Ψ_k workshop on

Strong electron correlation effects in complex d- and f-based magnetic materials for technological applications

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Strongly correlated metals, alloys and oxides, their surfaces, interfaces and heterostructures continue to be very creative, innovative and active research themes in condensed matter physics. These fields are progressing very fast and continue branching into increasingly wider areas of condensed matter. They involve the spintronics including the diluted magnetic semiconductors and spin-orbit related effects, the topological matter, the magnetoelectric coupling, the positive magnetic anisotropy, or the multiferroicity at oxide interfaces and heterostructures.

It is widely recognized that first-principles based calculations can give important clues to understanding the properties and behavior of different strongly correlated materials, and can have a remarkable impact both from the basic as well as from the technological point of view. This workshop focuses on the recent developments of the correlated band theory based on a combination of the density functional theory with the advanced many-body techniques such as the dynamical mean field theory. Special attention will be given to:

- The interplay of strong electron correlations with spin-orbit related phenomena and with the effects of symmetry breaking due to the presence of surfaces and interfaces.
- Calculations of the magnetic anisotropy in strongly correlated d- and f-based materials and nanostructures.
- The role of electron correlations in quantitative modelling of STM/STS, XMCD and RIXS/RXES spectra of d- and f-based materials and nanostructures.
- Applications of the correlated band theory to transport phenomena such as the spin-Hall effect, spin lifetime, spin-transfer torque, and spin dynamics.

Welcome to the Ψ_k workshop in Prague!

Alexander Shick, Jindřich Kolorenč, Sergii Khmelevskyi, and František Máca

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Abstracts are sorted alphabetically according to the family names of the presenting author.

PROGRAM

Monday, 30 June 2014

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Location: Lecture hall - Academy

(chairperson:)

09:00 – 09:10 A. Shick, F. Máca: *Workshop Opening*

09:10 – 10:30 **I. LDA+DMFT**

Location: Lecture hall - Academy

(chairperson: Jindřich Kolorenč)

09:10 – 09:50 Hubert Ebert: *Correlation effects in transition metal nano-systems treated by means of the LSDA+DMFT scheme*

09:50 – 10:20 Igor Di Marco: *Correlated electronic structure in LDA+DMFT: from transition metal oxides to rare earth compounds*

10:20 – 10:50 Coffee break

Location: Vestibule

10:50 – 12:00 **II. LDA+DMFT**

Location: Lecture hall - Academy

(chairperson: Peter M. Oppeneer)

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11:20 – 11:40 Ivan Leonov: *Importance of electronic correlations for the phase stability of V_2O_3*

11:40 – 12:00 Ondřej Šipr: *Effect of correlations on the magnetism and x-ray spectra of Heusler alloys*

12:00 – 14:00 Lunch

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Location: Lecture hall - Academy

(chairperson: A. Lichtenstein)

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15:10	– 15:30	David Blackbourn:	*A dynamical mean field theory study of self assembled diluted solids composed of strongly correlated d- and f- elements on a substrate*
15:30	– 15:50	Tim Wehling:	*Kondo physics and Hund's rule coupling in transition metal impurity systems*

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Location: Lecture hall - Academy

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16:50 – 17:10	David Jacob:	*Renormalization of magnetic anisotropy in adatoms by exchange coupling*
17:10 – 17:30	Soon Cheol Hong:	*Effects of strain, gas adsorption, and capping on magnetocrystalline anisotropy of Co(0001) and Fe(001) surfaces: A first-principles study*
17:30 – 17:50	Frank Freimuth:	*Direct and inverse spin-orbit torques from first principles*

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Location: Lecture hall - Academy

(chairperson:)

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08:30 – 09:00 Registration

Location: Vestibule

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Location: Lecture hall - Academy

(chairperson: Mikhail Katsnelson)

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09:30 – 09:50	Andrea Droghetti:	*Correlated zero-bias transport in nanostructures*
09:50 – 10:30	Jan Minar:	*Application of LDA+DMFT to HAXPES*

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Location: Vestibule

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Location: Lecture hall - Academy

(chairperson: Bedřich Velický)

11:00 – 11:40	Dieter Vollhardt:	*Structural Stability and Lattice Dynamics of Correlated Electron Materials*
11:40 – 12:10	Jindřich Kolorenč:	*Parquet approximations for disordered electrons*

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Location: Lecture hall - Academy

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14:40 – 15:10	Richard Hlubina:	*Unconventional metal-insulator transition in Fe(Si,Ge)*

15:10 – 15:40 Alexander Shick: *Unified picture of electron correlations in Pu and Pu115 family of unconventional superconductors*

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16:40 – 17:10 Georg Rohringer: *Diagrammatic routes to nonlocal electronic correlations*

17:10 – 17:40 Peter Markoš: *Metal-insulator Anderson transition: numerical results*

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08:30 – 09:00 Registration

Location: Vestibule

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Location: Lecture hall - Academy

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10:10 – 10:30	Alexander Poteryaev:	*Magnetic Properties of Iron*

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Location: Lecture hall - Academy

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11:00 – 11:20	Urszula D. Wdowik:	*Strong effect of defects on the electronic and dynamical properties of FeO*
11:20 – 11:40	Dominik Legut:	*Angular dependece of the X-ray magnetic linear dichroism of transition metals at L2,3 edges as a function of Hubbard U*
11:40 – 12:00	Leonid Sandratskii:	*The exchange splitting of surface and bulk electronic states in excited magnetic states of Gd*

12:00 – 14:20 Lunch + transfer to University

Location: Restaurant Slavia

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Location: Lecture hall - University

(chairperson:)

14:20 – 14:30 V. Sechovský, A. Shick: *Colloquium Opening*

14:30 – 15:30 **XI. Ab Initio Calculations**

Location: Lecture hall - University

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14:30 – 15:00 Pavel Novák: *Crystal field and magnetism with Wannier functions: rare-earth intermetallics and low symmetry systems*

15:00 – 15:30 Leon Petit: *First principles study of valence and structural transitions in rare earth compounds under pressure.*

15:30 – 16:00 Coffee break

Location: Lecture hall - University

16:00 – 17:40 **XII. Ab Initio Calculations**

Location: Lecture hall - University

(chairperson: Alexander Shick)

16:00 – 16:20 Jan Tomczak: *Rare-earth based pigments and colors from first principles*

16:20 – 16:40 Vojtěch Chlan: *Charge localization in La, Pr and Nd substituted Sr hexaferrites*

16:40 – 17:00 Sergii Khmelevskyi: *Study of complex magnetic states and phase transitions with Lichtenstein method*

17:00 – 17:20 Yaroslav Kvashnin: *Effective inter-site exchange interactions from DFT+DMFT*

17:20 – 17:40 David Jacob: *Interplay between Kondo effect and molecular quenching in magnetic molecules at metal substrates from first principles*

Invited Talks

Constituents of magnetic anisotropy and screening of spin orbital coupling in magnets

Vladimir Antropov and Liqin Ke

Ames Laboratory, ISU, Physics dept, A508 Zaffarano, Ames, USA

We propose a new quantum mechanical scheme to analyze the origin and spatial distribution of magnetic anisotropy in itinerant and correlated magnets. This method uses approximate perturbation theory and exact integration over parameter techniques. A simple relation between a total magnetic anisotropy and spin orbital coupling anisotropy has been obtained for different crystal symmetries. We analyze the effective screening of spin orbital coupling in solids and demonstrate practical use of this effect. A novel version of the virial theorem has been introduced to analyze separate contributions to magnetic anisotropy from kinetic, potential and spin orbital coupling terms in the effective Hamiltonian. This theory has been applied for many popular magnets: FePt, CoPt, MnBi, MnAl, FeNi, where a microscopic explanation of high anisotropy has been obtained. This analysis has shown that in the itinerant magnets there is very strong intersite orbital anisotropic interactions, that often provide unexpected large and dominant contributions to magnetic anisotropy. We have shown that single-ion anisotropy model is not suitable for many itinerant magnets, while an addition of two-ion anisotropy, due to large orbital interatomic coupling, creates a very consistent description of anisotropic magnetic properties. An extension of proposed technique for the implementation in the many body methods is proposed.

