC in the Han purple compound

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The quasi-2D, antiferromagnetic exchange coupled spin-1/2 dimer compound $BaCuSi_2O_6$ (Han purple) is considered as a prototype of the magnetic field induced Bose-Einstein Condensation (BEC) of triplet excitations on a lattice. Recently, $BaCuSi_2O_6$ has been claimed to exhibit unusual reduction of dimensionality of the BEC from 3D to 2D when lowering the temperature, induced by frustration between adjacent planes [1]. However, due to a structural transformation at 90 K, different intradimer exchange couplings and different gaps exist in every second plane along the *c*-axis. Our ²⁹Si Nuclear Magnetic Resonance (NMR) experiments have shown that this leads to a modulated population of bosons in adjacent planes [2]. More recently, a better model has been presented, which takes into account both frustration and quantum fluctuations [3]. This leads to a non-zero population of *uncondensed* bosons in every second plane. We compare this model to our new ²⁹Si and ⁶³Cu NMR results, obtained at high magnetic fields (23-27 T) and low temperatures (50 mK) [2].

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⁵⁷Fe NMR and Mössbauer spectroscopy in bentonite/iron oxide composites

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Magnetic or superparamagnetic iron oxide particles of submicron and nanoscale dimensions are materials widely used in various fields, e.g. in biotechnology and catalysis. Although they are applied also as MRI contrast agents, these materials as such are studied by NMR only rarely.

We report ⁵⁷Fe NMR investigation of composite bentonite/iron oxide samples. Composite samples were prepared by isothermal calcination of powder composed of bentonite and precursor containing ferric acetate. We focused on spectral region corresponding to ⁵⁷Fe NMR in maghemite and monitored its evolution with temperature of calcination T_{calc} . Spectra were recorded at 4.2 K using CPMG pulse sequence.

One of the main findings is that the spectral features characteristic for maghemite become more distinct with increasing T_{calc} up to 420 deg, which is most likely connected with higher degree of atomic/vacancy ordering in maghemite spinel structure.

Evaluation of integral intensities in NMR spectra allowed us to determine the relative content of maghemite phase in particular samples of the series: the content rapidly grows for T_{calc} up to 420 deg. For higher temperatures a presence of hematite is detected while the amount of maghemite phase decreases, in accordance with results obtained by Mössbauer spectroscopy.

Resonant G'-band and D-band Raman scattering in graphene

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The second-order Raman scattering has been widely used to determine the dispersions of optical phonons in different sp^2 based carbon materials. Physical grounds for the dispersive behavior of these Raman signals in graphite have been explained in terms of the double-resonant (DR) response theory. In the present work we consider the G'-band and D-band Raman scattering in graphene, by using the complete form of the Raman matrix elements and show that the contribution to these matrix elements of the triple-resonant scattering channel is one order of magnitude larger than the DR contribution. This results in enhancement of two orders of magnitude in the G'-band and D-band Raman intensity with respect to the DR theory. The theory used in the analysis is very general and can also be used to study different anomalies observed in the intraband and interband optical conductivity in graphene.

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Critical dynamics in the S=1/2 Heisenberg chain compound copper pyrazine dinitrate – NMR experiment versus effective field theory

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Copper pyrazine dinitrate (CuPzN) is known as one of the best realizations of the antiferromagnetic S=1/2 Heisenberg chain model with a relatively small coupling constant $J/k_{B}=10.7$ K [1]. Here, a field-driven quantum critical point (QCP) at $B_c = 14.6$ T marks the transition between a Luttinger liquid state and a ferromagnetically polarized phase. We present a comprehensive 13C-NMR study of CuPzN, with an emphasis on the parameter regime of the QCP. A comparison of our experimental findings with both numerical (quantum Monte Carlo) and analytical (conformal field theory) approaches is made and yields a very good agreement. In particular, a well-defined maximum of $1/T_1(B,T)$ below B_c is revealed as the signature of essential spin-spin interactions in the Luttinger liquid phase [2,3]. The ${}^{14}N$ -nuclei were used as a second probe in this compound. From an angular-dependent study of the NMR-observables in the low-field regime, the absolute contributions of the quadrupolar and magnetic terms in the total nuclear Hamiltonian could be disentangled, allowing a precise determination of the local EFG and local distribution of spin moments. The magnetic ${}^{14}N - 1/T_1$ -data sets confirm the ${}^{13}C$ -nuclei as suitable probes for the electronic spin dynamics in this compound.

