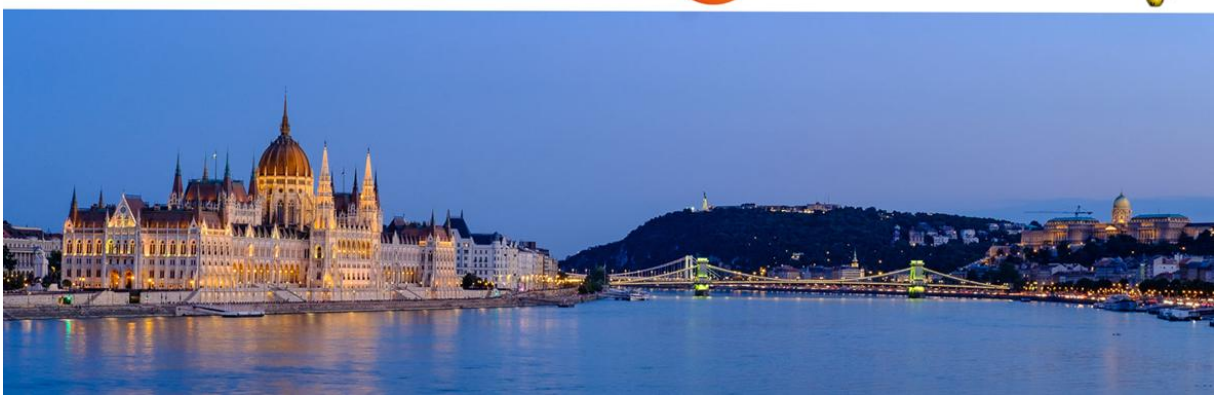
WE Heraeus Workshop on ab-initio methodologies for complex magnetism and magneto-superconductivity

15-18th September 2025,
Budapest, Hungary

MARTIN-LUTHER-UNIVERSITÄT HALLE-WITTENBERG

WILHELM UND ELSE HERAEUS-STIFTUNG

Psi-k Network



Program and Abstract Book

Program Overview

15.09. Monday	16.09. Tuesday	17.09. Wednesday	18.09. Friday
Arrival and registration	9:00-9:50 Hubert Ebert	9:00-9:50 Olle Eriksson	9:00-9:50 Christian Heiliger
	9:50-10:40 Jan Minar	9:50-10:40 Antonio Sanna	9:50-10:40 Stefan Blügel
	10:40-11:00 Coffee break	10:40-11:00 Coffee break	10:40-11:00 Coffee break
	11:00-11:50 Julie Staunton	11:00-11:50 Zeila Zanolli	11:00-11:50 Balázs Újfalussy
11:30-12:20 Rudolf Zeller	11:50-12:40 Stephen Dugdale Revealing the electronic	11:50-12:40 Tom G Saunderson	11:50-12:40 Gábor Csire
12:20-13:10 Markus Eisenbach	12:40-14:10 Lunch	12:40-14:10 Lunch	12:40-14:10 Lunch
13:10-14:30 Lunch	14:10-14:40 Flash poster presentations	14:10-15:00 Marjana Ležaić	Departure
14:30-14:40 Stefan Jorda			
14:40-15:30 Annica Black-Schaffer	14:40-16:00 Poster session	15:00-15:50 Tamio Oguchi	
15:30-16:20 Mario Cuoco	16:00-16:20 Coffee break	15:50-16:10 Coffee break	
16:20-16:40 Coffee break	16:20-17:40 Poster session	16:10-17:00 Anders Bergman	
16:40-17:30 Manuel dos Santos Dias		18:00-21:00 Conference dinner	

Abstracts

Forces and total energies in the KKR method

Rudolf Zeller

Peter-Grünberg-Institut, Forschungszentrum Jülich

The reasons will be identified that make the calculation of good forces and total energies and their consistent behavior in the KKR method difficult. It will be discussed how well the isoparametric integration scheme of Alam, Wilson and Johnson (PRB 84, 205106, 2011) can be used to solve these problems. A novel scheme leading to rapid convergence with the angular momentum channels taken into account will also be presented.