This research is supported in part by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office, through the Ames Laboratory. Ames Laboratory is operated by Iowa State University under contract DE-AC02-07CH11358.

I2

Correlated electronic structure in LDA+DMFT: from transition metal oxides to rare earth compounds

Igor Di Marco, Patrik Thunstrom, and Olle Eriksson

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In the last decade the combination of dynamical mean-field theory (DMFT) with density functional theory in local density approximation (LDA) has emerged as one of the most powerful methods to study the electronic structure of strongly correlated materials. In this talk I will present the details of a LDA+DMFT implementation based on a full-potential linear muffin-tin orbital method (FP-LMTO). The construction of an appropriate set of local orbitals and the applicability of different impurity solvers such as Hubbard I, exact diagonalisation and SPTF will be discussed with a few examples. First, the ground state and spectral properties of SrRuO3 will be analysed, in order to understand the role of the local correlation effects on the itinerant 4d states of Ru. Then, the high degree of localization of the 4f-states in rare earth elements and compounds, e.g. TbN or Ce-pnictides, will be discussed. It will be shown that the Hubbard I approximation can give an excellent description of the most important physical properties. Finally the versatility of the exact diagonalization solver will be illustrated through the understanding of the electronic structure of the transition metal monoxides and Mn doped GaAs.

Correlation effects in transition metal nano-systems treated by means of the LSDA+DMFT scheme

Hubert Ebert[1], Jan Minar[1,3], Svitlana Polesya[1], Sergiy Mankovskyy[1], and Ondrej Sipr[2]

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[2]*Institute of Physics, Academy of Sciences of the Czech Republik, Praha, Czech Republic*
[3]*New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic*

The combination of local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provides a very powerful basis to treat correlations beyond plain LSDA. A fully self consistent implementation on the basis of the multiple scattering Green function formalism (KKR-GF) allows in particular to investigate the impact of correlation effects for nano-systems. In addition, the use of a fully-relativistic formulation permits to study spin-orbit-induced properties. This platform is used for an investigation of various transition metal surface systems. The first part of the contribution deals with the magnetic properties of the surfaces of the pure ferromagnets Fe, Co and Ni and some magnetic surface films, while the second part of the talk is devoted to deposited magnetic clusters on non-magnetic substrates. The focus will be in particular on the influence of correlation effects on the spin-orbit induced magntic moments and spectroscopic properties. Accordingly, the corresponding LSDA+DMFT-based results are compared to those obtained using the LSDA and (in some few cases) the LSDA+U method.

I4

Unconventional metal-insulator transition in Fe(Si,Ge)

Richard Hlubina

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When the interaction strength in a metal is increased to a critical value, the charge degrees of freedom may freeze in an insulating phase. In this usual type of metal-insulator transitions, magnetic ordering of the more correlated phase is only a by-product of the transition in the charge sector. However, in the isoelectronic and isostructural alloys Fe(Si,Ge) a completely different phenomenology is observed: the less correlated compound FeSi is insulating, whereas the more correlated compound FeGe is metallic. On the other hand, from the magnetic point of view, the phase transition in Fe(Si,Ge) is conventional: FeSi is paramagnetic, whereas FeGe is magnetically ordered.

In this talk, after describing the relevant experimental data for the Fe(Si,Ge) alloys, I will argue that the metal-insulator transition in this system forms a novel universality class, one in which it is the magnetic instability of the paramagnetic insulator which drives the charge delocalization. Afterwards I will introduce what we believe to be a minimal microscopic model for this universality class. I will further demonstrate that an approximate treatment of the minimal model leads to qualitative agreement with several experiments on the Fe(Si,Ge) alloys, but also on the related system of FeGe under pressure. Finally I will conclude by listing some of the open questions in this problem.

A Typical Medium Dynamical Cluster Approximation for the Study of Anderson Localization in Three Dimensions

Mark Jarrell

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We develop a systematic typical medium dynamical cluster approximation that provides a proper description of the Anderson localization transition in three dimensions (3D). Our method successfully captures the localization phenomenon both in the low and large disorder regimes. As a function of cluster size, our method systematically recovers the re-entrance behavior of the mobility edge and obtains the correct critical disorder strength for Anderson localization in 3D. It also greatly reduces the computational cost required to study localization, enabling first principles calculations and calculations including the effect of interactions.

I6

Spin dynamics and magnetic interactions from the first- and second-principles calculations

Mikhail Katsnelson

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Magnetic ordering and related phenomena are of essentially quantum and essentially many-body origin and require strong enough electron-electron interactions. Also, they are very sensitive to the details of electronic structure of specific materials. This makes a truly microscopic description of exchange interactions a challenging task. Usually, one cannot use any natural perturbation parameters related with the strength of interactions. Long ago we suggested a general scheme of calculations of exchange interactions responsible for magnetism based on the "magnetic force theorem", when one considers a response of a system on small rotations of spins with respect to a (collinear) ground state magnetic configuration. It was formulated originally as a method to map the spin-density functional to effective classical Heisenberg model, the exchange parameters turned out to be, in general, essentially dependent on initial magnetic configuration and not universal. However, they are directly related to the spin-wave spectrum and, thus, can be verified experimentally. Now it is the standard scheme used for many different classes of magnetic materials, from dilute magnetic semiconductors to molecular magnets. This approach also lies in the base of "ab initio spin dynamics" within the density functional approach.

It is well known now that this scheme is, in general, insufficient for strongly correlated systems and should be combined with the mapping to the multiband Hubbard model and use of, say, dynamical mean-field theory to treat the latter. Our original approach can be reformulated for this "second-principle" method, the results are expressed in terms of Green's functions and (local) electron self-energy. It can be also generalized to the case of relativistic magnetic interactions, such as Dzyaloshinskii-Moriya interactions. Very recently, we have extended this scheme to the case of time-dependent Hamiltonians which opens a way to a consequent microscopic theory of laser-induced spin dynamics in strongly correlated systems.

