Final report for “The New Generation in Strongly Correlated Electrons Systems” conference

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(Organizing committee)

This is the final payment report for the 2011 edition of the conference “The New Generation in Strongly Correlated Electrons Systems” in relationship with the grant received from the European Science Foundation through its programme “Intelbiomat.” The structure of this report is the following. In the first section we briefly summarize the most relevant aspects of the conference. In the second section we recapitulate the scientific program and discussions that took place in the conference. In the third section we mention the possible effects of the conference in the future development of the field. Finally we append the full program of the conference, including the abstracts for each scientific contribution.

Summary.

The 2011 edition of the conference “The New Generation in Strongly Correlated Electrons Systems” took place in the campus of the University of Santiago de Compostela (Spain) from July 3 to July 8, 2011. The conference is the second of a series started in 2010 in Lanzarote (Spain). The aim of these conferences is to bring together emergent researchers in the field of strongly correlated electrons and promote collaborations between them in a friendly atmosphere.

The final number of participants was 63. We had several last-minute cancels and thus the number was slightly smaller than our goal of 75. Most of participants were young scientists: graduate students (24%), postdocs or young professors. They came from Europe excluding Spain (50%), Spain (26%), and the US (20%). 18% (21%) of participants (invited speakers) were female.

All participants were asked to present a scientific contribution. We had 32 talks and 23 posters. Invited speakers (14) presented 45-minute talks (plus 15 minutes of discussion), half of the time devoted to introduce a technique, method, or physical phenomenon, the other half to present their research. The rest of the speakers (18) presented 20-minute research talks (with 10 minutes of discussion). Poster contributors were asked to present them in a flash-poster session (two-minute presentation using two slides each), followed by a one-hour regular poster session for discussion. All posters were on display for the duration of the conference to stimulate discussion during breaks. The scientific content of the conference is discussed in the next section.

The University of Santiago de Compostela supported the conferences strongly. First we had access to the facilities of the new “Center for Research in Biological Chemistry and Molecular Materials” (CIQUS), which included a full-equipped conference room. Second the CIQUS itself took charged of some expenses such as printing the abstract books, and renting of boards for displaying posters. Third the University provided local administrative support (for billing, accounting, etc...), and a discounted price for 20 rooms in one of its residence halls.

Besides this Intelbiomat grant, the conference was funded also by the Spanish Ministry of Science and Innovation within the framework of its “Subprogram for Complementary Actions to Non-oriented Fundamental Research Projects” through grant FIS2010-12330, for an amount of 8000€. Another source of funding were the fees charged to participants. Regular participants (all but the organizers and invited speakers) were charged with a 150€ registration fee used to cover the social events (excursion, conference dinner, and reception.) We intentionally keep the registration fee as low as possible since most participants are young scientists who often lack strong financial support.

A website (http://ngsces2011.cesga.es) was created for the conference. It served as administration and communication tool, and in the future will be kept online to store the scientific program, including the slides of each talk. Initially we planned to videotape the talks and make them available to the general public through the website. This turned unfeasible due to technical difficulties. We also opened a Twitter channel to post news about the conference.

Scientific content

The conference was open to any topic in the strongly correlated electron arena, but focussing in four main points: superconductivity, including pnictides and cuprates; oxide heterostructures; topological insulators and topological order, and graphene. Being a general conference, we tried to keep a good balance between theory and experiment. In this section we summarize its scientific content by describing each of sessions. We start by describing the introductory (half-)talks given by the invited speakers.

Introductory half-talks

As it was said above we asked the invited speakers to use half of their time to present in an introductory and pedagogical way a technique, method, or phenomenon relevant to their research. This introductory talks were proved very useful taking into account that many of the attendees are graduate students and young postdocs, making this part of the conference similar to an advanced school.

We have several talks discussing theory. Capone and Kunes presented a very concise introduction to Dynamical Mean Field Theory (DMFT), Density Functional Theory (DFT) and the interplay and recent attempts to merge them in a method that allows to solve the strong correlated electron problem using *ab initio* input. Later Johannes explained the application of DFT to pnictides. Melko introduced a new method developed in his group to calculate entanglement in strongly correlated systems using Quantum Monte Carlo (QMC) techniques. Sengupta and Chern discussed the basics of frustration in magnetically frustrated systems and some techniques to treated them, focussing in mean-field solution and Chern-Simons theories (Sengupta) and in the emergence of gauge fields and fractionalized particles (Chern).

On the experimental side, we have several talks on spectroscopic techniques. Deisenhofer gave a nice introduction to optical spectroscopy, specifically in the THz and far-infrared range. Bobroff explained nicely the basics of Nuclear Magnetic Resonance (NMR) in condensed matter. Santander introduced Angle Resolved Photoemission (ARPES).

There were also a few talks introducing different types of materials. Vorontsov discussed the physics of pnictides. Rossier gave a primer on the physics of graphene. Caviglia presented the most relevant aspects of the physics of oxides heterostructures and interfaces. Zapf gave an introduction to new multiferroic materials. Hébert presented a review on thermoelectric oxides.

There was also a special talk on outreach given by Bobroff. He explained how to do outreach in quantum physics using the example of superconductivity and the materials that a team leaded by him have develop to commemorate the centennial of the discovery of superconductivity. It was a very encouraging talk on an aspect of the scientific work that it's sometimes underestimated.

Monday session (research)

Monday session was dedicated in part to high-temperature superconductivity. Capone presented a unified view on superconductivity of fullerides. Vorontsov discussed the competition of spin-density-wave and superconductivity in a weak-coupling approach to pnictides. Valenzuela discussed the origin of the anisotropy in the conductivity of pnictides

relating it to the anisotropy in the magnetic, rather than in the orbital order. There were also talks on other topics. Mazzoli presented diverse experimental results that clarify the magnetic order in the frustrated compound $Ca_3Co_2O_6$. Brzezicki presented a cluster mean-field theory analysis of the Kugel-Khomskii Hamiltonian in mono- and bilayers. Kunes showed the results of his DMFT calculations on the two-band Hubbard model to describe the high-spin to low-spin transition in $LaCoO_3$. Deisenhofer presented optical spectroscopy measurements on several frustrated magnets and low-dimensional magnets, analyzing in particular their magneto-optical excitations.

Tuesday session (research)

Tuesday session was entirely dedicated to high-temperature superconductivity. Johannes open the session by discussion the role of spin-fluctuations on the superconductivity of pnictides. Based on her DFT calculations, she proposed an explanation for the relation between the magnetic and structural transitions in pnictides. Bobroff explained how using NRM spectroscopy on pnictides one can distinguish between the different segregation states induced by Ru or Co doping of $BaFe_2As_2$. Park presented his work using muon-spin-resonance spectroscopy to analyze a novel tetragonal phase found in Mn-doped $BaFe_2As_2$. Monney discussed his measurements using Resonant Inelastic X-ray Scattering to analyze the energetics of the Zhang-Rice singlets and triplet excitations on Li_2CuO_2. Gadermaier presented a unified view on the role of the electron-phonon interaction on both cuprate and pnictides. Bauer discussed the presence and origin of the low energy kinks in the electronic dispersion of cuprates and its evolution with doping.

We closed the superconductivity chapter of the conference with an open discussion leaded by Batista and Rivadulla with the participation of all the participants. The most debated points were the origin of the pseudo-gap, the similarities between hole- and electron doped cuprates phase diagram, and whether pnictides can be considered as moderate correlated systems due to Coulomb or Hund coupling.

Wednesday session (research)

Wednesday session was entirely dedicated to oxide heterostructures and interfaces. Santander presented the recent paper of his group on the appearance of a metallic two-dimensional electrons gas on the surface of $SrTiO_3$ obtained by cleaving an insulating $SrTiO_3$ crystal. Caviglia analyzed the two-dimensional superconductivity state at the interface between $LaAlO_3/SrTiO_3$ and how to tune it to a quantum critical point applying static electric fields. He also showed how the limitations of this approach can be overcame by inducing ultrafast lattice excitations in the system. Perucchi discussed the optical properties of heterostructures of $(SrMnO_3)_n(LaMnO_3)_{2n}$ with the variation of the number of layers n, pointing to the appearance of a novel electronic state at the interfaces as an explanation of his results. Bach showed measurements proving the enhancement of the superconducting critical temperature on diverse multilayer thin film cuprate heterostructures in comparison to their single phase film counterparts. Zhou discussed how by measuring RIXS spectra in heterostructures made out of ferromagnets (manganite) and superconductors (cuprate), an orbital reconstruction at the interface is observed.

Thursday session (research)

Thursday session covered a range of topics. Rossier discussed several phenomena appearing in nanostructures made out of graphene, such as the magnetism in graphene

nano-ribbons edge or the influence of spin-orbit coupling on them. Castro analyzed the appearance of a topological fermi liquid in the doped honeycomb lattice. Grushin presented a very original work on the possibility of tuning the character of the Casimir force between plates of 3D topological insulators from an attractive to repulsive interaction. Melko showed how new techniques to measure quantum entanglement within QMC allow to characterize topological ordered states. Dil presented spin-resolved ARPES measurement on topological insulators. Andújar presented his work on metal organic frameworks focussed on its dielectric properties. Sengupta discussed the formation of magnetization plateaus in some compounds described by the Shastry-Sutherland model. Chern discussed the formation of orbital ice (an analogous to spin ice) in p-band Mott insulators in the diamond lattice.

Friday session (research)

Friday session was dedicated to several topics. Zpaf discussed new possibilities on the physics on multiferroic materials. Hébert presented new advances made on her group on the field of oxide thermoelectrics. Bisogni presented RIXS and EELS measurements to analyze the Zhang-Rice excitations in $CuGeO_3$. Inosov presented inelastic neutron scattering measurements in CeB_6 antiferroquadrupolar spin resonance mode. Radwanski presented his calculations on the effect of the crystal-field interaction on several 3d- and 4f-electron materials, including heavy fermion systems. Ivanshin showed electron spin resonance measurements on $YbRh_6P_4$.