Scalable First Principles Multiple Scattering Calculations for Complex Material

Markus Eisenbach

National Center for Computational Sciences, Oak Ridge National Laboratory

Complex materials incorporating defects, disorder and chemical complexity can exhibit new and unexpected electronic and magnetic behavior that are of great fundamental and technological interest. Current high performance computer systems, such as Frontier at the Oak Ridge Leadership Computing Facility, are providing unprecedented opportunities for the quantitative exploration of these complex materials. Here I will present our implementation of multiple scattering theory for first principles density functional calculations. This approach directly obtains the single particle Green's function of the Kohn-Sham equation, either in reciprocal space (Korringa-Kohn-Rostocker i.e. KKR) or real space (Localy-Selfconsistent Multiple Scattering i.e. LSMS). The KKR method allows an efficient description of random solid solution alloys using the Coherent Potential Approximation (CPA), while our LSMS code allows for scalable large scale first principles density functional calculations of materials. A fundamental science driver for scalable, large scale, first principles calculations of materials is the need to understand states beyond periodic crystalline lattices. For large simulation cells, needed to describe extended electronic and magnetic orderings, defect states or disorder in alloys, the cubic scaling of traditional first principles methods have prevented direct calculations. The linear scaling nature of the LSMS ab initio code enables the treatment of extremely large disordered systems from the first principles using the largest parallel supercomputers available, such as calculations for O(10,000 – 1,000,000) atoms on current high performance computing architectures. For exascale systems, we have extended the use of accelerators to enable efficient calculations at scale. Additionally, we utilize the Kubo-Greenwood formalism for the linear response theory calculation of electric conductivity in these materials. The linear scaling nature of the LSMS ab initio code enables us to calculate the residual resistivity of large systems with complex order from first principles. Here we present calculations for pure elements and binary alloys, that we compare to both experimental results and first-principles effective medium methods (the Korringa-Kohn-Rostoker coherent potential approximation). Additionally, we will present calculations for concentrated solid solution alloys and quasicrystals.

These computational capabilities are available in our Multiple Scattering Theory suite (MuST) [https://github.com/mstsuite]

This work was supported in part by the Office of Science of the Department of Energy. This research used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

About the Wilhelm and Else Heraeus Foundation

Stefan Jorda

Wilhelm and Else Heraeus Foundation

Superconductivity in altermagnets

Annica Black-Schaffer

Uppsala University

Recently, a new form of magnetism, called altermagnetism, has been discovered, beyond the previously well-established ferro- and antiferromagnetism possibilities. Altermagnets break spin-degeneracy, as in a ferromagnet, but with a momentum dependent spin splitting resulting in zero net magnetization, as in antiferromagnets. Due to their unique magnetization, altermagnets also produce intriguing possibilities for other ordered phases of matter. Magnetism and superconductivity are two of the most celebrated quantum phases of matter and usually have a 'friend-foe' dichotomous relation, but combining superconductivity with altermagnetism turns out to open for new exceptional possibilities. In this talk I will show several novel effects occurring when superconductivity appears in an altermagnet, including finite momentum pairing, field-induced superconductivity, and a perfect superconducting diode effect, as well as demonstrate constraints on the possible superconducting pairing.

Superconducting orbitronics: phase engineering, magneto-electric and nonreciprocal effects

Mario Cuoco

CNR-SPIN, Università di Salerno

In this seminar, I will start presenting the concepts of orbital moments and orbital currents, and contextualize them within the framework of Cooper pairs. The common view of superconductivity centers on Cooper pairs, which can exist in either a spin singlet state or a spin triplet state. Typically, magnetic fields and magnetic materials are extensively utilized to convert spin singlet states into spin triplet states, serving both fundamental research purposes and applications for superconducting spintronics. In this context, I will pursue an entirely different approach by elucidating and demonstrating how to attain superconducting quantum states with high orbital angular momentum, thus prone to non trivial orbital magnetism. To achieve this goal, I focus on the importance of electrical and mechanical methods over magnetic forces in designing superconducting orbitronic effects. The use of orbital degrees of freedom introduces a completely new range of quantum phases and phenomena. For instance, I will discuss the electric-versus-magnetic dichotomy in superconductors by demonstrating that novel forms of non Abrikosov vortices can be generated using electric or strain fields rather than magnetic fields. I demonstrate that colossal magneto-electric effects can be achieved by exploiting the orbital Edelstein effect. For multiorbital superconductors orbital antiphase pairing and π-Josephson coupling can be effectively realized without violating time-reversal symmetry. Finally, I discuss nonreciprocal phenomena in the context of multiorbital and multicomponents superconductors.