Excitonic condensation in systems of strongly correlated electrons

Jan Kunes and Pavel Augustinsky

Institute of Physics, AS CR, Cukrovarnicka 10, Praha 6, Czech Republic

The ordered electronic phases are typically characterized by modulations of spin or charge density on inter-atomic scale, although exceptions like superconductivity are well known. Excitonic condensation is a specific type of 'unconventional' instability which leads to spin-multipole or spin-current order. We have used the dynamical mean-field theory to investigate possible long-range order in systems close to a spin-state transition. We will report the results of several types of studies: i) unbiased search for divergences of the particle-hole susceptibility in the two-band Hubbard model, ii) direct simulation of the ordered phases of the same model and iii) static-mean field (LDA+U) calculations for real materials. The main result is an observation of condensation for spinful excitons both in the model [1] and materials [2]. The excitonic phase is characterized by spontaneous appearance of hybridization between atomic states with different spin quantum numbers, i.e., breaking the spin rotational symmetry. We will summarize our numerical data and discuss the concept of the spin-triplet excitonic condensation.

[1] J. Kunes and P. Augustinsky, Phys. Rev. B 89 (2014) 115134

[2] J. Kunes and P. Augustinsky, arXiv:1405.1191

I8

Non-local electronic correlation effects

Alexander Lichtenstein

University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany

Dynamical mean field theory (DMFT) in combination with the first-principle LDA-scheme is an optimal starting point to go beyond static density functional approximation and include effects of spin and charge fluctuations in strongly correlated materials. In order to go beyond the local approximation we investigate a cluster generalization of the DMFT scheme as well as analytical dual-fermions scheme which include a full interaction vertex of impurity problem and spin fluctuations in the ladder approximation. We discuss non-local correlation effects in real materials which have anomalies in the energy spectrum.

Metal-insulator Anderson transition: numerical results

Peter Markoš

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Disorder induced transition from the metallic to the insulating regime was predicted by P. W. Anderson (1958) who showed that randomly distributed impurities can prevent the propagation of electron across the sample. Electron becomes localized in certain region of the lattice. Physical origin of the localization lies in the quantum character of electrons. The localization of electrons is crucial for the understanding of transport properties of mesoscopic structures at low temperatures.

While the transport of electrons in weakly disordered structures can be described analytically, the quantitative description of the localization, in particular the critical regime between the metallic and localized phases is still not complete. There is no agreement between results of analytical theories and numerical simulations.

We numerically demonstrate main phenomena observed in studies of the electron localization: absence of diffusion, the metal-insulator transition, sensitivity to small fluctuations, absence of self-averaging of physical quantities, and summarize main ideas and results of the scaling theory of localization obtained by the analysis of the electron conductance and the inverse participation ratio. Then we discuss possible origin of discrepancies between predictions of the analytical theories and numerical data.

[1] P. Markoš: Numerical analysis of Anderson localization. acta physica slovaca 56, 561 (2006); cond-mat/0609580

[2] J. Brndiar and P. Markoš: Character of eigenstates of the three-dimensional disordered Hamiltoniann Physical Review B 77, 115131 (2008) arXiv 0801.1610

[3] P. Markoš: Comment on the paper I. M. Suslov: "Finite Size Scaling from the Self Consistent Theory of Localization" JETP 142 (2012) iss. 6, paper ID:2206 arxiv:1205.0689

I10

Application of LDA+DMFT to HAXPES

Jan Minar[1,2], Juergen Braun[1], and Hubert Ebert[1]

[1]*LMU Munich, Butenandtstr. 5-13, Munich 82152, Germany*
[2]*New Technologies - Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic*

Angle resolved as well as angle integrated photoemission in the soft and hard X-ray regime became a very important tool to investigate the bulk properties of various materials [1]. Contrary, bulk sensitivity can be achieved by so called threshold photoemisison, e.g. by using for example laser light at 405 nm [2]. The increased bulk sensitivity might lead to the impression that the LSDA band structure or density of states can be directly compared to the measured spectra. However, various important effects, like matrix elements, the photon momentum or phonon excitations, are in this way neglected. Here, we present a generalization of the state of the art description of the photoemisison process, the so called one-step model that describes excitation, transport to the surface and escape into the vacuum in a coherent way. A short introduction to the main features of the one-step model implementation within the Munich SPR-KKR program package will be given. Special emphasis will be put on the spin-polarised relativistic mode that allows to deal with magnetic dichroism. Also, the possibility to account for correlation effects and chemical disorder using the LSDA+DMFT (dynamical mean field theory) scheme in combination with the Coherent Potential Approximation (CPA) method [3] will be demonstrated by various examples. For photon energies, even in the soft-x-ray regime, a considerable effect of lattice vibrations is present [4]. Here, we discuss a theoretical description of lattice vibrations which is based on the CPA. These aspects will be discussed in an detail using various examples [5]. In the last part of my talk I will show prediction that HAXPES is possibly valuable tool to study topological surface states and rashba effect [6].

[1] A. Gray, etl al., J. Minar et al., Nat. Mat. 10, 759 (2011).

[2] M. Kronseder, Ch. Back, J. Minar et al., Phys. Rev. B 83, 132404 (2011)

[3] J. Minar, J. Phys.: Cond. Mat. Topical review 23, 253201 (2011), H. Ebert et al., Rev. Prog. Phys. 74, 096501 (2011)

[4] J. Braun, J. Minar et al., Phys. Rev. B 88, 205409 (2013)

[5] A. Gray, J. Minar et al., Nature materials 11, 957 (2012), Fujii et al., Phys. Rev. Lett. 111, 097201 (2013)

[6] J. Braun et al., New J. Phys 16, 015005 (2014)

Transverse Hall and Nernst effects in thin films from first principles

Yuri Mokrousov

FZ-Juelich, Institute for Advanced Simulation, Juelich, Germany

The importance of transverse transport effects which are driven by spin-orbit interaction has been constantly rising in the past years owing to the key role these effects play for possible applications in future spintronics devices. Here, we will focus on the physics of the Hall and Nernst family of effects as accessed from first principles in thin films of transition metals. We will discuss the origins of the transverse currents in disordered media and the ways these currents can be manipulated by proper nano-structuring taking as an example the spin Nernst effect. Moreover, we will discuss the interplay of the topological Hall and anomalous Hall effect in thin films with non-collinear magnetic order and relation of the topological charge to the transverse thermoelectric properties in such systems. Finally, we will show how the topological concepts allow us to formulate the thermoelectric analog of the spin-orbit torque in ferromagnets, and we will discuss the magnitude of this thermal spin-orbit torque in thin transition-metal films.

I12

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

Pavel Novák

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

The method uses the density functional theory based band structure calculation, followed by a transformation of the Bloch to the Wannier basis and expansion of the local Hamiltonian in terms of the spherical tensor operators. It contains a single adjustable parameter that characterizes the hybridization of RE(4f) states with the states of oxygen ligands. In the present contribution the method is applied to $NdFe_{14}B$ and to R:LaF_3 (R=Ce, Pr, ... Yb). In LaF_3 the rare earth site has a low symmetry and 27 crystal field parameters are needed to describe the crystal field.

Ab-initio theory of ultrafast laser-induced demagnetization

Karel Carva[1,2], Ritwik Mondal[1], Marco Battiato[1], Dominik Legut[3], and Peter M. Oppeneer[1]

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[2]*Charles University, Dept. of Cond. Matter Physics, CZ-12116 Prague 2, Czech Republic*
[3]*Nanotechnology Centre, VSB-TU Ostrava, CZ-708 33 Ostrava, Czech Republic*

More than a decade ago it was discovered that excitation of a metallic ferromagnet with an intensive femtosecond laser-pulse causes an ultrafast demagnetization within 300fs [1]. Until today, the mechanism(s) underlying the fs demagnetization could not be uncovered and remain a controversial issue. Several theories have been proposed – mostly based on the assumption that there must exist an ultrafast channel for the dissipation of spin angular momentum. One of the proposed fast spin-flip channels is the Elliott-Yafet electron-phonon spin-flip scattering [2].