Poster sessions

Poster sessions presented a variety of topics. Most of the posters were presented by students, and there was fruitful interaction between participants. It's important to take into account that the fact that most of the participants are in the similar group age favor interactions, eliminating the intimidation factor that sometimes hampers them in larger conferences.

Open discussion (Friday)

There was a session (the last one of the conference) dedicated to assess the results of conference and to discuss the issues that the participants (as young scientists) feel there are more relevant to their work. In particular, the focus was in finding a way of continuing this series of conferences as well as in finding new and better way of collaboration among them.

Assessment of the results and impact of the event on the future direction of the field

Different group leaders, postdocs and PhD students from Europe, USA and Asia came to the conference The New Generation in Strongly Correlated Electron Systems to present their latest results in this exciting field of research. This conference was conceived as a place of exchange of ideas between young researchers, in a friendly atmosphere, at a time in which new experimental capabilities revitalized the field of high temperature superconductivity, and the discovery of superconducting pnictides added more exciting materials to the field.

To give the possibility to young people to discuss their ideas, sometimes risky hypothesis that can have a hard time to make it to the front line in a larger conference, is something that must be encouraged for new ideas to come into the field. We are absolutely satisfied with the result at this respect, given the large amount of time dedicated to discussion and debate, after each of the sessions of the conference. Also, as a result of the exchange of ideas, new collaborations were established among the participants.

Apart from the pure scientific exchange there are two results of the conference that should be mentioned. First given the success of the conference organized in Santiago de Compostela (as well as that of the first edition organized in Lanzarote in 2010), there was a proposal by Gadermaier and Capone, among others, to organize the third edition next year in Slovenia. Some other people started to plan the fourth edition in 2013. We consider that this can be establish this conference as one of the places for scientific exchange for young scientists in the field of strongly correlated electron systems.

The second result was the idea of organizing more stable collaborating structure around the conference. An idea that was discussed was to apply for funding to create a collaboration network through the COST program (sponsored by the EU.) A small team of 5 people was named to analyze the possibilities of establishing such a network.

The New Generation in Strongly Correlated Electron Systems

Santiago de Compostela, July 3rd to 8th 2011

Organizing Comittee:

Iván González (*Centro de Supercomputación de Galicia*),
Francisco Rivadulla (*Universidade de Santiago de Compostela*),
Víctor Pardo (*University of California at Davis*), and
Cristian BAtista (*Los Alamos National Lab*).

For updates on this program, see: http://ngsces2011.cesga.es, http://twitter.com/#!/ngsces2011.

Time	Monday	Tuesday	Wednesday	Thursday	Friday
8:45-9:00	Opening				
9-10	Capone (invited)	Johannes (invited)	Santander (invited)	Rossier (invited)	Zapf (invited)
10 -11	Mazzoli, Brzezicki	Bobroff (invited)	Caviglia (invited)	Castro, Grushin	Hébert (invited)
11-11:30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:30- 12:30	Kunes (invited)	Park, Monney	Perucchi, Zhou	Melko (invited)	Bisogni, Inosov
12:30- 1:30	Deisenhofer (invited)	Gadermaier, Bauer	Bach	Dil, Sánchez-Andújar	Radwanski, Ivanshin
1:30 - 3:30	Lunch	Lunch	Lunch	Lunch	Lunch
3:30- 5:00	Posters & coffee	Posters & coffee	Excursion	Sengupta (invited) & coffee	Open discussion & closing
5:00-6:30	Vorontsov (invited), Valenzuela	Open discussion	Excursion	Chern (invited)	

Dynamical Mean-Field Theory and Strongly Correlated Superconductors: Can repulsion favour superconductivity?

Massimo Capone

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The most striking realizations of superconductivity have been uncovered in materials where electron-electron correlations are strong, leading to Mott insulating states. This is an intuitively surprising situation, because superconductivity requires attractive interactions and Mott physics arises from strong repulsion. While this link between superconductivity and correlations is almost universally recognized for copper-oxides, it has been revealed recently also for organic superconductors like the alkali-metal doped fullerides such as Cs_3C_{60}, despite the pairing in these materials is likely driven by phonons.
We discuss how superconductivity can be favoured by electron-electron repulsion by solving models for these two families of superconductors using Dynamical Mean-Field Theory (DMFT), a powerful nonperturbative approach for correlated materials. For the case of fullerene superconductors, our calculations predicted a transition between superconductor and a Mott insulator [1] and several properties that have been confirmed experimentally in later experiments [2]
The first part of the talk will be devoted to a brief introduction to DMFT and to its use for superconductors. In the second part we will present results for fullerenes and discuss the relevance of our theory for different compounds including potassium-doped picene, another surprising organic superconductor [3].

[1] M. Capone, M. Fabrizio, C. Castellani and E. Tosatti, Rev. Mod. Phys. **81**, Rev. Mod. Phys. 81, 943 (2009); Science **296**, 2364 (2002)
[2] Y. Takabayashi et al., Science 323, 1585 (2009); A.Y. Ganin et al. Nature Materials 7 367 (2008)
[3] R. Mitsuhashi et al. Nature 464. 76 (2010); G. Giovannetti and M. Capone, Phys. Rev. B **83**, 134508 (2011)

Frustrated Magnetism: The $Ca_3Co_2O_6$ Paradigm

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In solids, magnetic frustration can lead to exotic states of matter. In this sense, $Ca_3Co_2O_6$ is a textbook case showing unprecendent magnetic state coexistence, dynamics and step like magnetization dependence on magnetic field. Our investigation by means of resonant X-ray diffraction [1-3], neutron diffraction [4-5] and NMR [6] has finally clarified both the magnetic ground state and the peculiar dynamical properties, allowing for a careful determination of the magnetic interaction at play. In particular, the previous scheme of a simple quasi 1D frustrated system has been proven insufficient to describe the complexity of this system and a much more complex picture of magnetic interaction has been proposed.

[1] Phys. Rev. B 77 (2008) 140403R
[2] Phys. Rev. B 78 (2008) 100406R
[3] Phys. B 404 (2009) 3042
[4] Phys. Rev. Lett. 101 (2008) 097207
[5] Eur. Phys. Lett. 90 (2010) 67006
[6] Phys. Rev. B, accepted (DOI: 10.1103/PhysRevB.83.104408)

Entangled Spin-orbital Phases In The d^9 Model

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The phase diagram of the spin-orbital (SO) Kugel-Khomskii (d^9) model posed a challenging theoretical problem [1], yet it is still unknown [1]. Here we investigate the phase diagrams of the d^9 model, depending on Hund's exchange J_H and the e_g orbital splitting E_z, for a bilayer and a monolayer square lattice using Bethe-Peierls-Weiss method with exact diagonalization of a cubic or square cluster coupled to its neighbors in ab planes by the mean-field (MF) terms. The cluster MF method confirms existence of singlet phases similar to those obtained by variational wave functions [2], and enables finite SO order parameter independent of spin and orbital ordering. For a bilayer we obtain phases with interlayer spin singlets stabilized by holes in $3z^2 - r^2$ orbitals and with alternating plaquette valence-bond (PVB) as well as two new phases with SO entanglement, in addition to the antiferromagnetic (G-AF, A-AF) and ferromagnetic (FM) order. For a monolayer we obtained at temperature $T = 0$: (i) the PVB phase, (ii) two AF phases with either $3z^2 - r^2$ or $x^2 - y^2$ orbitals occupied, and (iii) a FM phase. However, after including thermal fluctuations ($T > 0$) we found the same entangled SO phases as for a bilayer at $T = 0$. This shows that both quantum and thermal fluctuations can stabilize phases with exotic SO order while the classical spin order is destroyed.

[1] L. F. Feiner, A. M. Oleś, and J. Zaanen, Phys. Rev. Lett. **78**, 2799 (1997).
[2] A. M. Oleś, Acta Phys. Polon. A **115**, 36 (2009).

Disproportionation At High-spin–low-spin Transition In $LaCoO_3$

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Emergence of the local magnetic moments is one of the typical features of the systems with strong electronic correlations. Common in transition metal oxides at ambient conditions, the local moment formation competes with effects such as band broadening or crystal field splitting when pressure is applied. $LaCoO_3$ is a well known and much studied example of a system where two spin states S=0 and arguably S=2 are almost degenerate. This results in a strongly temperature dependent conductivity and magnetic susceptibility. We will present a dynamical mean-field study of a simple two-band Hubbard model, which mimics the electronic structure of $LaCoO_3$. We calculate the one-particle spectra and the local as well as uniform spin susceptibility, in qualitative agreement with experimental observations. Our main finding is the observation of a disproportionation into magnetic and non-magnetic sites at intermediate temperatures. We provide an explanation of this behavior in terms of a simplified spin model and discuss its implications for presence of a gap in the one-particle spectrum.

Magneto-optical Excitations In Systems With Frustrated Spin And Orbital Degrees Of Freedom

Joachim Deisenhofer

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Optical spectroscopy is a highly sensitive tool to investigate the elementary excitations in correlated systems with coupled spin, lattice and orbital degrees of freedom. For example, low-lying electronic excitations of electric and magnetic origin in the THz range can provide information on the electronic level splitting due to orbital ordering. The coupling of spin and orbital degrees of freedom to the lattice can be traced by infrared spectroscopy. The infrared optical phonons reflect the influence of magnetic exchange interactions and magnetic ordering via spin-phonon coupling which often is the decisive interaction to release magnetic frustration. In addition, the magnetic excitation spectrum of antiferromagnetically coupled spin systems can be directly accessed via cooperative exciton-magnon transitions involving a pair of magnetic ions. As exciton-magnon transitions can occur already when short-range order develops, these excitations are particularly promising probes of the spin-wave spectrum in frustrated magnets where finite spin correlations persist up to the Curie-Weiss temperature.
As a first part basic concepts of THz and FIR spectroscopy will be discussed and an overview of magneto-optical excitations accessible by these techniques will be given. In the second part the emphasis will be on recent work in specific archetypical systems e.g. transition-metal monoxides, highly frustrated magnets such as $ZnCr_2O_4$, and low-dimensional spin systems.