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Absence of hyperfine field in magnetic zinc and chromium ferrites nanoparticles

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Two groups of ferrites namely zinc ferrite and chromium ferrites were synthesized in the nanosize range by taking their citrate salts. X-ray diffraction results show that all the synthesized samples possess good spinel structure [1]. We have chosen above samples because Zn is diamagnetic and prefers tetrahedral site, while Cr is arrange themselves in anti-ferromagnetic fashion in metallic phase and prefers octahedral position in the spinel ferrite. Interestingly the samples with smaller particle size are strongly attracted by a permanent magnet and give large magnetization in VSM measurement. However, we don't get any magnetic hyperfine splitting in the Mössbauer spectrum. The doublet of zinc ferrite was not split into any sextet even at 12K. Similar behaviour was found for the chromium ferrite also down to 16K. The saturation magnetization ZnF is found to be larger than that of Cr ferrite of comparable particle. The value sensitively depends on the particle size but the Mössbauer parameters get only slightly affected by particle size. Even at the highest magnetization of 28 A-m2/kg (Zn ferrite 13 nm sample), the magnetic splitting is not seen in the Mössbauer spectra. The relation between the magnetic ordering in the VSM measurement and internal hyperfine field therefore needs to be investigated with greater care.

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Phase transition and conduction mechanism in the ionic conductor Cu₂HgI₄

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The ionic conductor copper(I)-tetraiodomercurate(II) has been known for several decades due to its near-room temperature insulator-conductor transition and striking colour change at the transition temperature [1]. However, the transition details and conduction mechanism have been debated [2]. We present the first combined NMR and conductivity study of this material, revealing extensive pretransition fluctuations and suggesting a new conduction mechanism in the conductive phase.

 63 Cu spin-lattice relaxation times show an anomalous decrease starting ~ 50K below the transition temperature and a sharp drop of two orders of magnitude at the transition, accompanied by substantial line broadening; careful relaxation measurements indicate that a fast process is already present several K below the transition. Pretransitional disordering also influences the 63 Cu chemical shift, which shows power-law behaviour close to the transition. The 199 Hg line is, however, significantly narrowed in the conducting phase, unexpectedly implying that the large and heavy Hg²⁺ diffuses through the material contributing to the ionic conduction process. This was confirmed by spin-spin relaxation measurements on 199 Hg in a constant field gradient, which produced a faster-than-exponential decay function characteristic for spin diffusion.

This work has been done using the equipment purchased within FP7 project no. 229390 SOLeNeMaR.

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Pressure study of Co_{1/3}**NbS**₂

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Systems in which magnetic ordering is suppressed to low temperatures due to competing interactions have attracted much attention in recent years. In $Co_{1/3}NbS_2$, the cobalt atoms are intercalated within the layered structure of the parent compound 2H-NbS₂, forming the triangular lattice between NbS₂ layers. At ambient pressure, spins on the Co atoms show antiferromagnetic ordering at 26 K, with ferromagnetic chains formed along one plane direction. Hydrostatic pressure suppresses the ordering at a rate of $dT_N/dp = 1.2$ K/kbar.[1] Recent investigations indicate the occurrence of a quantum critical point at p = 2.6 GPa, as well as nonmonotonous pressure dependence of the Kondo-type behavior. The ordering mechanism is not fully understood yet, although the competition of super-exchange and RKKY interactions are natural candidates. Notably, ordering takes place within the metallic host, and the possibility exists that the suppression of the ordering proceeds via the Doniach mechanism in which the magnetic moment is screened by the conducting electrons. In this contribution we present an extensive set of measurements characterizing the transport properties of Co1/3NbS2 under pressure. We also touch upon the high-pressure facilities that are currently being developed in our laboratory. Future direction of investigation will be highlighted, as well as other ways to affect magnetic subsystems. The possible role of NMR in helping to resolve the mysteries of this, and related systems, will also be discussed.

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HP NMR Measurements on *Cs*₃*C*₆₀

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Three years ago, the discovery of the largest member of the alkali-doped fulleride family (Cs_3C_{60}) revitalized the research on the fullerene superconductors [1]. The hyper-expanded lattice places this member over the metal-insulator transition (MIT) to the insulator state. The metallic ground state could be obtained only under the pressure of 3 kbar, becoming superconducting (SC) at low temperatures with maximum T_c of 38 K at 7 kbar. A non-monotonic behavior of the T_c versus pressure cannot be explained within the standard BCS theory, thus calling for a detailed investigation of the superconductivity close to the MIT. To study the fcc Cs_3C_{60} we measured a high-pressure ¹³C NMR. A precise in-situ pressure calibration allowed us to exactly determine the position of our NMR measurements on the phase diagram. We show that the superconducting ratio $2\Delta/k_BT_c$ for small unit cell volumes yields a BCS value of 3.5, however closing to the Mott state the ratio is increased up to the value of 5. From the $1/T_1T$ values just above the superconductor transition we observed an increase in the spin susceptibility, which is in best agreement with the dynamic mean field theory DMFT calculations [2], where the electron correlations are taken into the account. The remaining discrepancy can be attributed to the antiferromagnetic spin correlations.