From electronic structure to magnetisation dynamics

Olle Eriksson

Uppsala University

Magnon spectroscopy of complex magnetic materials from first principles

Manuel dos Santos Dias

STFC Daresbury

Magnons are the elementary collective excitations of magnetic materials. They make a fundamental contribution to their quantum and thermal properties and can act as spin carriers for emergent magnonic devices. This motivates their systematic experimental investigation using inelastic neutron scattering (INS) and more recently resonant inelastic x-ray scattering (RIXS), and the development of theoretical methods for determining and understanding their behaviour. In this talk, I will present results for selected materials that have been experimentally investigated, highlighting what can be learned even when the agreement between theory and experiment is less than quantitative and identified challenges for first-principles simulations.

Magnons are typically obtained from linear spin wave theory based on a specified spin Hamiltonian, with the respective exchange interaction parameters determined either by fitting to experiment or by first-principles simulations for the material of interest. For the latter, applying the infinitesimal rotation approach using the Korringa-Kohn-Rostoker Green function (KKR-GF) method is quite natural and has proven very successful [1], for instance using the full-potential relativistic implementation developed in Jülich [2].

The first example is Mn5Ge3, a harmless ferromagnetic unlike its cousin Mn5Si3 which is an antiferromagnet with a complicated phase diagram [3]. For Mn5Ge3 the simulations were performed prior to the INS experiment and made the crucial prediction that the magnon bands would be affected by the Dzyaloshinskii-Moriya interaction (DMI), despite its centrosymmetric space group. This was verified by INS and it was further shown that the magnon gap at the K-point of the Brillouin zone could be manipulated by applying an external magnetic field, providing experimental evidence for the DMI mechanism and its topological implications [4].

The second example is CrSb, a metallic altermagnetic with the potential to also exhibit a strong altermagnetic splitting of its magnon spectrum, lifting the degeneracy expected for collinear antiferromagnets. Its magnon properties were investigated with RIXS and a strong circular dichroism was found at the magnon peak, while the conventional x-ray magnetic circular dichroism vanishes. This was explained by a minimal theory relating the x-ray photons to the spin excitations, and complemented with KKR-GF calculations for its magnetic exchange interactions [5].

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[4] dos Santos Dias et al., Nat. Commun. 14, 7321 (2023); DOI:10.1038/s41467-023-43042-3

[5] Biniskos et al., arXiv:2503.02533 (2025)

Calculating response quantities using the KKR Green function formalism

Hubert Ebert

Ludwig-Maximilians-University Munich

Sergey Mankovsky

Ludwig-Maximilians-University Munich

Alberto Marmodoro

Czech Academy of Sciences

Ján Minár

University of West Bohemia

We demonstrate the use of the fully relativistic KKR multiple scattering Green function formalism to calculate response quantities for complex systems with an emphasize on effects caused by spin-orbit coupling and/or missing inversion symmetry. This very flexible approach allows in particular to account for the perturbation caused by a static or frequency dependent electric field that is reflected by corresponding changes of material properties.

Quantum Materials and Magnetic Phenomena Studied by Spin-Resolved ARPES: Theoretical perspectives

Ján Minár

University of West Bohemia

Quantum materials exhibit a complex interplay between electronic correlations, topology, and magnetism, placing them at the forefront of condensed matter physics and quantum technology. Understanding these systems requires disentangling spin-orbit coupling, electron-electron interactions, and magnetic fluctuations under realistic conditions, including finite temperatures and structural disorder. Spin- and time-resolved angle-resolved photoemission spectroscopy (STARPES) is a crucial technique for probing electronic and spin structures in magnetic and topological materials. However, quantitative interpretation of spin-ARPES data necessitates advanced theoretical models that accurately capture electronic states, spin textures, and dynamic responses to external fields.

I will present a theoretical framework based on the fully relativistic multiple-scattering Green function KKR method [1], effectively modeling spin-dependent photoemission. This approach includes correlation effects via dynamical mean-field theory (DMFT) [2] and describes spin fluctuations using the alloy analogy model [3]. I will also discuss advances in calculating light-induced electronic excitations [4], highlighting their relevance to spin-ARPES studies of topological and magnetic quantum materials.

A novel application is the one-step model of photoemission in studying altermagnets and kagome magnetic materials. Altermagnets, exhibiting unconventional time-reversal symmetry breaking without net magnetization, are explored in RuO2 and MnTe [5,6]. Spin-ARPES combined with the one-step model provides insights into lifted Kramers spin degeneracy, revealing their potential for spintronics. In kagome magnetic materials, persistent flat band splitting and selective band renormalization are observed in FeSn thin films [7], highlighting unique correlation effects and topological phenomena. These developments offer a comprehensive framework for exploring magnetic phenomena and spin dynamics in complex quantum materials.