Anisotropy In The Magnetic State Of Undoped Iron Pnictides

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The recently discovered high temperature superconductors iron pnictides present singular magnetism. The undoped compound is metallic with $Q = (\pi, 0)$ columnar ordering instead of being a Mott insulator with Néel order as in cuprates. It presents a very low magnetic moment[1], even lower than predicted in ab-initio calculations. Another interesting aspect is a strong anisotropy found in transport[2], optical[3] and inelastic neutron experiments[4]. In particular, the resistivity anisotropy is the opposite to the expected one since the system conducts better in the antiferromagnetic x direction than in the ferromagnetic y direction. This situation has put forward orbital ordering as a possible theoretical scenario to understand the anisotropies found in these experiments. Orbital ordering is also consistent with the dominance of zx orbital at the Fermi surface in ARPES[5]. In our work we calculate the mean field $Q = (\pi, 0)$ magnetic phase diagram using a five orbital tight-binding model[6]. For intermediate values of the interaction, two different metallic regimes with low and high magnetic moments arise. Orbital ordering is concomitant with magnetism in both regimes. The low moment state is characterized by on-site antiparallel orbital magnetic moments[7]. This metallic low moment state is consistent with the strong exchange anisotropy found in neutron experiments. The orbital ordering found in the metallic region of the phase diagram reproduces the large zx weight seen around Γ in ARPES experiments. We also calculate the ratio of the Drude weight along the x and y directions, D_x/D_y[8]. We find that D_x/D_y ranges between $0.2 < D_x/D_y < 1.7$ for different interaction parameters. Large values of orbital ordering favor an anisotropy opposite to the one found experimentally. On the other hand D_x/D_y is strongly dependent on the topology and morphology of the reconstructed Fermi surface. This anisotropy extends to higher frequencies and changes direction as seen in optical experiments. Our results points against orbital ordering as the origin of the observed conductivity anisotropy, which may be ascribed to the anisotropy built by the magnetic state[8,9].

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[2] Chu et al. Science 329, 824 (2010)
[3] Dusza et al, EPL 93 37002 (2011)
[4] Zhao et al., Nat. Phys. 5, 555 (2009)
[5] T. Shimojima et al., PRL 104 057002 (2010)
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[7] E. Bascones, M.J. Calderón, B. V., PRL 104 , 227201 (2010)
[8] B. Valenzuela, E. Bascones, M.J. Calderón, PRL 105, 207202 (2010)
[9] G. León, E. Bascones, M.J. Calderón, B. Valenzuela, in preparation

Superconductivity, Magnetism, And Spin Fluctuations In Fe-based Superconductors.

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Since the discovery of a high temperature superconducting transition in ferropnictides approximately two years ago, the highly magnetic character of these compounds and the close relationship between superconductivity and magnetism has been widely recognized and intensely studied. Initially, debate about the nature of the magnetism was split into two camps: localized moments (as in cuprates) and pure itineracy (a spin-peierls type transition). But closer investigation shows that magnetism in pnictides and in the related chalcogenides is between these two extremes, consisting of Hund's rule (or Stoner) derived moments on the Fe atoms. Using density functional theory (DFT) calculations, it is shown that the ordering mechanism is not Fermi surface driven and is also unlikely to be of superexchange origin. From a computational perspective, it can be explained how the magnetic and structural transitions are related and doping and pressure dependent quantities can be compared to experiment. Many quantities are well reproduced and explainable using DFT, though remaining questions need to be answered before magnetism, superconductivity and their relationship can be considered as understood. Spin fluctuations are widely understood to be the driving force behind the superconductivity with magnetic order as a competing, and therefore detrimental, phase. In this context, spin fluctuation scheme, known as the nematic phase, could explain why the structural transition appears either in conjunction with or before the magnetic transition. Spin fluctuations are also likely related to the suppression of LRO order with pressure and doping.

NMR in pnictides

Julien Bobroff

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We will first present the basic principles and the uses of Nuclear Magnetic Resonance in Solid State Physics and especially in strongly correlated materials based on a few examples. NMR is a local probe which enables to get unique informations about magnetism, superconductivity, spin or charge distribution and local static and dynamic susceptibilities. In addition, t is not sensitive to spurious phases and probes the full volume of the sample.
The second part of the talk will be devoted to recent NMR results obtained in pnictide superconductors. In the Co-doped $BaFe_2As_2$, we will show how NMR unambiguously demonstrates the atomic coexistence of superconductivity and an incommensurate spin density wave. In comparison, we will show the peculiar case of Ru doping. Ru and Co apparently induce the same phase diagram despite the fact that Ru is isovalent while Co gives one electron to the FeAs layer. However, from the NMR local point of vue, the situation is very different: Ru induces an intrinsic spatial distribution in the FeAs layer which results in a strong distribution of the local properties, such as the ordered magnetism or the superconductivity, resulting in a segregated situation.

Novel Tetragonal Antiferromagnetic Phase In $Ba(Fe_{1-x}Mn_x)_2As_2$.

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In 122-ferropnictides, superconductivity can be induced either by iso- or aliovalent chemical substitution or by applying a mechanical pressure to the antiferromagnetic parent compounds. In particular, one can introduce extra electrons or holes into the FeAs layers by replacing Fe with Co [$Ba(Fe_{1-x}Co_x)_2As_2$] or Ba with K [$Ba_{1-x}K_xFe_2As_2$], respectively. In the case of Mn substitution, one might naively expect a hole-doped system similar to $Ba_{1-x}K_xFe_2As_2$, but in reality a completely different phase diagram is observed [1]. It exhibits no superconductivity, but contains a novel antiferromagnetic phase that does not break the tetragonal symmetry of the crystal, in contrast to the spin-density-wave (SDW) state in the parent compound. Additionally, the magnetic transition temperatures above 10%-Mn doped $BaFe_2As_2$ start to increase, evidencing that this magnetic state is strongly related to the presence of Mn. However, its microscopic origin still remains unexplained up to now. Thus, we carried out complementary experimental methods μSR and neutron spectroscopy on 12%-Mn doped $BaFe_2As_2$ to investigate the magnetic property of such novel phase, and observed the distinct behavior of magnetism in sharp contrast to the SDW in the $BaFe_2As_2$ compound. In this talk, we will discuss about possible origins of novel magnetic phase in 12%-Mn doped $BaFe_2As_2$.

[1] M. G. Kim *et al.*, Phys. Rev. B **82**, 220503(R) (2010).

Probing The Local Magnetic Structure Of A Quasi-1d Cuprate With Resonant Inelastic X-ray Scattering

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The quasi-one-dimensional cuprate Li_2CuO_2 is a prototype edge-sharing chain compound [1]. The Cu^{2+} ions in this strongly correlated material give rise to one spin 1/2 per CuO_4 plaquette with a nearest neighbor Cu-O-Cu bond angle close to $90\,^{circ}$ implying weak superexchange coupling between Cu spins. As a result, spins order antiferromagnetically between the chains below T_N∼9K, but ferromagnetically in the chains. We have performed Resonant Inelastic X-ray Scattering (RIXS) at Cu L_3 and O K-resonances at the ADRESS beamline on this compound. Our momentum resolved RIXS measurements at the Cu L_3-edge allow analyzing orbital excitations with high sensitivity. At the O K-edge, the RIXS spectra display a complicated interplay of low-energy excitations from charge, orbital and lattice degrees of freedom. In particular, we discuss charge transfer related spectral components in the scenario of exotic Zhang-Rice (ZR) singlet and triplet excitations which can be reached in the final state with O K-edge RIXS [2,3]. Our recent temperature dependent measurements evidence clear opposite temperature behavior for these two features, in good agreement with optical conductivity calculations [4]. Comparing the excitation energy of both ZR features allows to directly read the binding energy of the Zhang-Rice singlet in Li_2CuO_2 from the spectra. Furthermore, this study suggests RIXS as an excellent probe for investigating local magnetic order.

[1] R. Neudert et al., Phys. Rev. B 60, 13413, (1999).
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T_c In Pnictides And Cuprates Correlates With The Electron-phonon Relaxation Times

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The pairing mechanism in high critical temperature (T_c) superconductors is one of the outstanding mysteries of condensed matter physics. Here we show that for cuprates and pnictides both electron-phonon interaction (EPI) and electron-electron interaction (EEI) are necessary ingredients. To investigate the role of EPI in the superconducting mechanism we need an experiment that yields a direct measure of the EPI strength. EPI is the dominant mechanism of electron energy relaxation, which we study using femtosecond optical pump-probe spectroscopy. Systematic investigation of different compound families and different doping levels shows that T_c depends universally on two phenomenological parameters: the relative doping level x/x_{opt} as a measure of EEI, and the lattice-temperature corrected electron-phonon relaxation rate T_l/τ_{e-ph} as a measure of EPI. This identifies high T_c superconductivity as a collaborative action of EEI and EPI, which puts strong constraints on a possible theory of the pairing mechanism.