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Static solid state NMR and NQR investigation of niobium halide clusters

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Hexanuclear metallic clusters $[(M_6L_{12}^i)L_6^a]^{n+}$ (n= 2, 3, 4) are worth studying due to many interesting properties, ranging from superconductivity or antiferromagnetism to thermoelectric properties. Physical properties of metallic halide clusters depend on their oxidation states. The simplest case are diamagnetic (n=2)clusters. They can be taken as reference compounds for study of n=3 clusters which exhibit magnetic interactions. To obtain reference NMR parameters, we have studied two diamagnetic clusters, $[Nb_6Br_{12}(H_2O)_6][HgBr_4] \cdot 12H_2O$ and Nb₆Cl₁₂(H₂O)₄(OH)₂·4H₂O, whose structures were previously determined [1]. Static ⁹³Nb and ³⁵Cl NMR powder spectra have been obtained in magnetic field of 12 T. In addition, zero field NOR measurements of ⁹³Nb, ⁷⁹Br, and ⁸¹Br have given precise EFG parameters. Independent GIPAW-DFT calculations of NMR and NQR parameters have been conducted using program CASTEP-NMR [2], and compared to experimentally obtained parameters.

This work has been done using the equipment purchased within FP7 project #229390 SOLeNeMaR.

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Study of local field distribution on the surface of single-molecule magnet

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Single-molecule magnets (SMMs) are candidates for many applications, such as quantum computation, high-density magnetic data storage and magnetoelectronics[1],[2]. In order to develop these applications, it is important, among others, to investigate when they are in contact with other dissimilar materials because it is expected that their wave functions and/or magnetic fields extend considerably outside the physical structure[3]. This also implies to improve detection of magnetic field on their surface i. e. magnetic field generated by the crystal in the vicinity of its surface. Magnetic properties of SMM at temperatures above blocking temperature, $T > T_B$, can be considered as a superparamagnetic properties. In superparamagnetic systems the observed magnetic behavior strongly depends on the value of the measuring time, t_m , of the employed experimental technique with respect to intrinsic characteristic relaxation time, τ , of magnetization. Therefore, it can be expected wide variation in the employing time "window", which varies from large values as in magnetization measurements (typically 100 s) to the very small ones, like in ac-susceptibility or spectroscopy (10 ns). Detection and estimation of such distribution of local fields on surface at very short time interval (0.1 ns) as a function of orientation of SMM crystal in the external magnetic field by employing paramagnetic probes are in the focus of this presentation.

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NMR study of quantum critical point in the DTN spin chain compound

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The NiCl₂-4(SC(NH₂)₂) compound (DTN) presents a Bose-Einstein Condensation (BEC) if we apply a magnetic field parallel to its *c* axis [1]. We have studied this compound close to its second critical field (H_{c2}) with proton NMR at very low temperatures in a dilution refrigerator. Analysing the proton spectra we determine the precise orientation of the sample with respect to the field, which is important for the existence of a BEC. We have determined the phase diagram, that is the dependence of the critical temperature T_c on the field, allowing us to determine the zero temperature H_{c2} value. We have performed T_1 measurements as a function of temperature for differents fields above H_{c2} . These data define the evolution of the gap versus the field, presenting a significant residual gap at H_{c2} , apparently in contradiction with the BEC scenario. In the low temperature 3D ordered (BEC) phase, we have determined the field dependence of the order parameter, as well as the temperature dependence of T_1 providing an information on the spin dynamics of this phase.

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NMR in Substituted Magnetite

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In the past, NMR has significantly contributed to understanding of complicated physics of pure magnetite (Fe_3O_4). Equally intriguing is the behaviour of magnetite containing low concentration of nonmagnetic cations. In these compounds, the NMR may shed light on the localization of the charge carriers near the impurities and on modification of the Verwey transition.

This work concerns ⁵⁷Fe NMR study of series of single crystal samples of magnetite with small concentration of Ti, Al, Zn and Ga. Various types of substitution enter into different crystallographic sites: Ti^{4+} and Al^{3+} ions replace iron ions $Fe^{2.5+}$ in octahedral (B) sites, while Zn^{2+} ions enter into tetrahedral (A) sites replacing ferric ions and Ga^{3+} ions preferentially occupy also the A sites. Due to the modified hyperfine field, resonance frequencies of nuclei in the neighbourhood of the substitution ions are shifted, thus satellite lines appear in NMR spectra.