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Statistical physics of multi-component alloys using the KKR-CPA

Julie B. Staunton

Department of Physics, University of Warwick

Christopher D. Woodgate

H. H. Wills Physics Laboratory, University of Bristol

We describe an ab initio theoretical framework for modelling compositional order in multicomponent alloys driven by the electronic structure. The theory is an extension of the S(2) theory developed for binary alloys and has its groundings in statistical physics and in the seminal papers on concentration waves authored by A.G.Khachaturyan, and by B.L.Gyorffy and G.M.Stocks. It is based on a Landau-type expansion of the free energy of the system and implemented with multiple scattering KKR techniques and the construct of an inhomogeneous effective medium (CPA) to carry out averages over atomic configurations. Effects on alloy electronic structure and on the rearrangement of charge, owing to an applied inhomogeneous chemical perturbation as ordering occurs, are fully included [1]. The inclusion of these effects is similar to the approach taken in Density Functional Perturbation Theory (DFPT), used to describe ab initio lattice dynamics and response functions for phonons, etc. We illustrate the approach via applications to the famous Cantor CrMnFeCoNi [2], AlxCrFeCoNi [3] and refractory VNbMoTaW [4] high entropy alloys.

We highlight the method's highly efficient and effective way of exploring the phase space of candidate multicomponent alloys and KKR Green function basis which enables the atomic short range order dependence of properties to be accessed. When compared to high-throughput calculations on supercells using DFT evaluations of energies, our method uses two orders of magnitude less CPU hours to discover the same physics. Furthermore, we report how the method can quickly generate representative configurations reflecting realistic atomic short-range order for subsequent study via further supercell DFT calculations. This approach has recently been demonstrated by training a machine-learned interatomic potential for the prototypical austenitic stainless steel, Fe7Cr2Ni4 [5] and FeNi alloys.

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Revealing the electronic structure of high-entropy alloys

Stephen B. Dugdale

University of Bristol

Although understanding the electronic structure and magnetism of so-called high- and medium-entropy alloys is crucial to developing a picture of the behaviour of the electrons in these materials, traditional experimental tools such as quantum oscillatory methods or angle-resolved photoemission are essentially precluded due to astonishingly short electronic mean free paths or the challenge of obtaining a suitable surface . Using experimental techniques such as Compton scattering, magnetic Compton scattering and x-ray magnetic circular dichroism, all in conjunction with first-principles calculations, it has been possible to reveal the underlying electronic structure and magnetism of these fascinating metallic alloys. Here, the results of our study of a range of fcc-based alloys are presented, including the manifestation of heavily smeared Fermi surfaces.

Electronic structure of superconducting nickelates from first-principles

Antia S. Botana

Arizona State University

The physics behind high-temperature superconductivity in the cuprates remains a defining problem in condensed matter physics. Among the myriad approaches to addressing this problem has been the study of alternative transition metal oxides with similar structures and electron count. After a 30-year quest, the first nickelate superconductor was discovered in 2019: hole-doped $NdNiO_2$. Given that this material is one of the members of a larger series (of so-called low-valence layered nickelates), this result opened up the possibility of uncovering a new family of superconductors. By means of first-principles calculations, we have analyzed the similarities and differences between this family of low-valence planar nickelates and the cuprates. Our results show that low-valence layered nickelates offer a new way of interrogating the cuprate phase diagram and are singularly promising candidates for unconventional superconductivity.

Ab initio methods for superconductivity beyond GW

Antonio Sanna

Max Planck Institute of Microstructure Physics

Martin Luther University Halle-Wittenberg

Camilla Pellegrini

Max Planck Institute of Microstructure Physics

Nature Publishing Group

Unlike encouraging results in hydrides under pressure, recent works seem to suggest that room temperature superconductivity at low pressure may be possible only with an unconventional pairing mechanism [1]. This calls for appropriate extensions of ab initio methods for superconductivity, which have traditionally focused on the prediction of superconducting critical temperatures (Tcs) and gaps in phononic superconductors. I will briefly discuss our extensions of Eliashberg theory and superconducting density functional theory (SCDFT) based on the GW approximation for the ab initio calculation of plasmonic effects on the superconducting properties [2, 3]. In both frameworks retardation effects in the phonon-mediated and screened Coulomb interaction are treated on the same footing by keeping their characteristic frequency dependence. I will then consider the problem of going beyond the GW approximation for the treatment of the Coulomb interaction in the superconducting state. This is in fact an unjustified and severely limiting approximation which neglects spin fluctuations effects, but is commonly adopted because the brute force inclusion of higher-order self-energy corrections would be computationally prohibitive. Our solution here consists in employing the Kukkonen and Overhauser (KO) ansatz for the Coulomb propagator W, which through dynamical local-field factors includes, in an effective yet rigorous way, electron-electron interactions mediated by both charge and spin density fluctuations, opening the path towards practical Tc and gap predictions for spin fluctuation mediated superconductors [4].