Low Energy Kink In The Cuprates And Effective Interaction For Systems With Competing Electron-electron And Electron-phonon Coupling

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Motivated by the observation in the copper-oxide high-temperature superconductors, we investigate the appearance of kinks in the electronic dispersion due to coupling to phonons in the presence of a strong electronic repulsion. To model this strong coupling situation we present controlled calculations for the Hubbard-Holstein (HH) model within the framework of the dynamical mean field theory combined with the numerical renormalization group.
We find that contrary to the conventional electron-phonon theory, the position of the kink can be shifted to energies larger than the renormalized phonon frequency ω_0^r. This can be understood in terms of an effective U at low energy, which is only weakly renormalized by the phonons, such that phonon effects are visible only at higher energy. When including antiferromagnetic correlations for small doping we find a pronounced kink at ω_0^r due to a cooperative effect. Our results provide a scenario of a kink position increasing with doping, which is consistent with recent photoemission experiments on Bi-based cuprates [1].
Within a similar framework we also analyze other situations which can be understood in terms of an effective low energy interaction. The ground state phase diagram of the HH model at half filling shows antiferromagnetic and charge order. The phase boundary is shown to be determined by an effective electronic interaction. Interestingly, there can be direct continuous transitions between the two ordered states [2,3]. Finally we allude to recent results from an analysis of the limitations of Morel-Anderson retardation effects for phonon induced superconductivity when the Coulomb repulsion becomes large [4].

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Angle-Resolved Photoemission Spectroscopy and its application to the study of the electronic structure of some correlated-electron systems

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In solids with strongly-interacting electrons, the competition between the different degrees of freedom leads to competing quantum ground states, from which a rich variety of macroscopic phenomena emerge. In many cases, these phenomena arise from phase transitions described by exotic (or even unknown) order parameters and underlying novel states of matter. Examples of such physical richness are the high-temperature superconductivity in cuprates, the colossal magneto-resistance in manganites, the multiferroic behaviour in bismuth ferrites, the numerous quantum-critical transitions in heavy-fermion materials, or the recently discovered 2D metallic electron gases (2DEGs) at the interfaces of insulating transition-metal oxides.
A direct approach to understand the physics of strongly-correlated materials is to study their band structure and how the many-body interactions and phase transitions affect it. The technique of angle-resolved photoemission spectroscopy (ARPES) does precisely that. ARPES gives access to the band structure, the effective masses and the scattering-rate of electrons (hence the effects of many-body interactions) in the occupied states of the solid.
In this talk, I will first introduce the basic aspects of the ARPES technique. Then, I will discuss its application to the study of two paradigmatic problems of correlated-electron materials. The first is the enigmatic phase transition to a "hidden-order" state of yet unknown nature occurring at $T_0 = 17.5$ K in the heavy-fermion semi-metal URu_2Si_2. Recent ARPES results have provided direct evidence that a large reorganization of heavy-electron bands occurs at the Fermi surface of URu_2Si_2 during the hidden-order transition [1,2], highlighting the importance of the "dual" localized-itinerant character of electrons in this material in the understanding of such mysterious transition. The second problem is the nature and electronic structure of the 2DEGs in $SrTiO_3$-based interfaces. Such 2DEGs are not only a novel playground to study fundamental aspects of the physics of doped correlated-electron systems, but also offer interesting perspectives in applications aiming at functionalizing the numerous properties of transition-metal oxides. Here, very recent ARPES experiments have unveiled the existence of a metallic 2DEG at the surface of insulating $SrTiO_3$ [3], providing detailed information about its electronic structure, and hinting to a novel route to generate 2DEGs at surfaces of functional oxides.

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Tuning the electronic properties of oxide heterostructures using electrostatic gating and coherent light

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Complex oxide heterostructures exhibit functional electronic properties such as magnetism and superconductivity. An important step toward the use of quantum materials in real-word applications is to achieve on-demand control of their ground state. One strategy consists in applying static electric fields to the material, in the spirit of the field effect transistor. I will discuss this approach on the control of the ground state of the two-dimensional electron gas found at the $LaAlO_3/SrTiO_3$ interface [1]. Another innovative strategy is based on the use of coherent light sources. Recent developments in laser technology have made it possible to generate pulses of light in the mid infrared and THz range, indeed at intensity levels that make possible to substantially perturb the properties of a solid [2]. Thus, we are now in a position to control the dynamics of the low-energy excitations of complex solids and, most notably, to control their macroscopic electronic properties. This technique will be applied on $NdNiO_3/LaAlO_3$ heterostructures, where the electronic properties can be tuned by coherent vibrational excitation.

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Optical Properties of $(SrMnO_3)_n/(LaMnO_3)_{2n}$ Insulator-to-Metal Transition Observed In The Absence Of Disorder

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We measure the optical conductivity, $\sigma_1(\omega)$, of $(SrMnO_3)_n/(LaMnO_3)_{2n}$ superlattices (SL) for $n = 1, 3, 5$, and 8 and $10 < T < 400$ K. Data show a T-dependent insulator to metal transition (IMT) for $n = 3$, driven by the softening of a polaronic mid-infrared band. At $n = 5$ that softening is incomplete, while at the largest-period $n = 8$ compound the MIR band is independent of T and the SL remains insulating. One can thus first observe the IMT in a Manganite system in the absence of the disorder due to chemical doping. Unsuccessful reconstruction of the SL optical properties from those of the original bulk materials suggests that $(SrMnO_3)_n/(LaMnO_3)_{2n}$ heterostructures give rise to a novel electronic state.

Enhancement Of The Superconducting Transition Temperature In Cuprate Heterostructures

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We observe enhancement of the superconducting transition temperature in heterostructures of superconducting oxides. Fabrication of multilayer thin films of $La_{2x}Ce_xCuO_4$ (LCCO) and $Pr_{2-x}Ce_xCuO_4$ (PCCO) paired over-doped and under-doped (or un-doped) layers of various layer thicknesses. An increased T_c was observed, significantly above that of single-phase films with dopings corresponding to the under- or over-doped layers. We report transport measurements on these mulitlayer films in order to investigate the mechanism of this T_c enhancement. This work was supported by BSF Grant 2006385 and the Center for Nanophysics and Advanced Materials (CNAM).

Orbital Reconstruction At YBa2Cu3O7/La2/3Sr1/3MnO3 Interfaces Revealed By Resonant Inelastic X-ray Scattering

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Transition metal oxide hetero-interfaces have been attracting great attention due to extraordinary phenomena not exhibited by either of the constituent materials alone. A particularly fascinating system is the ferromagnetic/superconducting heterostructure which has vast application in the area of spintronics. Recent studies on YBa2Cu3O7/La2/3Ca1/3MnO3 superlattices have revealed an extensive rearrangement of magnetic domain structure as well as a likely electronic orbital reconstruction at its interface. To testify whether orbital reconstruction is a general characteristics of the YBCO/ferromagnet heterostructures, we investigate YBa2Cu3O7/La2/3Sr1/3MnO3 multilayers grown by pulsed laser deposition. Resonant inelastic x-ray scattering at Cu L3-edge is used to address this issue as which is particularly sensitive to orbital excitations. By probing directly the angular dependence of 3d orbital excitation, we unambiguously reveal that Cu 3d3z2-r2 orbital is reconstructed to create a molecular bond at the interface as the former strongly hybridizes with Mn 3d3z2-r2 orbital. The associated charge-transfer and modification of dynamic magnetic structure at Cu sites are also discussed in terms of proximity effect at the interface.

Exotic electronic phases in graphene nanostructures

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Graphene is a zero gap semiconductor with a very large Fermi velocity and low energy bands made of p-orbitals. Therefore, the influence of correlation effects and spin-orbit coupling on the electronic properties is not expected to be large. In this talk I show how this is not the case in graphene nanostructures and I discuss two exotic electronic phases that arise in graphene zigzag nanoribbons. One of them has persistent charge currents driven by magnetic order and spin-orbit coupling [1]. The other is a half-metal with vanishing total magnetic moment, whose metallic character arises only when Coulomb repulsion between the electrons are taken into account, in dramatic contrast with the usual interaction-driven metal-to-insulator transition. Possible experimental realization of the predicted phases is discussed.

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Topological Fermi Liquids In The Doped Honeycomb Lattice

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We study spontaneous symmetry broken phases of spinless electrons in the Honeycomb lattice using a tight binding model with nearest neighbors Coulomb interactions V. When the unit cell is enlarged to allow non-zero, selfconsistent currents inside it we find within a variational mean field approach a metallic phase with broken time reversal symmetry T around 1/3 filling, very close in parameter space to a Pomeranchuk instability. Within the T broken region the predominant configuration is an anomalous Hall phase with non zero Hall conductivity, a realization of a topological Fermi liquid. A T broken phase with zero Hall conductivity is stable in a small region of the parameter space for lower values of V.

Tunable Casimir repulsion with three dimensional topological insulators

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In this work, we show that switching between repulsive and attractive Casimir forces by means of external tunable parameters could be realized with two topological insulator plates. We find two regimes where a repulsive (attractive) force is found at small (large) distances between the plates, canceling out at a critical distance. We also study the effects of temperature and uniaxial anisotropy in our findings.

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Computing Entanglement In Quantum Matter

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Condensed matter physicists have recently begun exploiting the properties of entanglement as a resource for studying quantum materials. At the forefront of current efforts is the question of how the entanglement of two subregions in a quantum many-body groundstate scales with the subregion size. The general belief is that typical groundstates obey the so-called "area law", with entanglement entropy scaling as the boundary between regions. This has lead theorists to propose that sub-leading corrections to the area law can provide new indications of universal physics at exotic quantum phases and phase transitions. However, away from one dimension, entanglement entropy is difficult or impossible to calculate exactly, leaving the community in the dark about scaling in all but the simplest systems. In this talk, I will discuss recent breakthroughs in calculating entanglement entropy in two dimensions and higher using advanced numerical simulation techniques. This paves the way for future work in calculating new universal quantities derived from entanglement, which can be used as a diagnostic for detecting exotic physics in a variety of condensed matter systems.