We probe several of the proposed mechanisms using ab-initio caluclations. To examine the electron-phonon spin-flip scattering we compute ab-initio the spin-flip Eliashberg function, from which we calculate the spin-flip probability and demagnetization for various situations, viz. equilibrium distributions, hot electron distributions in the thermalized regime, and laser-induced non-equilibrium conditions [3]. Hot electron distributions in the electron-thermalized regime are calculated to lead only to a very small demagnetization rate. A larger net demagnetization is computed for laser-induced non-equilibrium conditions, however, also this contribution is not sufficient to explain the measured fs demagnetization. Following a different rationale we have developed a model for fs laser-induced magnetization dynamics, based on the high mobility of laser-excited spin-polarized electrons [4]. We establish the influence of fast electron dynamics of excited non-equilibrium electrons and show that this provides spin-transport in the super-diffusive regime, causing effectively a demagnetization. We find that super-diffusive flow of hot electrons can account for the experimentally observed demagnetization within 200fs in Ni.

[1] E. Beaurepaire, J.-C. Merle, A. Daunois, J.-Y. Bigot, Phys. Rev. Lett. 76 (1996) 4250.

[2] B. Koopmans, G. Malinowski, F. Dalla Longa, D. Steiauf, M. Fähnle, T. Roth, M. Cinchetti, M. Aeschlimann, Nature Mater. 9 (2010) 259.

[3] K. Carva, M. Battiatio, D. Legut, P.M. Oppeneer, Phys. Rev. B 87 (2013) 184425.

[4] M. Battiato, K. Carva, P.M. Oppeneer, Phys. Rev. Lett. 105 (2010) 027203.

I14

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

Leon Petit[1], Axel Svane[2], Martin Lueders[1], Zdzislawa Szotek[1], V Kanchana[3], Ganapathy Vaitheeswaran[4], and Walter Temmerman[1]

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

Diagrammatic routes to nonlocal electronic correlations

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Strong electronic correlations play a crucial role in the physics of important and technologically relevant classes of materials such as, for example, transition metal oxides or rare earth compounds. From the theoretical side, in the last two decades, a big step forward was achieved by the dynamical mean field theory (DMFT), which accounts non-perturbatively for an important part of the electronic correlations, namely the local ones. However, many fascinating phenomena such as, e.g., unconventional superconductivity or quantum criticality originate (or are at leas strongly affected by) nonlocal correlations. In this walk I will discuss a class of extensions of DMFT which are based on a systematic resummation of specific classes of nonlocal Feynman diagrams. These so-called diagrammatic methods allow for an inclusion of nonlocal electronic correlations on all length scales in addition to the local ones of DMFT. I will emphasize the applicability of such approaches using the example of the Dynamical Vertex Approximation (DΓA)[1]. Adopting this technique for the analysis of the critical behavior[2] of the three-dimensional half-filled Hubbard model demonstrates its strength in capturing the effects of nonlocal correlations. More specifically DΓA predicts a sizable reduction of the transition temperature to the antiferromagnetically ordered state compared to DMFT. Its validity is further confirmed by an investigation of the critical exponents which can be shown to be consistent with those of the three-dimensional Heisenberg universality class.

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I16

Many-body phenomena in correlated systems.

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By definition, correlated electrons cannot be reduced to a single-particle description. Indeed, the most successful theory of electronic correlations, Dynamical Mean-Field Theory (DMFT), essentially takes on-site electron-electron interaction in the account. However one can note that most of the DMFT calculations yield single-electron Green's function and related quantities, and not collective many-body excitations, like plasmons or magnons. We argue that such an asymmetry is related with a local nature of the DMFT theory. Whereas local single-electron self-energy appears to be a very reasonable approximation, an assumption about the locality of, for example, polarization operator violates the charge conservation law. Thus a conservative theory for many-body quantities should necessarily be non-local in space. We construct a minimal theory of this kind, that is based on the ladder series expansion in so-called dual variables. The results for plasmonic dispersion in correlated films are presented. Other related problems will be discussed also.

Structural Stability and Lattice Dynamics of Correlated Electron Materials

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How does the lattice structure of a solid depend on the correlations between the electrons? To answer this question we compute the total energy of correlated materials as a function of the atomic positions and unit cell parameters within the DFT+DMFT scheme, which combines density functional theory with the many-body dynamical mean-field theory. Results are presented for the equilibrium crystal structure and phase stability of paramagnetic Fe, in particular near the α - γ phase transition [1]. Furthermore, by combining the DFT+DMFT scheme with the method of frozen phonons the lattice dynamics and phonon dispersion relations are determined [2]. Electronic correlations are found to be essential for the explanation of the electronic and structural properties of iron.

Finally, a brief introduction into a new approach for the calculation of interatomic forces and structural distortions in strongly correlated materials is presented, which is based on the implementation of LDA+DMFT within the linear-response formalism [3]. Thereby one is able to calculate the equilibrium lattice structure of correlated systems even in the vicinity of a Mott metal-insulator transition — a computation which was not feasible up to now.

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Contributed Talks

A dynamical mean field theory study of self assembled diluted solids composed of strongly correlated d- and f- elements on a substrate

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We endeavour to investigate the properties of self assembled dilute super-lattices of d- and f-orbital elements on a metallic surface, within a fully self consistent DFT+DMFT (Dynamical Mean Field Theory) framework, that is able to fully capture the local strong correlations of magnetic rare earth and transition metal elements while also being able to capably converge the total electronic density.

We are motivated in this task by the experimental realization of a stable Ce super-lattice on Ag(111) [1]. Such a system is a promising candidate for the development of nanoscale magnetic memory devices, where the ad-atom states could possibly be controlled independently, allowing atomic scale information storage. Such devices are a subject of interest in academic and industrial sectors, with IBM successfully storing data using anti-ferromagnetic arrangements of Fe atoms [2]. This was done by individually placing atoms using an STM tip, but achieving success through self assembly mechanisms is obviously a desirable progression.

This is a difficult problem due to the multitude of possible phenomena at play. Experimental data suggests that the Kondo effect plays a role in the low electron density regime, and screening of the magnetic moment is indeed expected of the highly localised f-electron of Ce. There is the possibility of indirect exchange between the moments on adatoms giving rise to RKKY interactions, and a previous tight binding study has shown the importance of the ionic potential [3].

With all these possible effects present, it has been necessary to develop an advanced DMFT model using exact diagonalisation and cluster DMFT techniques to correctly take them all into account, and adequately treat the strongly localised d- or f-electron. These methods come with considerable computational costs, and so work has also been done to optimize the algorithms used.

While motivated by the Ce/Ag(111) lattice, our developing framework is universal and parameters can easily be changed to study numerous possible super-lattices of different transition and rare earth elements, on a variety of substrates. We hope that this can eventually be used as guiding tool for experimentalists, able to predict where in a complex phase space of temperature, adatom and substrate elements and competing interaction regimes, stable super-lattices might form and what regions of this space warrant further investigation.