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Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code

Zeila Zanolli

Utrecht University

I this talk, we will present SIESTA-BdG [1], namely the theoretical development and code implementation of the simultaneous solution of the Bogoliubov-de Gennes (BdG) and density functional theory (DFT) problem in SIESTA, a first-principles method and code for material simulations which uses pseudopotentials and a localized basis set . This unified approach describes both conventional and unconventional superconducting states, and enables a description of inhomogeneous superconductors, heterostructures, and proximity induced superconductivity [2]. We demonstrate the validity, accuracy, and efficiency of SIESTA-BdG by computing physically relevant quantities (superconducting charge density, band structure, superconducting gap features, density of states) for conventional singlet (Nb, Pb) and unconventional (FeSe) superconductors [3]. We find excellent agreement with experiments and results obtained within the KKR-BdG computational framework. SIESTA-BdG forms the basis for modeling quantum transport in superconducting devices and including—in an approximate fashion—the superconducting DFT potential of Oliveira, Gross, and Kohn.

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First Principles Approches to Superconducting Orbitronics and their application to chirality

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Institute of Physics, Martin Luther University Halle-Wittenberg

Samir Lounis

Institute of Physics, Martin Luther University Halle-Wittenberg

To overcome the technological challenges of the age, new devices must be conceived which depart radically from the current state-of-the-art. Superconductors have recently shown promise, exhibiting diode behaviour [1], and dramatic spin-current enhancements [2]. Similarly, orbitronics dominates the physics of many device setups, eclipsing the efficiencies of spintronics [3]. Superconducting orbitronics (see e.g. [4]) enriched with chirality concepts provide an exciting playground for cryogenic applications but current methods fall short as most theory combining both superconductivity and orbitronics relies too heavily on model formulation. In this talk I will showcase our methodology which combines superconductivity in a first principles Green function-based formulation. Using this flagship method I will show our recent results combining superconductivity with broken inversion symmetry and chiral systems.

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Complex magnetism of orthorhombic iridates

Marjana Ležaić

Forschungszentrum Jülich

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Leonid Pourovskii

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Regina Dittmann

Forschungszentrum Jülich

In 5d transition-metal oxides, correlations and spin-orbit coupling meet at the same energy scale, creating optimal conditions for exotic physics, sensitive to various external stimuli. In perovskites, the interplay of relativistic phenomena and correlations has been intensively studied on the Ruddlesden-Popper series, Srn+1IrnO3n+1 which offers the opportunity to understand the formation of the relativistic jeff=1/2 state and a Mott gap, the changes of the correlation strength, the size of the gap, and the magnetic ordering for the different structures, defined by the number of the perovskite units, n, within the materials' unit cells.

We present our study of a 5d-transition metal oxide, CaIrO3, in the form of thin perovskite films grown on SrTiO3, employing a combination of ab-initio tools and the resonant inelastic X-ray scattering. The results indicate that the films likely lie in the semimetallic regime. Ordering of higher-order atomic magnetic multipoles, taking place at an unusually high temperature, is shown to play an important role in the formation of a small bandgap.

We will discuss the conditions necessary for stabilizing magnetism in this material as well as the importance of various approximations that are routinely applied in the codes based on the density functional theory for the treatment of transition-metal oxides.

Magnetocrystalline anisotropy in MnGa alloys

Tamio Oguchi

The University of Osaka

Magnetocrystalline anisotropy (MCA) is among the magnetic properties having fundamental significance and application importance. Its microscopic origin has long been interpreted closely linked to the orbital magnetic moment, but it has recently been pointed out that spin magnetic dipoles are more important in some magnetic materials. Tetragonal MnGa alloys are such a prototypical magnetic system showing large MCA despite negligibly small orbital moments of magnetic Mn ions [1]. In this study, the magnetic properties including MCA are investigated for the tetragonal MnGa alloys with several compositions by means of first-principles density-functional-theory calculations with the all-electron FLAPW method, especially by directly evaluating the spin magnetic dipoles [2]. In addition, MCA in MnGa with L10-type structure possessing interfaces with Fe layers is also examined with a view to device applications.