Spin Structure Manipulation In Three Dimensional Topological Insulators

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Topological insulators are a novel phase of condensed matter physics with unique spin structures [1]. Due to strong spin-orbit interaction he bulk of the material is insulating, but at the surface spin-polarized edge states are formed. The Fermi level crossing of these surface states is protected by the topology of the material and time-reversal symmetry. Spin and angle-resolved photoemission spectroscopy is a powerful tool for the characterization of topological insulators because it can simultaneously determine the topology and the details of the spin structure [2].

In order to fully utilize the promises which topological insulators hold for developments in spintronics and fundamental physics, it is important to gain control over the details of the spin structure. Here we will show how the spin structure is directly linked to the crystal structure and can thus be influenced by it. Especially the occurrence of an out-of-plane spin component increases the number of potential applications because of the less stringent requirements on the injected spin direction. Furthermore we will discuss the influence of the exact surface termination on the spin structure and the possibility to manipulate the electronic and spin structure.

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Functional Properties Of Metal Organic Frameworks With Perovskite Structure

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Hybrid materials that combine inorganic and organic components and that contain cavities and channels the so-called metal organic frameworks (MOFs) have been extensively studied in the last decade in view of their interesting potential applications, for example, in catalysis and gas storage [1]. In addition to nanoporous MOFs, dense hybrid framework structures have also been discovered and are receiving increasing attention as they can display a wide range of interesting functional properties (magnetic, optical, dielectric, etc.) [2-4]). In this context, the recent discovery of a sharp dielectric transition in the perovskite-like ABX3 compounds with A: (CH3)2NH2+ (DMA), B: Zn+2 or Mn+2, X: HCOO- Zn(HCOO)3[(CH3)2NH2] [3] and Mn(HCOO)3[(CH3)2NH2] [5] has spurred the interest in this family of compounds and has opened a new direction in the search for novel dielectric and even multiferroic materials as the Mn-compound also shows weak ferromagnetism. In this work, we report the most outstanding results found in our group on Mn(HCOO)3[(CH3)2NH2] and the synthesis, structure, magnetic, transport and dielectric properties of other new hybrid inorganic-organic compounds with perovskite-like structure.

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Novel magnetization plateaus in frustrated quantum magnets

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Geometrically frustrated spin systems are known to exhibit novel quantum phenomena. One example is the unique non-monotonic field dependence of the magnetization and the associated emergence of magnetization plateuas in a class of frustrated spin compounds commonly known as the Shastry-Sutherland compounds after their underlying magnetic lattice. In this talk, I shall discuss the underlying mechanism for the formation of these plateaus. In the first half of the talk, I shall compare the quantitative predictions from our recently developed unconstrained Chern-Simons theory with experimental observations in SrCu2(BO3)2. Interestingly, our theoretical calculations predict that at the plateaus, the elementray magnetic excitations, triplons, form well-defined stripes. Evidence of such stripes have recently been reported in TmB4, another compound belonging to this family. In the second half of the talk, I shall discuss the formation of magnetizaion plateaus in a new family of Shastry-Sutherland compounds, viz., the rare-earth tetraborides. The bare Shastry-Sutherland model needs to be supplemented by additional longer range interactions to describe the magnetic properties of these compounds. I shall discuss he underlying microscopic models and our recent studies of these models.

Orbital Ice: p-band Mott insulators on an optical diamond lattice

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The Mott-insulating states of p-orbital spinless fermions in a three-dimensional optical lattice exhibit an unusual degeneracy due to the anisotropic orbital interaction and geometrical frustration. Here we demonstrate the existence of orbital Coulomb phase as the exact ground state of the p-orbital exchange Hamiltonian on the diamond lattice. We show that the extensively degenerate orbital configurations of this Coulomb phase can be mapped to Ising spins obeying the ice rule on the pyrochlore lattice. An experimental signature is the pinch-point singularities in diffusion-scattering measurement which originate from a dipolar-like correlation function in the orbital ice state.

Bose-Einstein Condensation in Magnetic Spin Systems

Vivien Zpaf

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I will review Bose-Einstein condensation in quantum magnets. In these materials a field-induced quantum phase transition to XY antiferromagnetic order can be mapped onto Bose-Einstein Condensation. This gives us the opportunity to study BEC in the thermodynamic limit, as well as an interesting case where magnetic field rather than temperature can be the tuning parameter for BEC transition. I will focus in particular on the metal-organic quantum magnet $NiCli_2$-$4SC(NH_2)_2$. Here the $S = 1$ Ni system orders antiferromagnetically between $H_{c1} = 2.1$ and $H_{c2} = 12.6$ T and a wide range of experimental techniques suggest the BEC universality class. We also find that that mass of the bosons that condense can be strongly suppressed by quantum fluctuations, resulting in a remarkable asymmetry between the properties at H_{c1} and H_{c2}. I will present magnetization, thermal conductivity and specific heat data to probe BEC. I will also mention follow-on topics like the BEC to Bose-Glass phase transition, and spin supersolidity.

The Seebeck coefficient in oxides: the example of misfits and related compounds

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Thermoelectric materials can be used to generate electricity directly from waste heat, but the efficiency of thermoelectric devices is small and only niche applications are developed today. The search for thermoelectric materials with improved properties is thus very active. To combine the three following antagonistic properties : (i) small electrical resistivity, (ii) large Seebeck coefficient and (iii) small thermal conductivity, different approaches are followed, such as nanostructuration to reduce thermal conductivity and/or enhance the Seebeck, or the use of strong electronic correlations to generate large Seebeck. I will first briefly present these approaches, and will then focus on the work we have been doing on oxides. The importance of spin and orbital degeneracies, and the importance of electronic correlations will be evidenced. The different classes of new materials that are investigated as potential thermoelectric materials will be discussed.

Charge Dynamics In $CuGeO_3$: A Combined RIXS And EELS Study

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Model compounds of the high temperature superconductors (HTCS) are considered of big interest for the understanding of superconductivity but also for their fascinating, tunable magnetic and electronic properties. Thanks to the low dimensionality, these model systems allow for a thorough theoretical analysis enabling to achieve a good understanding of the interactions at work. $CuGeO_3$ is a well known realization of one-dimensional antiferromagnetic S=1/2 spin chain, made of edge-sharing CuO_4-plaquettes, and undergoing a Spin-Peierls transition at $T \approx 14$ K. Recently, thanks to the improved energy resolution, soft x-ray resonant inelastic scattering (RIXS) has demonstrated to be a suitable tool for the study of the HTCS. We performed RIXS experiments on $CuGeO_3$ at the ADRESS beamline of the Swiss Light Source. Intra-site d-d excitations can be clearly observed at the Cu-L edge, while inter-site Cu-O charge transfer processes are enhanced at the O-K edge. Temperature dependent studies unambiguously identify the presence of two Zhang-Rice (ZR) singlet excitons in $CuGeO_3$. The strong variation of their spectral weight with temperature can be directly linked to the local magnetic correlation at the ground state. Complementary data measured with high resolution electron energy loss spectroscopy (EELS) at the IFW Dresden support the RIXS results. Finally RIXS calculations are in qualitative good agreement with our measurements by presenting two temperature dependent features in the same energy range as the experiment: therefore the theory allows for a direct interpretation of the different ZR singlet excitons, respectively formed between nearest neighbor and next nearest neighbor plaquettes.

Antiferroquadrupolar Resonance Mode In CeB_6 Revealed By Inelastic Neutron Scattering In Zero Magnetic Field

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Since decades, rare-earth hexaborides are famous for their anomalously low work functions, making them ideal materials for electron-emitting cathodes. Nevertheless, fundamental understanding of their many unusual physical properties still remains hazy. The heavy-fermion metal CeB_6 stands out as the only material in this family that develops an exotic antiferroquadrupolar (AFQ) order at temperatures between 2.3 and 3.3 K, whose microscopic origin is still debated. Our inelastic-neutron-scattering data suggest the existence of an unusual spin resonance mode that emerges at the AFQ wavevector in the antiferromagnetic ground state of CeB_6 out of a broad continuum of itinerant paramagnetic fluctuations. The weakly dispersing tails of the main peak extend in momentum space, forming a rich anisotropic three-dimensional structure. The resonant mode is sharply peaked in energy around 0.5 meV, below the onset of the charge gap, and is followed by a weaker second peak around 1.1 meV at the same wavevector. At lower energies, a suppression of the magnetic spectral weight marks the opening of a spin gap. The temperature evolution of this new mode bears striking resemblance to the spin resonance in unconventional superconductors, which could turn out to be a key to the understanding of the mysterious AFQ phase in CeB_6.

Ground State And The Low-energy Electronic Structure Of NiO And In UPd_2Al_3

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NiO and UPd_2Al_3 are considered as prototype compounds with very strong electron correlations, not well theoretically described so far. We have consistently described properties of NiO, reconciling its insulating ground state and a strong (antiferro-)magnetism with TN of 525 K. We calculated low-energy electronic structure associated with eight 3d strongly-correlated electrons at the Ni site in the incomplete 3d shell. For intermetallic UPd_2Al_3 we have proved the existence of the strongly-correlated 5f3 configuration (U3+ ion). Our result is in agreement with inelastic-neutron-scattering experiment which reveals a low-energy structure below 20 meV.From consistent description of basic properties of such different compounds as NiO and UPd_2Al_3 are I conclude that the strong correlations are mainly related with 1) the charge transfer during the formation of the compounds and with 2) the intra-atomic correlations responsible for the formation of the strongly-correlated atomic-like systems 3dn, 4fn or 5fn. For successful description the multipolar charge potentials, described customarily as the crystal field, and relativistic spin-orbit interactions are fundamentally important. According to the developed Quantum Atomistic Solid-State Theory (QUASST) I claim that the crystal-field interactions should be evaluated the first for any meaningful description of magnetic and electronic properties of any 3d/4f/5f compound. QUASST is supported by a recent EPR experiment on heavy-fermion metal $YbRh_2Si_2$ - the strongly-correlated 4f13 configuration has been found to exist at 1.5 K, i.e. at temperature being 15 times lower than the Kondo temperature.My approach is well suited for the New Generation of theoretical understanding of Strongly-Correlation Electron Systems.