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C2

Charge localization in La, Pr and Nd substituted Sr hexaferrites

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

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

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Correlated zero-bias transport in nanostructures

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In the recent years, scanning tunnelling microscope as well as break-junctions experiments have opened new routes in the study of the Kondo effect and how it affects the transport properties of nano-devices. Similarly,the Kondo effect in graphene and 2D topological insulators (TI) [1] has also attracted considerable interest because of to the peculiar electronic properties of these systems: while an impurity spin in graphene interacts with the Dirac fermions of the lattice, an impurity on the edge of a 2D-TI interacts with the helical edge liquid. Here we first describe (within the tight-binding formalism) the electronic structure of several graphene and 2D-TI model nanostructures, which incorporates magnetic impurities. In particular, we discuss how electron correlation effects on the transport properties of these systems can be studied by combining continuous time quantum Monte Carlo with the Green function transport theory and the existing schemes, which allows for the calculation of the electrodes hybridization function [2]. Then, we highlight how the same method can be combined with density functional theory in the Smeagol electronic transport code [3] in order to include material specific properties. Finally we present some preliminary results about our in-progress implementation.

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C4

Direct and inverse spin-orbit torques from first principles

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Under application of electric currents, ferromagnetic (FM) layers asymmetrically sandwiched between nonmagnets (NM1, NM2) in NM1/FM/NM2 films experience spin-orbit torques (SOTs) on the magnetization, which can serve to switch the magnetic state of the FM layers. Using density-functional theory calculations we study SOTs by means of the Kubo linear response formalism [1]. Comparing SOTs in NM1/FM films for different choices of NM1 (Pt, W, Ta, Ir, Au) we show that the sign of the spin Hall effect in these transition metals correlates with the even ("damping-like") component of SOT. Resolving torques and spin-fluxes on the atomic scale allows us to elucidate further the role of spin-currents in mediating the SOTs and to identify an additional spin-current independent component. Varying the thickness of the Co and Pt layers as well as the choice of NM2 in NM2/Co/Pt(111) films we find a strong sensitivity of the odd ("field-like") component of SOT, while the even component is less sensitive. Estimating extrinsic contributions from a scalar disorder model [2] we argue that intrinsic effects prevail. Our results on the NM2/Co/Pt(111) systems are in very good quantitative agreement with recent experiments [3] on AlO/Co/Pt(111) films.

Besides the direct SOT also its inverse effect is currently of great interest. While the direct SOT allows us to control the magnetization via applied electric current pulses, the inverse effect consists in the generation of current in the presence of a time-dependent magnetization. We discuss exact relationships between direct and inverse SOTs within the Kubo linear response formalism. An important contribution to the inverse SOT is the conversion of pumped spin current into charge current via the inverse spin Hall effect. We focus in particular on the spatial decay in the NM1 layer of the spin current pumped into NM1 via the ferromagnetic resonance of the FM layer and its conversion into a charge current, which is a question that so far has been addressed only within phenomenological models. Finally, we consider the adiabatic inverse SOT, which allows us to relate the intrinsic even SOT to the Dzyaloshinskii-Moriya interaction [4,5].

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Effects of strain, gas adsorption, and capping on magnetocrystalline anisotropy of Co(0001) and Fe(001) surfaces: A first-principles study

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Intense scientific efforts to increase information density in devices such as magnetic-resistance access memory (MRAM) have been paid during last few decades. Recently, so-called spin transfer torque random access memory (STT-RAM) has been emerged in a nano-scaled magnetic tunnel junction (MTJ) with advantages of good selectivity in writing, low power consumption, and high scalability over conventional MRAM. Two key factors of (1) high thermal stability and (2) low critical current density for switching of magnetization orientation should be satisfied to realize commercialized STT-RAM. An MTJ with strong perpendicular magnetocrystalline anisotropy (PMCA) is indispensable for the two key factors [1]. In this talk, some suggestions will be given to enhance MCAs of the typical magnetic systems of Co(0001) and Fe(001) surfaces, based on our first-principles studies on effects of strain, gas adsorption, capping of 4d/5d transition metal on the MCAs. Physical origins will be discussed in terms of single particle energy spectra.

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C6

Renormalization of magnetic anisotropy in adatoms by exchange coupling

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The coupling of a magnetic adatom to the conduction electrons of the underlying substrate can lead to the screening of its spin by formation of a Kondo singlet state if the coupling is strong enough. The Kondo effect is signaled by the appearance of a sharp and strongly renormalized peak in the spectral density right at the Fermi level, the so-called Kondo resonance. On the other hand for weak coupling, magnetic anisotropy (MA) induced by the local environment of the adatom leads to inelastic spin flip excitations visible as steps at the corresponding excitation energies in the STM spectra. Recently, it we have shown experimentally and theoretically [1] that the exchange coupling of a Co adatom to the conduction electrons of the substrate also leads to the renormalization of MA and the corresponding spin flip excitations. Hence the effective MA of a single ion can be tuned by tailoring its coupling to the substrate. Here we extend our theory presented in [1] to the case of Fe and Mn adatoms. We calculate the spectra of Co, Fe and Mn adatoms in dependence of the coupling to the substrate, by solving the generalized multi-orbital Anderson impurity model including MA in the One-Crossing Approximation. This allows us to treat the strong electronic correlations leading to the Kondo effect and the MA leading to inelastic spin-flip excitations on the same footing. We find that the spectra evolve from purely inelastic spin-flip at weak coupling, via the coexistence of Kondo effect and inelastic spin flips at intermediate coupling, to pure Kondo effect at strong coupling. As the coupling increases, the inelastic spin flip steps broaden and shift to lower energies, and finally merge into a single Kondo peak at strong coupling. Hence Kondo effect and inelastic spin-flip excitations are really two sides of the same coin.

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

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

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C8

Study of complex magnetic states and phase transitions with Lichtenstein method

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The first-principle calculations of the magnetic exchange constants using the magnetic force theorem (so-called Lichtenstein method) is allowed to investigate the microscopic mechanism of the complex magnetic phase formations and phase transitions. We illustrate this using as examples the complex non-collinear ground state in NpCoGe compound, predictions of novel type of meta-magnetic transition in (Mn,Cr)Au_2 alloy and evaluation of magnetic compensation temperature in $DyCo_5$ compound. On the basis of Lichtenstein method the state-of-the-art ab-initio calculations one may predict a novel materials with superior magnetic properties. The experimental invention of high-temperature antiferromagnets Mn_2Au (T_{Neel} > 1200K), which for over two decade has been regarded as non-magnetic compound, has been initiated by the theoretical predictions on the basis of Lichtenstein method. Another example is the prediction of the one-dimensional metallic ferromagnetism in MnB_4 will be discussed.

Parquet approximations for disordered electrons

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The Anderson model of noninteracting disordered electrons is studied using the diagrammatic perturbation technique formulated in terms of Green's functions averaged over all configurations of the disorder. We utilize the topological nonequivalence of the two-particle scattering channels to formulate self-consistent equations for the two-particle vertices, the so-called parquet scheme. The vertices then determine transport coefficients in the framework of the linear response theory.