Temperature dependences of spectra were measured above the Verwey transition in a zero external magnetic field. A special care was taken to detect satellite patterns and pronounced satellite signals were assigned to corresponding crystallographic configurations of the resonating nucleus and the substitution. Dependences of frequencies of main and satellite lines on temperature were compared for different types of substitution and also cationic vacancies. An analysis comprising a confrontation with the mean field based calculations was performed. Moreover, temperature dependences of widths of A lines above the Verwey transition are reported and discussed.

Peculiar high-field quantum magnetism in the frustrated s = 1/2 spin chain cuprate linarite

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We present an experimental and theoretical study of the quasi-onedimensional s = 1/2 Heisenberg magnet linarite PbCuSO₄(OH)₂, with competing ferromagnetic nearest-neighbor and antiferromagnetic nextnearest- neighbor exchange interactions. It includes magnetization and NMR studies as well as theoretical simulations for the determination of the leading exchange couplings, which are about an order of magnitude higher as determined previously.[1] Furthermore, a manifold of field-induced phases are probed, from which we draw a preliminary phase diagram. Notably, spin-lattice relaxation investigations indicate that linarite might undergo a magnetic quadrupolar spin liquid phase transition as recently predicted for such materials.[2]

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NMR study of magnetism and superconductivity in pnictides

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Unconventional superconductivity has now been evidenced in a wide variety of materials, high Tc cuprates, cobaltates, heavy fermions, organic conductors. Despite their differences, all these compounds share a common unexpected feature: in all their phase diagrams, superconductivity is always adjacent to a long range magnetic ordered phase, usually antiferromagnetic (AF). The Recent discovery of pnictides gives hope to understand how these two phases interact. These Fe-based materials display a spin density wave (SDW) magnetic ordering which turns into a high temperature superconductor when doping or pressure is applied.

We present a ⁷⁵As NMR study on various pnictides family in fixed and sweep field experiments up to 14 Tesla. We study the effect of the distance between Fe-As plans on the electron behavior and superconductivity by comparing Co-doped Sr_2ScO_3FeAs (1111, high inter-plan distance) and Co-doped $BaFe_2As_2$ (small interplan distance). We also study the nature of the magnetic state versus doping in electron doped $Ba(Fe_xM_{1-x})_2As_2$ (M=Co, Ni) high quality single crystals to decide whether disorder or incommensurability can explain the observed magnetic state.

EPR studies of the 3D networks {[**Cu(bpy**)₃][**M**₂(**C**₂**O**₄)₃]·**H**₂**O**}_n

P-22

 $(\mathbf{M} = \mathbf{C}\mathbf{u}^{2+}, \mathbf{M}\mathbf{n}^{2+})$ Dijana Žilić¹, Boris Rakvin¹, Marijana Jurić¹

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The homometallic {[Cu(bpy)₃][Cu₂(C₂O₄)₃]·H₂O}_{*n*} (*1*) and the heterometallic {[Cu(bpy)₃][Mn₂(C₂O₄)₃]·H₂O}_{*n*} (*2*) compounds (bpy = 2,2'-bipyridine) have been synthesized. The structures of both compounds consist of a 3D, polimeric anionic network $[M_2(C_2O_4)_3]_n^{2n-}$ (where M = Cu²⁺ or Mn²⁺) with cations [Cu(bpy)₃]²⁺ occupying the vacancies of the framework. So far, only a few singlecrystal structures of this type of 3D metal oxalates have been described.

Electron paramagnetic resonance (EPR) measurements performed by an Xband spectrometer on a polycrystalline sample of 1 and on a single crystal of 2, in the temperature range 300–5 K, are presented.

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PROGRAMME

	Monday	Tuesday	Wednesday	Thursday	Friday
8:45-9:00	opening				
9:00-9:50	M. Takigawa	V. Kataev	MH. Julien	M. Takigawa	D. Arčon
9:50-10:40	W. Halperin	Y. Furukawa	M. Poggio	F. Bert	N. J. Curro
10:40-11:10	Coffee	Coffee	Coffee	Coffee	Coffee
11:10-12:00	A. Keren	P. Prelovšek	A. Smontara	M.Horvatić	De Renzi
12:00-12:30	F. Hammerath	L. Bossoni	A. Zorko	E. Kermarrec	Closing
12:30-13:30	Lunch	Lunch	Excursion	Lunch	Board meeting
13:30-16:00					Lunch
16:00-16:50	H. Mukuda	I. Eremin		F. Mila	
16:50-17:20	M. Klanjšek	G. Koutrolakis		I. Heinmaa	
17:20-17:50	Coffee	Coffee		Coffee	
17:50-18:40	K. Ishida	. Ishida H. H. Klauss		Poster session	
18:40-19:10	T. Shiroka	B. Perić			
19:10-20:00					
20:00				Banquet	