Electron Spin Resonance Of Some Dense Strongly Correlated Electron Systems

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One of the most important problems in condensed matter physics involves the microscopic understanding of how localized electrons at high temperatures turn into itinerant heavy quasi-particles in a low temperature metallic state. The fundamental mechanism of this evolution lies at the heart of heavy-electron physics and depends on the Kondo coupling between the conduction electrons (CE) and the localized d or f electrons. Electron spin resonance (ESR) probes microscopically both the local moment (LM) spins and CE in different strongly correlated electron materials such as high-temperature superconductors, pnictides, heavy fermion systems. LM ESR is observed in compounds with paramagnetic ions and localized electrons. CE spin resonance (CESR) can be detected in metallic systems based on light elements exhibiting an enhanced Pauli susceptibility. We discuss here the ESR studies in several undoped Yb-, Ce-, and Eu-based intermetallics which share the nature of both, the LM-like and CESR-like ESR signals. Moreover, ESR measurements in the new ternary phosphide $YbRh_6P_4$ are reported. Different theoretical approaches which were proposed to explain the origin of such unexpected ESR behavior are discussed.

$La_4Ru_2O_{10}$ And $La_{3.90}Ce_{0.10}Ru_2O_{10}$: Rapidly Fluctuating Orbital Occupancy Above Their Orbital Ordering Transition

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Several spin systems with low dimensionality develop a spin-dimer phase within a molecular orbital below T_S, competing with long-range antiferromagnetic order. Very often, preferential orbital occupancy and ordering are the actual driving force for dimerization, as in the so-called orbitally-driven spin-Peierls compounds ($MgTi_2O_4$, $CuIr_2S_4$, etc.). In this framework, we focus on the layered ruthenate compounds $La_4Ru_2O_{10}$ and $La_{3.90}Ce_{0.10}Ru_2O_{10}$. Wu et al. [1] proposed that in $La_4Ru_2O_{10}$ an orbital ordering: $[d_{xz}\uparrow\downarrow, d_{xy}\uparrow, d_{yz}\uparrow]$ (S=1) introduces a strong exchange anisotropy that drives the system electronically 1D, and forms Ru^{4+}-Ru^{4+} spin-singlets below $T_S \sim 160$ K. This anisotropy is reflected in alternating short/long Ru-O bond-lengths in the low temperature (spin-gapped) phase. However, these bond-distances are also compatible with an $S \sim 0$ at each Ru^{4+} site ($d_{xz}\uparrow\downarrow, d_{xy}\uparrow\downarrow, d_{yz}0$), as originally proposed by Khalifah et al. [2]; and to distinguish between these scenarios is a difficult task [3]. Through a microscopic analysis of the thermal conductivity $k(T)$ in these compounds, we show that the orbital occupancy fluctuates rapidly above T_S, resulting in an orbital-liquid state. The strong orbital-lattice coupling introduces dynamic bond-length fluctuations that scatter the phonons to produce a $k(T) \sim T$ (i.e. glass-like) above T_S. We have also studied their temperature dependence of the magnetic susceptibility under pressure and their transport properties.

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Electronic And Magnetic Phase Diagram Of $Cr_{1-x}V_xN$

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In this work we investigate the electronic and magnetic phase diagram of $Cr_{1-x}V_xN$. Stoichiometric CrN is a narrow gap, correlation-induced, semiconductor that orders antiferromagnetically below 286 K. The changes in the chemical bond associated to the magnetic order result in a non-activated behavior of the resistivity in the antiferromagnetic state, showing some similarities with other materials proposed to be itinerant-AF, like $CaCrO_3$. Doping this state with holes drives the system towards itinerant electron behavior through a series of inhomogeneous magnetic/electronic states. Given the chemical and structural simplicity of this system, it could provide an interesting place to study the evolution from an antiferromagnet with a non-thermally activated charge transport to a paramagnetic metal in a non-oxide material.

Angle-resolved Photoemission Study Of The Electronic Structure And Hidden-order Transition Of URu_2Si_2.

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The heavy-fermion system URu_2Si_2 presents a second-order phase transition at $T_{HO} = 17.5$ K from a paramagnetic to a so-called hidden-order state. Early specific heat measurements already suggested the opening of a gap of about 10 meV over more than 40% of the Fermi surface [1]. Yet, despite intense experimental and theoretical work, the nature of the associated order parameter is so far unknown.

We have used high-resolution angle-resolved photoemission spectroscopy (ARPES) to study the changes in the electronic structure of URu_2Si_2 across the hidden-order transition. Our first results demonstrated the important role played by itinerant heavy electrons into the Fermi surface reconstruction at the Γ point [2]. In this work, we present our measurements of heavy quasi-particles contributing to the Fermi surface at other high-symmetry points. We discuss their temperature dependence and their associated gap structures.

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Crystal Growth Of The 1111 Iron-pnictide Superconductors: The Sn-flux Technique

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Although superconductivity (SC) in the Iron pnictides was initially discovered in the so-called 1111 compounds, i.e. doped LaFeAsO, most of the in-depths studies carried on in the last two years were performed on the 122 compounds (AFe_2As_2) systems, because there large single crystals are available. However, the 1111 family presents by far the highest SC transition temperature T_c, up to 56 K, in comparison to 30 K in the 122 systems. Therefor a detailed investigation of the 1111 is crucial in order to resolve the origin of those exceptionally high T_cs. This is impeded by the lack of larger, high quality single crystals. The 1111 compounds are in-between intermetallic compounds and oxides, therefor the methods adapted for oxides and those adapted for intermetallic compounds all present some problems, in general a very low solubility for one of the constituent. A promising approach is the Sn-flux growth technique used in our laboratory. In the case of CeFeAsO we were able to grow very high quality single crystals, with unprecedented sharp transitions. We shall review the different techniques presently used for the growth of 1111 compounds, discuss their respective advantage and disadvantage, and present our achievements with the Sn-flux technique.

Internal Electric Field In $SrTiO_3/LaAlO_3$ Heterostructures Probed With Hard X-ray Photoemission Spectroscopy

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The origin of the conducting layer at the interface between insulating $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) is still widely debated. The alternatingly charged layers within the LAO blocks give rise to an internal electric field, which at some point has to be screened. This built-in potential is predicted to close the LAO bandgap at a critical thickness of 4 layers of LAO. Using hard x-ray photoemission spectroscopy we study the core levels of these systems as a function of the LAO layer thickness. By measuring the La 4d and Al 2s core levels with respect to the Sr 3d core level we carefully determine the core level shifts for samples with 2 to 6 layers of LAO. Although the observed shifts are an order of magnitude smaller than predicted, we do find an interesting increase of the core level shifts for samples with more than 4 layers. We perform DFT slab calculations to show that oxygen vacancies can significantly reduce the potential build-up. Our results suggest that in real materials the electronic reconstruction is pre-empted by other effects of which oxygen vacancies are one possibility.

Conduction-Electron Spin Resonance in CoS_2

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$CoS_2$and its alloys (Fe, Se, etc) were intensively studied during the last years due to prospect of presenting a large spin polarization that make them attractive as sources of spin-polarized electrons above liquid nitrogen[1].On the other hand, CoS_2 is one of the classic examples of weak itinerant ferromagnet (WIFM), according to Moriya's spin fluctuation theory (SFT) [2]. In these systems the thermodynamic and transport properties are completely determined by the temperature dependence of the amplitude of the local spin density, $\langle S_L^2 \rangle$. In this regime strong exchange interaction between the spin density fluctuations are expected to increase the spin relaxation time, another ingredient needed for spintronic applications. However, an experimental determination of the spin relaxation time T_1^{-1}in CoS_2 is lacking. Here we report the existence of an observable conduction electron spin resonance (CESR) at X-band in metallic $CoS_{2-x}Se_x (x \leq 0.1)$ in a wide temperature range above T_C. We demonstrate that the strong exchange interaction between the spin fluctuations suppresses very much the spin-lattice relaxation via spin-orbit coupling increasing T_1^{-1}enough so as to make CESR observable in CoS_2. The linewidth (intensity) increases (decreases) very fast up to $T^* \approx 2T_C$, where it first distorts and then becomes unobservable. The results indicate a transition from a $\langle S_L^2 \rangle \sim T$ to a saturated regime ($\langle S_L^2 \rangle$ =constant) above T^*, as predicted by SFT.

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The XAS Study Of Ca Doped $BaNi_xCo_{1-x}S_{2-y}$

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The doping induced distortion of $BaNi_xCo_{1-x}S_{2-y}$ polycrystal was sintered in vacuum-sealed quartz tube. The temperature dependent electric transport and magnetization curve were measured. The antiferromagnetic-aramagnetic and semiconductor-metallic phase transition was observed. The resistivity reduced upon doping level indicates the electronic structure tuned by the structure distortion. The change of ligand state with doping level is verified by S k-edge X-ray absorption spectrum. We also find the Co L-edge shift before and after phase transition. The electronic structure tuning of $BaNi_xCo_{1-x}S_{2-y}$ by controlled structure distortion by doping was proved in this project. (The project was supported by National Science Council, Taiwan, contract No. NSC-97-2112-M-606-001-MY3).