The classification of the two-particle diagrams into non-equivalent channels is possible only if the one-particle Green's functions entering the diagrams are non-local, which is achieved by considering all local contributions as being irreducible. Since the sum of all local scatterings corresponds to the coherent potential approximation (CPA), the parquet scheme takes the form of an expansion around the CPA and thus offers a systematic way to incorporate non-local quantum coherence into the description of disordered electrons.

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C10

Galvanomagnetic properties of ordering L_{10}-FePt alloy

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The effect of the long-range order (LRO) on the longitudinal (ϱ[xx], ϱ[zz]) and anomalous Hall (ϱ[xy]) resistivities as well as on the anisotropic magnetoresistance (AMR) in ordering L_{10} -FePt alloys is studied from first-principles. The linear-response theory as formulated in the framework of the relativistic tight-binding linear muffin-tin orbital method which includes both the Fermi-surface and Fermi-sea terms is used. The effect of disorder is treated by means of the coherent potential approximation. The main result is a weak dependence of the anomalous Hall conductivity σ[xy] on the LRO which is, however, compatible with the resistivities ϱ[xx] and ϱ[xy] which both depend strongly on the disorder present in the system. The resistivity and the AMR are predicted to increase with increasing degree of the LRO. We also investigate the effect of spin fluctuations on studied quantities using a simple model of the spin disorder. We have found a good agreement between the theory and recent experiment.

Effective inter-site exchange interactions from DFT+DMFT

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

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

In the last part of my presentation I will show some particular applications of the method. A special attention will be given to the case of $SrRuO_3$. The impact of correlation effects and structural changes on the J-parameters in this system will be discussed.

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C12

Importance of electronic correlations for the phase stability of V_2O_3

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We report results for V_2O_3 obtained by a novel implementation of the LDA+DMFT approach for the computation of the total energy of materials with strongly interacting electrons. It includes a fully self-consistent calculation of the charge density, whereby correlation-induced changes in the effective Kohn-Sham Hamiltonian are taken into account. This scheme is employed to study the electronic structure and phase stability of V_2O_3 near a pressure-induced Mott-Hubbard metal-insulator transition. To explore structural transformations as a function of pressure, we use the experimentally determined atomic positions for the metallic and insulating phases, respectively, and calculate the total energy as a function of volume. We find that the structural stability depends very sensitively on changes of the lattice volume. In agreement with experiment, we observe that the metal-insulator transition is accompanied by a remarkable change of the c/a ratio. Full charge self-consistency is shown to be important to understand the phase stability of V_2O_3 near the Mott-Hubbard metal-insulator phase transition.

Magnetic Properties of Iron

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The properties of iron have fascinated mankind for several thousand years already. Iron has been an exceptionally important material for the development of modern civilization and its technologies. Nevertheless, even today many properties of iron are still not sufficiently understood. Therefore iron remains at the focus of active research. In particular, the problem of origin of magnetism of iron in different phases attracts a lot of attention, despite long time of its investigations. By performing LDA+DMFT calculations in the paramagnetic phase of α-iron we find that Coulomb interaction and, in particular Hund exchange, yields the formation of local moments in e_g electron band, which can be traced from imaginary time dependence of the spin-spin correlation function. This behaviour is accompanied by non-Fermi-liquid behaviour of e_g electrons and suggests using local moment variables in the effective model of iron [1]. In γ-iron, the frequency dependence of the electronic self-energy has a quasiparticle form for both, t_2g and e_g states, such that local moments are not formed at low temperatures. At the same time, in the temperature range T=1200-1500 K, where γ-iron exist in nature, the effect of weak temperature dependence of local magnetic moments can be observed in the local magnetic susceptibility [2].

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C14

The exchange splitting of surface and bulk electronic states in excited magnetic states of Gd

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Recent pump-probe experiments provide time evolution of the bulk and surface electronic states in Gd exited by the laser pulse. These new experiments are in close connection with earlier spectroscopic experiments probing temperature dependence of the exchange splitting of the bulk and surface states. The two types of electronic states show very different behavior. Most of the researchers suggest to treat the bulk states within a Stoner model whereas the surface states show clear non-Stoner behavior and remain exchange-split above the Curie temperature. We report first-principles study of the electronic states in both thermally excited Gd and Gd subjected to the laser irradiation. We model the excited states of the system by the noncollinearity of the 4f spin moments where stronger excitations correspond to larger noncollinearity of the neighboring 4f moments. We provide arguments for ultra-fast character of the 4f-moments disordering by hot electrons and discuss the possible ways of the treatment of the induced 5d6s moments. In agreement with experiments we obtained strong difference in the dynamics of the bulk and surface states. We apply the concept of spin-mixing to characterize the electronic states of the excited system. The surface states remain weakly spin-mixed with respect to the local atomic spin axes that explains the presence of the exchange splitting in highly excited systems. On the other hand the bulk states are strongly spin-mixed with respect to the local atomic axes and average the influence of the atomic spin-up and spin-down potentials. This results in the properties that are usually associated with the Stoner model. We analyze quantitatively the dynamics of the electronic states and compare the numerical results with the results of the recent experiment.

Drag of supercurrent in three-contact hybrid structure on surface of 3D topological insulator

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In our work we consider a model of a three-contact quantum interferometer of Fabri-Perot type which has two neutral 1D Majorana leads and a normal one. This three-contact setup is supposed to be a hybrid structure fabricated on 2D surface of a 3D topological insulator. The hybrid structure is the combination of magnetic islands and superconducting leads where the proximity effect with 2D surface results in formation of profiles with gapless 1D chiral channels. Namely, in our model we suppose that 2D surface electrons of a topological insulator are described by Dresselhaus or Rashba type Hamiltonian which couples momentum and real spin and have single Dirac cone in low energy spectrum. It is common that applied homogeneous Zeeman field or superconducting pairing potential induces a gap in 2D Dirac spectrum. Indeed, magnetic domain walls, where Zeeman field changes sign, or boundaries between magnet and superconductor support non-trivial gapless 1D chiral channels with charged or neutral Mejorana fermions. Quantum interferometers constructed from such a 1D channels have attracted a great interest recent years because they reveal unusual transport properties if they support Majorana states. Despite that Majorana excitations are neutral, their presence at the edges of two superconductors strongly affects the character of Cooper pair tunneling, resulting, for example, in anomalous 4 π-Josephson effect. In our three-contact hybrid structure the superconducting leads with 1D Majorana channels and the interferometer loop are coupled through a tunnel point contacts. We find that if the coupling between them is quite strong then voltage bias in the normal lead results in a strong drag of supercurrent between two superconducting leads, with the current in the normal contact being zero. We derive scattering matrices for the tunnel contacts of the interferometer and calculate analytically the drag current as a function of superconducting phase difference and voltage bias in the normal lead.