Investigation of Thermodynamic and Magnetic Properties of Periodic Anderson Model by Irreducible Green Function Method

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The two-band Periodic Anderson Model was considered in the wide range of electron concentrations, local hybridizations and on-site interactions. We applied the improved higher-order approximation for irreducible Green functions that takes into account resonance broadening and band shifting inter-orbital exchange effects. Such an approach resulted in the appearance of four spectral density moments and four- or five-subbands in the density of states. The three peaks obtained in specific heat were shown to be connected to the maximums of the temperature derivatives of the interaction, kinetic and mixing terms of the Hamiltonian and to the charge and spin fluctuations. It was found that intermediate maximum formed by mixing term can drift and overlap with low- or high-temperature peaks as hybridization strength and/or other model parameters change. The direct calculation of the magnetic moments for the localized and conduction electron systems as well as localized spin-flip cor! relation function allowed us to investigate the pressure-temperature phase diagrams and discuss the controversy existing in publications about the association of Kondo temperature and singlet formation with various peaks in specific heat of some rare earth compounds.

Vortex States In High Parallel Magnetic Fields In Mesoscopic $Bi_2Sr_2CaCu_2O_{8+a}$ single Crystals

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Vortex states in high Tc superconductors have been an attractive subject for condensed-matter scientists over the past two decades. Novel intriguing phenomena have been observed in the layered $Bi_2Sr_2CaCu_2O_{8+x}$ single crystal that could be described as a stack of weakly coupled Josephson junctions commonly referred to as intrinsic Josephson junctions (IJJ's). A combination of a large anisotropy and a variation of the order parameter across the layers has led to the occurrence of unusual vortex states such as a pancake vortex (PV), Josephson vortex (JV) and vortex lock-in state while in the oblique magnetic fields, observations have shown a vortex crossing lattice (CL), tilted lattice, chain phase, mixed chain and lattice state, etc. In order to investigate the interaction between Josephson vortices and pancake vortices in a layered $Bi_2Sr_2CaCu_2O_{8+x}$ superconductor, c-axis resistivity measurements were carried out on fabricated mesoscopic single crystals for two experimental geometries, when an applied high magnetic field of 14 T is perpendicular (Bex$\perp$L) and parallel (Bex|L) to the width of sample. In the first case, the angular dependence of the resistance obtained near the ab-plane at $T = 30$ K exhibited hysteretic non-monotonic behavior with local maxima at 0.6o degrees away from the ab-plane and dips and spikes at 0.2o degrees marking a vortex lock-in transition. In the second geometry (Bex|L), instead of a local maximum, peculiar resistance shoulders were observed. At higher temperatures, hysteresis is reduced, while the vortex lock-in transition becomes considerably broader indicating the interaction of pancake and Josephson vortices.

PACS codes: 74.60.Ec; 74.72.Hs; 74.25.Dw; 74.25.Ha Keywords: Vortex phase diagram; Crossing lattices; c-axis resistance Bi2Sr2CaCu2O8+x

Evidence For An Anisotropic Fluctuation-induced Diamagnetism Above The Superconducting Transition In A $Ba_{1-x}K_xFe_2As_2$ Single Crystal

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The magnetization around T_c was measured in a high-quality single crystal $Ba_{1-x}K_xFe_2As_2$ with magnetic fields applied along and transverse to the crystal ab layers. These measurements allowed to observe, for the first time in iron-pnictides, the precursor diamagnetism associated to Cooper pairs created by thermal fluctuations. This effect, anisotropic in amplitude about a factor 3, is explained at a phenomenological level in terms of a Gaussian Ginzburg-Landau approach for three-dimensional anisotropic superconductors (3D-AGL) under a total-energy cutoff in the fluctuation spectrum. As a check of consistency, the values found for the superconducting parameters are in agreement with the ones resulting from the 3D-AGL scaling of the data in the critical region.

J. Mosqueira et al., Phys. Rev. B 83, 094519 (2011)

On The Origin Of The $\chi(T)$ Temperature Dependent Magnetic Susceptibility And Large Thermoelectric Power In Metallic Layered-cobaltites

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We report a detailed analysis of the magnetic susceptibility, , and thermoelectric power, S, of metallic Na_xCoO_2 and $Ca_3Co_4O_9$, as representative examples of layered cobalt oxides with a triangular lattice. We will show that the magnetic and transport properties are mostly determined by CoO_2 planes, what explains the similar phenomenology found in different 2D cobalt oxides based on hexagonal Co arrangments, particulary the puzzling temperature dependent $\chi(T)$ and large thermoelectric power combined with a metallic resistivity. We will also demonstrate that the temperature dependence of the magnetic susceptibility in triangular lattice Co-oxides cannot be justified assuming a spin localized model. We suggest that the origin of the temperature dependence of the magnetization is due to the temperature dependence of the spin fluctuations of itinerant electrons, $\langle S_L^2 \rangle$, which dominates paragmanetic χ in nearly ferro/antiferromagnetic metals. Also we will discuss the applicability of previous models based on a large spin and orbital entropy contribution to $S(T)$ in mixed valence $Co^{3+/4+}$ systems, showing that this contribution is much lower than previously thought. We discuss the origin of $S(T)$ in the whole temperature range.

Chemical Magnetic/Electronic Phase Separation In Perovskite Manganites

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One paradigmatic system exhibiting phase separation is La1-xCaxMnO3 perovskite. This material has been thoroughly studied and there are plenty of experimental evidences of a dynamic magnetic/electronic phase separation at low temperature near $x \approx 0.2$ and $x \approx 0.5$. We have studied a structure with Ca doping levels close to $x \approx 0.2$ (exactly $x = 0.1875$) via "ab initio" calculations, using density functional theory. We have set up several large superstructures based on the unit cell $La_{0.8125}Ca_{0.1875}MnO_3$ and have explored various magnetic configurations, including magnetically phase separated states produced by embedding one of these magnetic phases into the other. Our calculations show that the purely ferromagnetic structure is the most stable one, more than the magnetically phase separated scenarios. Initially, we have assumed that the La and Ca atoms (the dopants) are distributed in a perfectly homogeneous manner throughout the crystal. However, experimentally, this might not be the case in the nanoscale. To test the possibility of chemical inhomogeneities, we have constructed four different structures, each with a different Ca dopant distribution, relaxing the atomic positions in each case. The most stable structure corresponds to an intermediate case between a homogeneous and a totally inhomogeneous case. These chemical inhomogeneities will be accompanied of magnetic homogeneities, leading to a nanoscale magnetic phase separation that could be observed experimentally. Our results show important evidences about the origin of the chemical magnetic/electronic phase separation close to a magnetic phase transition. Chemical inhomogeneities are an important player in driving the phase separation.

Surface States Control And Thermoelectric Properties Of CrN Films.

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In recent years, the manipulation of the electronic structure of a material by quantum confinement has attracted much attention, e.g. the appearance of topological surface states or the novel phenomena at the interface between two insulating oxides. CrN is a degenerate semiconductor with large thermoelectric power in the bulk. We have performed DFT electronic structure calculations in thin CrN films (1-3 nm thick) within the LDA+U formalism. We have studied the evolution with film thickness of the electronic structure and conduction properties (obtained using the Boltzmann transport theory). When nanostructured, almost conducting surface states arise. Due to the dangling bonds around the Cr atoms in the surface, the Cr d levels split and appear well separated from the bulk states. For the non-relaxed structures, the surface states lead to a gap reduction with respect to its bulk value being almost constant with the thickness. When the films are relaxed, the surface states can actually become gapless as the thickness is increased, leading to conducting surface states. These states are not affected by the introduction of spin-orbit coupling. We have analyzed the role of spatial confinement in the thermoelectric properties of CrN. A large Seebeck coefficient is predicted even in a thin film geometry. This, together with the increased conductivity from the surface states, could lead to a larger figure of merit of the system if the thermal conductivity can be reduced by nanostructuring.

Structural And Magnetic Characterization Of Ln_2MnCoO_6 Mixed Oxides (Ln=Y, Lanthanide)

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Ln_2MnCoO_6 (Ln = Y, lanthanide) mixed oxides crystallize in the perovskite structure with two cations (Mn and Co) occupying the B positions. These compounds, particularly La_2MnCoO_6, have been extensively studied in view of their interesting magnetic and electrical properties. Nevertheless, for a given compound, results reported in the literature by different groups are often very diverse and even contradictory. From the structural point of view these compounds have been sometimes characterized as pseudo-cubic, sometimes as orthorhombic, monoclinic or even biphasic. This variety of results is related (leaving apart the characteristics and limitations of the technique used: X-ray diffraction, neutrons), to the conditions used to synthesize the compounds, parameters which have a very big influence on the chemical, compositional, structural and microstructural characteristics (oxygen content, degree of Mn/Co ionic order, cation valences) of the obtained materials. As a result, samples with the same nominal composition but obtained under different conditions, can be very different from the microscopic point of view. In this work and with the aim of clarifying the existing controversy, we present a comparative study of the magnetic properties of Ln_2MnCoO_6 (Ln = Y, lanthanide) compounds, that we have carried out on well characterized samples that we have obtained under carefully controlled synthetic conditions.

Thermal Conductivity In Frustrated Spin Systems: The Spinels ACr_2O_4 (A=Zn, Cd, Mn, Mg)

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The materials ACr_2O_4 (A=Zn, Cd, Mn, Mg) are antiferromagnetic oxide-spinel systems, in which the M^{2+} cations occupy the tetrahedral (A) sites and the Cr^{3+} cations occupy the octahedral (B) sites.