C16

Unified picture of electron correlations in Pu and Pu115 family of unconventional superconductors

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PuCoGa5, discovered in 2002, has the highest critical temperature of 18.5 K among heavy-fermion superconductors, that is one order of magnitude higher than for typical heavy-fermion compounds. In this work we address electron correlation effects in $PuCoGa_5$ making use of a combination of the local density approximation (LDA) with an exact diagonalization (ED) of the Anderson impurity model. The band structure obtained by the relativistic version of the full-potential linearized augmented plane wave method (FP-LAPW) is extended to account for the f-orbital atomic multiplets and their hybridization with the conduction bands. We show that the unconventional character of superconductivity in the Pu-115 compounds and the unusual physical properties of delta-Pu, in particular the unexpected absence of magnetism, may have a common origin in the intermediate-valence nature of the Pu 5f-electron ground state. The local 5f magnetic moment is compensated by a moment in the surrounding cloud of conduction electrons, and the Anderson impurity grounds state is a non-magnetic singlet. On the basis of these results, we discuss the role of spin and charge fluctuations for Cooper pairing, and the nature of the unconventional d-wave superconducting state in $PuCoGa_5$.

Effect of correlations on the magnetism and x-ray spectra of Heusler alloys

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Heusler alloys represent a class of systems for which the correlations between the d electrons may be important. We performed charge-selfconsistent LSDA+DMFT calculations of the electronic structure and x-ray spectra of stoichiometric Cu_2MnAl and non-stoichiometric $Ni_2Mn_{1+x}Sn_{1-x}$ systems, to study the combined influence of correlations and disorder. We show how hybridization affects orbital magnetic moments and x-ray absorption spectra also for those atoms for which the Hubbard U is zero. An pronounced impact of the way the double-counting is included is observed for the Cu $L_{2,3}$-edge spectra. The calculations are compared with experimental data.

C18

Rare-earth based pigments and colors from first principles

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

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Strong effect of defects on the electronic and dynamical properties of FeO

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Electronic structure and vibrational dynamics of FeO crystal containing cation vacancies are theoretically studied within density functional theory incorporating strong local Coulomb interactions at iron atoms. Our investigations show a strong effect of Fe vacancies on the structural, electronic, and vibrational properties of wustite [1]. They also uncover qualitative difference between stoichiometric and defected FeO containing either 3% or 6% of cation vacancies. The insulating gap of iron oxide is reduced by about 50% due to unoccupied electronic bands introduced by trivalent Fe ions stabilized by cation vacancies. Significant changes in the electronic structure along with atomic displacements induced by cation vacancies affect strongly phonon dispersions via modified force constants, including those at atoms beyond nearest neighbors of defects. It is shown for the first time that theoretical phonon dispersions and their densities of states reproduce the results of inelastic neutron and nuclear resonant inelastic x-ray scattering experiments [2,3] only when Fe vacancies and Coulomb interaction are both included explicitly in ab initio simulations.

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C20

Kondo physics and Hund's rule coupling in transition metal impurity systems

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We study the electronic structure of transition metal impurities (Mn, Fe, Co, Ni) in metallic hosts by combining density functional theory, many body impurity models and photoemission spectroscopy. While Mn and Co can be understood in terms of generalized Kondo models, Fe is shown to host sizable charge fluctuations and magnetic moments at the same time. In the latter case, there are no more well quantized magnetic moment and electronic correlations are largely driven by Hund's exchange J instead of Hubbard U. Fe in metal hosts realizes thus the single impurity limit of a Hund's metal. For this case, the dependence of the electronic excitation spectra and thermodynamic ground-state properties on hybridization between impurity and its surrounding is investigated systematically. Atomic multiplet peaks and exchange split many body satellites persist despite strong charge fluctuations and spin-freezing is observed.

Posters

Lattice dynamics and optical properties of GeS from first principles

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Phonon spectrum and optical properties were calculated for the orthorhombic dielectric compound of GeS. The results were obtained within the single-electron framework of density functional theory using the VASP code and generalized-gradient approximations for the exchange-correlation energy term. Phonon properties were obtained within the direct method approach which utilizes the calculated Hellmann-Feynman forces acting on atoms in a supercell. Special attention was paid to minimize errors of the calculated force constants, as the crystal is complex: it is strongly anisotropic, with two-dimensional layers having strong covalent Ge-S bonds. The interlayer coupling is, however, weak. The phonon dispersions and phonon density are in good agreement with results found in the literature. The dielectric function was also calculated and compared with available data.

P2

Ab-initio investigation of double fluoride $GdLiF_4$ under pressure

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Nowadays, solid-state laser materials with diode pumping are of great interest because of their possible use as a laser system of small size with high efficiency and long lifetime. Crystals $GdLiF_4$ doped with rare-earth ions are promising materials to create a such systems [1].

Recently, it was concluded that the effect of pressure on compounds with scheelite and fergusonite structures in oxides, fluorides, and compounds such as ABX_4 is not fully studied [2]. Thereby, the angular dispersion on the powder $GdLiF_4$ was investigated by X-ray as a function of pressure and temperature [3]. Decomposition of the compound into two components $Gd_{1-y}Li_yF_{3-2y}$ ($P6_3/mmc$, Z = 2) and LiF at a pressure of 13.1 GPa has been observed.

In the present work possible causes of decomposition of compound $GdLiF_4$ under pressure were explained. Ab-initio calculations were carried out based on the density functional theory using the module VASP 5.2 [4] (Vienna Ab-Initio Simulation Package), the interface software MedeA[1].

The order parameter was analyzed for two symmetries of $GdLiF_4$ structure $I4_1/a$ and $C12/c1$. The second rank components of the strain tensor were chosen as the primary order parameter. It is possible to use this kind of order parameter due to the fact that the structural model fergusonite (space group $C12/c1$) was obtained from the scheelite type (space group $I4_1/a$ [5]) based on the supergroups-subgroups relationships. Change the behavior of the order parameter was observed near 16 GPa. Enthalpy was also investigated for two symmetries $GdLiF_4$ compound $I4_1/a$ and $P12/c1$. The intersection of enthalpies was obtained near the pressure 18 GPa.

The obtained results indicate that the transitions of compound $GdLiF_4$ in the structures with given symmetries compete. This assumption can give a reason of the fact that the investigated compound undergoes to a structural decomposition, rather than the phase transition, which was observed in similar materials $LuLiF_4$ and $YLiF_4$.

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New discoveries in old magnetite

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Magnetite, first magnetic material discovered in Ancient Greece, is a ferrimagnetic spinel with anomalously high Curie temperature 850 K. Hence, it is viewed as an ideal candidate for room-temperature spintronic applications. It still attracts great attention due to puzzling properties of the Verwey transition that occurs at T = 124 K and is associated with a drop of electric conductivity [1] and a complex structural phase transition [2].

Our theoretical studies based on the LDA+U method demonstrated a strong interplay between the local electron correlations on Fe atoms and electron-phonon coupling, which plays a crucial role in the Verwey transition [3,4]. These results were confirmed by the inelastic x-ray scattering measurements at the ESRF in Grenoble that found anomalous, nonlinear broadening of low-energy phonons with decreasing temperature above the Verwey transition [5]. By a combination of these experimental results with ab initio calculations we revealed a strong anharmonicity induced by electron-phonon coupling. This anharmonic behavior is connected with the short-range fluctuations inherited from the long-range charge-orbital order observed below the Verwey transition [2].

Our recent diffuse scattering studies discovered very rich pattern in large areas of reciprocal space, which allows us to link the nature of short-range ordering with the long-range structure of the low-temperature phase [6]. It shows that whatever the electron localization pattern is, it partially survives up to room temperature as short-range correlations in the high-temperature cubic phase. Additionally, ab initio calculations reveal that characteristic features in the diffuse scattering pattern can be correlated with the Fermi surface topology.

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P4

Temperature dependence of uniform magnetic susceptibility of iron pnictides from dynamical mean-field theory

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The discovery of superconductivity in ferropnictides has sparked tremendous interest to the new class of superconducting materials. In addition to rather high critical temperatures the iron pnictides demonstrate unusual magnetic properties. Namely, in some cases the paramagnetic susceptibility shows unusual non-Pauli and non-Curie-Weiss temperature dependence. Therefore understanding of the microscopic mechanism for such an unusual temperature evolution of the susceptibility is a challenging task. In our work we present the LDA+DMFT (method combining Local Density Approximation with Dynamical Mean-Field Theory) results for magnetic properties of the parent superconductors LaFeAsO, BaFe2As2 and KFe2As2 in the paramagnetic phase. Calculated uniform magnetic susceptibility demonstrates quasilinear increase at low temperatures followed by a maximum and decrease at higher T. The increase is detected experimentally for LaFeAsO and BaFe2As2 while the increase, maximum and the decrease are observed in hole-doped KFe2As2. The calculated susceptibility curves and their evolution with doping are in agreement with experimental data. We show that the microscopic origin of this anomalous behavior is connected with thermal excitation of the states forming the peak of the spectral function located approximately 100 meV below the Fermi level. This peak is due to the weak dispersion of the two-dimensional bands associated with layered crystal structure of the pnictides. Our results demonstrate that the unusual temperature dependence of the static magnetic susceptibility in the pnictide superconductors is connected with their spectral properties and can be understood without invoking intersite magnetic fluctuations.

Optical properties of a monoclinic insulator $Cu(H_2O)_2(en)SO_4$, en=$C_2H_8N_2$

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$Cu(H_2O)_2(en)SO_4$ was recently identified as a quasi-one-dimensional $S = 1/2$ antiferromagnetic insulator with a theoretically predicted gap of about 2 eV [1]. We used the electronic structure of [1] to predict material's optical properties and, namely, study one aspect related to the structure's monoclinic symmetry (the angle β is 105.5°). The monoclinicity implies that (i) the material is optically biaxial, and (ii) the axes of the dielectric frame, defined as the frame where the real part of the (generally complex) dielectric tensor is diagonal, are not fixed by crystallographic symmetry (and actually depend on frequency). By means of Mueller ellipsometry we measured the system's optical properties, from which the orientation of the dielectric frame was inferred and compared to a prediction of DFT-based (GGA+U, with U=5.5 eV [1]) *ab-initio* calculations. The theoretical orientation was obtained by diagonalizing the dielectric tensor as calculated in the linear-response regime by the VASP code. For comparison we mainly concentrate on the static limit, $\omega \to 0$.

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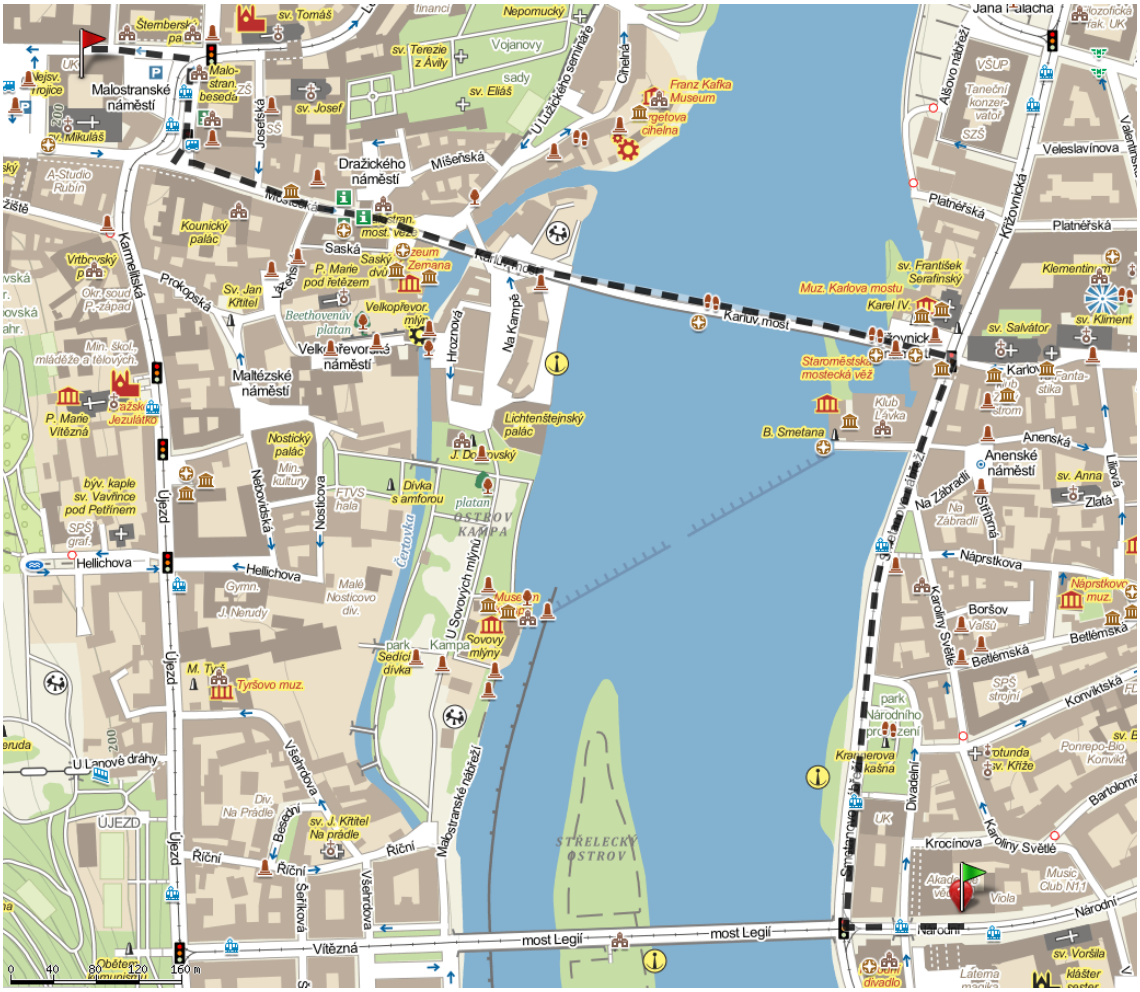
Maps



The conference takes place in the building of the Academy of Sciences of the Czech Republic, Narodni 3 (opposite to the National theater) in walking distance from the metro station Narodni (line B). The Academy building (tram stop Narodni divadlo) can be reached by tram No. 18 from the tram stop Hradcanska (near Vila Lanna).

The conference dinner will be served in the Restaurant Profesni dum, Malostranske namesti 25 (in the upper part of the square, the neighboring building of the St. Nicholas church). The map shows the walking route how to reach the restaurant, it is also possible to use the tram No. 22.

The Wednesday afternoon program will be organized at the Faculty of Mathematics and Physics of the Charles University, Ke Karlovu 5. There will be a small bus available for transport. The bus departure time is 13:45 and 14:00.