The antiferromagnetic oxide-spinel systems ACr_2O_4 (A=Zn, Cd, Mn, Mg) are prototypical examples for highly frustrated magnets, where the magnetic Cr^{+3} ions with spin $S = 3/2$ reside on the vertices of corner-sharing tetrahedra forming a pyrochlore lattice. An antiferromagnetic (AF) nearest-neighbor Heisenberg exchange on the pyrochlore lattice leads to inheret frustration and a multiply degenerate magnetic ground state. In most systems this degeneracy will be released at finite temperatures by coupling to others degrees of freedom and, indeed the spinel systems undergo a magnetostructural transition with antiferromagnetic order at 7.8 K (Cd), 12.5 K (Zn), 12.7 K (Mg) and 14 K (Mn), although their Curie-Weiss are 88 K, 400 K, 390 K, 51 K respectively.

In this study we present the results of the low temperature thermal conductivity of ACr_2O_4. We observed an important supression in the lattice contribution to the thermal conductivity due to the coupling between lattice and magnetic fluctuations. Below the magnetostructural transition, an extra contribution to the Debye lattice thermal conductivity can be identified.

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Spin-triplet Pairing Induced By Hund's Rule Exchange In Orbitally Degenerate Systems: Hartree-fock Approximation

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Spin-triplet pairing induced by the Hund's rule exchange was proposed some time ago [1], as well as its coexistence/competition with the ferromagnetic and orbital types of ordering within simplified models [2,3]. In this work we include the effect of interband hybridization and treat the problem by starting from an extended Hubbard model for doubly degenerate band and making the simplest Hartree-Fock approximation for the parts involving the pairing and the Hubbard terms. The conditions of stability of various phases are determined as a function of both band filling and microscopic parameters. The phase diagram contains regions of stability of the spin-triplet superconducting phase coexisting with either saturated or non-saturated ferromagnetism. For comparison, phase diagram for the cases of constant density of states and that of square lattice, have been presented. The influence of hybridization on the stability of considered phases as well as the temperature dependence of magnetic moment and the superconducting gap is also provided. One of the authors (M.Z.) acknowledges the scholarship from Interdisciplinary Ph. D. School financed by EU Program POIG. The authors acknowledge also the financial support of the Foundation for Polish Science (FNP).

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Numerical Simulation Of The Resistive Berezinskii-Kosterlitz-Thouless Transition In A Two-dimensional Superconductor With A Random Gaussian Distribution Of Critical Temperatures.

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We calculate numerically the electrical transport behaviour under a constant dc voltage V of a planar superconductor with a random distribution of critical temperature inhomogeneities. We focus our study on the strong spatial redistributions of the local current that occur around the Berezinskii-Kosterlitz-Thouless (BKT) transition when the applied bias current I or the temperature T are varied. We also discuss the corresponding broadening of the V-I curves, and of the resistance V/I, around the BKT transition.

Fluctuation Magnetoconductivity In A $BaFe_{1.9}Ni_{0.1}As_2$ Single Crystal

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We present measurements of the in-plane magnetoconductivity in a high-quality single crystal of the iron pnictide $BaFe_{1.9}Ni_{0.1}As_2$. For temperatures near the superconducting transition, these measurements allowed to observe the contribution associated with Coopers pairs created by thermal agitation. These experimental data agree with the existing Gaussian Ginzburg-Landau approaches for three-dimensional superconductors.

Origin Of The Magnetodielectric Coupling in $M_2V_2O_7$ (M= Co And Cu) Divanadates

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In this work we have synthesized and characterized two divanadates $M_2V_2O_7$ (M^{2+}, Co^{2+}, Ni^{2+} and Cu^{2+}), and we report their dielectric behavior. We have observed a magnetodielectric coupling - a change of the slope of the dielectric constant at the magnetic transition temperature. In the $Cu_2V_2O_7$ divanadate, the magnetodielectric coupling is due to the presence of weak ferromagnetism in a polar crystal structure and the behavior of ϵ_r as a function of temperature can be described with a free energy model, which suggests a nonlinear magnetoelectric coupling, with variation in ϵ_r proportional to M2. In the Co-compound the magnetodielectric effect appears to be due to a different mechanism: the magnetic anisotropy of Co^{2+} cations, which causes a non-collinear magnetic arrangement inside the chains and induces electrical polarization by magnetostriction.

Spin dynamics Of $YbCo_2Zn_{20}$ Probed By ESR

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After opening the unexpected well-resolved signals of electron spin resonance (ESR) below the Kondo temperature in heavy-fermion Kondo lattice $YbRh_2Si_2$, investigation of the ESR signal in some undoped alloys started to attract a considerable attention of experimentalists and theorists. It was previously assumed that the corresponding ESR lines are very broad and it is impossible to observe them. However, an unusual narrowing of the ESR lines in such systems according to recent theoretical studies can be explained due to hybridization effects between the localized f-electrons and conduction electrons in the presence of ferromagnetic (FM) correlations. We report the orientation-, temperature- and frequency-dependent ESR spectra in the $YbCo_2Zn_{20}$ single crystals in comparison with the ESR measurements in other dense intermetallic compounds. It should be noted that the strongly anisotropic ESR spectra have been recorded with the external magnetic field H rotated in th!ree different crystallographic planes.

Investigating The Kondo Lattice Compound CeTiGe: Two Related Modifications With Strikingly Different Physical Behavior

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CeTiGe is a paramagnetic Kondo lattice system with a large orbital degeneracy involved in the formation of the heavy fermion ground state. Recently we discovered that this compound presents a huge metamagnetic transition at $B_{\mathrm{MMT}} \approx 12.5\,\mathrm{T}$, with much larger anomalies in magnetization, magnetoresistance and magnetostriction than in the archetypical Kondo lattice metamagnet $CeRu_2Si_2$. Since CeTiGe forms in a pronounced peritectic reaction the growth of single crystals is difficult. We therefore studied the Ce-Ti-Ge ternary metallographic phase diagram to obtain a sound basis for future crystal growth attempts. Preliminary results of growth experiments based on these studies are promising and shall be discussed. In this phase, we have grown quite large single crystals of a new high temperature (HT) configuration of CeTiGe. Completely new physical properties appear although the HT form and the familiar CeTiGe phase crystallize in very closely related structure types. A detailed analysis of the magnetic, thermal and transport properties of HT-CeTiGe will be presented.

On Superconductivity In The Topological Insulator Bi_2Se_3 Intercalated By Cu

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Topological insulators provide a new tool for the realization of novel states of quantum matter. Recently, it has been recognized that the thermoelectric materials Bi_2Se_3 and Bi_2Te_3 are topological insulators: the bulk is insulating, but the surface states - protected by topology - are conducting. Surprisingly, it has been reported recently that these materials can be turned into superconductors by reacting with transition metal elements, like Cu or Pd [1]. However, superconductivity is fragile, as no complete superconducting transition was observed in transport measurements. Here we report our recent efforts to synthesize superconducting $Cu_xBi_2Se_3$ crystals with $x = 0.12 - 0.15$. All samples showed metallic behaviour with a carrier concentration $\sim 1.4 \times 10^{20}$ cm^{-3}. Only the samples rapidly cooled after annealing at 600 ^{o}C for $\sim$100 hours showed traces of superconductivity. The largest effect was obtained for a sample with $x = 0.14$ which showed a $\sim$15 % resistance drop below $T_c = 2.3$ K. The drop is gradually depressed in a magnetic field, as expected for a superconducting transition. Interestingly, similar transitions with limited resistance drops have been observed in $Pd_zBi_2Te_3$ with $0.15 \leq z \leq 1$ [1]. Susceptibility measurements to investigate the diamagnetic screening signal are underway. The results obtained so far indicate the superconducting properties depend sensitively on the sample preparation process. We will compare our data with the recent literature and discuss the possible evidence for bulk superconductivity in $Cu_xBi_2Se_3$.

[1] Y.S. Hor *et al.*, PRL 104, 057001 (2010); J. Phys. Chem. Solids, in press; arXiv:1006.0317v1

Evidence Of New Magnetic Phase Transitions In $PrBa_2Cu_3O_7$ At Low Temperature

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We have revisited specific heat $C_p(T)$ and entropy $S(T)$ properties of $PrBa_2Cu_3O_7$ or ($Pr123O_7$) at low temperature. Below the Néel temperature of the antiferromagnetic ordering (AFM), $T_N^{Pr} = 17.5K$, the low-critical temperature T_{cr}) recently reported on $Pr123O_{6.95}$ [1] appears clearly at the same value ˜$4.5 \pm 0.5K$ with an additional enhancement located at approximately $T_2 \approx 11 \pm 0.5K$ in the temperature dependencies of $C_p(T)/T$ and $C_p(T)/T^2$. The $S(T)/T$ and $S(T)/T^2$ curves show an inflexion point at T_2 between two different entropy behaviors below T_{cr} and above T_N^{Pr}. The ratio $C_{pmagn}(Pr)/C_p(T)$ is calculated using the Pr magnetic contribution $C_{pmagn}(Pr)$ obtained with the usual relation $394C_p(T) = C_p[Pr123O_7] - C_p[Y123O_7]$ where the C_p data of $Y123O_7$ are considered as the phonon and electronic contributions. The $C_p(T)/T$ versus T^2curve is well fitted below T_{cr} to the second order contribution $(T^2)^2$ where some modest non linear effects are evidenced. The previous spin reorientation transition [2] occurs at the transition temperature T^2 due to a small perturbation of both Pr and Cu(2) AFM ordering from the deduced $Pr2500Cu(2)$ magnetic coupling. All parameters are compared to previous results and a reordering of the Pr subsystem is suggested below T_{cr}.

[1] W. Younsi, M. Lahoubi, M.-L. Soltani, D. Schmitt and J. Hejtmánek: Journal of Physics: Conference Series 150, 052290 (2009).
[2] S. Uma, W. Schnelle, E. Gmelin, G. Rangarajan, S. Skanthakumar, J. W. Lynn, R. Walter, T. Lorenz, B. Büchner, E. Walker and A. Erb, J. Phys.: Condensed Matter 10, L33 (1998).

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