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Real-space descriptions of magnetic interactions and complex magnetism

Anders Bergman

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Broken symmetries and reduced dimensionality often provide an interesting and useful playground for complex magnetic behaviour; a standard example is the emergence of Dzyaloshinskii–Moriya interactions (DMI) in systems with broken inversion symmetry. This phenomenon also highlights the role that magnetic interactions play for a proper description of complex magnetic ground states and their magnetisation dynamics.

As this workshop emphasises, the theoretical exploration of complex magnetism is challenging, and it becomes even more demanding when impurities and disorder come into play. In this talk we will present recent applications and developments of a long-standing workhorse in this context: the real-space LMTO method.

Our examples include the observation of finite DMI in disordered Co/Pd multilayers; interdiffusion effects on magnetic interactions and magnetisation dynamics in Pd/Fe/Ir(111); configuration-dependent exchange and weak ferromagnetism in Mn_3Sn; and the extraction of spin–lattice coupling parameters in transition metals.

Electronic transport in magnetic materials

Christian Heiliger

Justus Liebig University Giessen

On the never-ending story of extracting effective tensorial spin Hamiltonians from ab initio

Stefan Blügel

Forschungszentrum Jülich

It has become common practice to map the energy landscape of the huge number of 2D and 3D magnets onto classical spin-lattice models with pairwise exchange interactions of the Heisenberg type, extended by the Dzyaloshinskii-Moriya interaction, single and two-ion anisotropy. This provides the basis for the study of their magnetic ground states, dynamics, magnon excitations, thermodynamics and phase diagrams. On the other hand, in the study of ultrathin magnetic films we witnessed additional interactions that had to be added to the established spin-models more and more often to explain the magnetic order (four-spin-three-site interaction [1,2], four-spin-four-site interaction [3], chiral-biquadratic interaction [4-7], topological chiral-chiral and spin-chiral interaction [8], etc.). This sounds like a very spontaneous unsatisfactory case-by-case procedure and it seems totally unclear whether all important interactions are captured or important ones are still missing. In this contribution, I present an attempt to derive systematically the spin Hamiltonian of all exchange interactions from the very general principle of indistinguishability of electrons in a many-electron system [9]. This provides a rigorous ansatz for reasonable spin-Hamiltonians without and with spin-orbit interactions whose expressions can be compactified in terms of tensorial interactions [10,11] and provide the starting point for energy functionals whose minimizer are topological spin-textures such as skyrmions, antiskyrmions etc.. The mapping of ab initio calculations onto the spin-models is far from trivial. Issues are e.g. the design of local and global spin models and the initial state dependence/bias of the model. I discuss here two approaches of mapping, one based on the total energy calculation of magnetic configurations [11] and one of the single particle energy using the LKAG approach [12, 13] in combination with a Green function method based on the Jülich KKR method [14].

Work was carried out in collaboration with Hiroshi Katsumoto, Juba Bouaziz and Yuriy Mokrousov.

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Proximity-Induced Superconductivity in Gd Layers on Nb: First-Principles Study with U term

Kyungwha Park

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Balázs Újfalussy

HUN-REN Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, H-1525 Budapest, Hungary

Orientation-Dependent Surface States in the Superconducting Phase of Sr_2RuO_4

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Yuri Fukaya

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The superconducting order parameter of Sr_2RuO_4 has remained elusive for decades. While it was long considered a prime candidate for chiral p-wave spin triplet pairing, recent reanalysis of Knight shift measurements has cast serious doubt on this interpretation. In our work, we present results from soft point-contact Andreev-reflection (PCAR) spectroscopy, which further contradict the chiral p-wave scenario. These spectroscopic features, undetected in earlier STM studies, reveal novel low-energy surface states inconsistent with previously proposed chiral p-wave pairing state.

To explain the new experimental observations, we introduce superconducting pairing models with dominant interorbital components which is crucial to account for the observed anisotropy of Andreev states. The calculated surface spectra based on this model show strong orientation dependence providing new constraints for theoretical models of the superconducting state. Moreover, to reproduce the experimental PCAR data, we solve the Dirac-Bogoliubov–de Gennes equations within a density functional theory framework. This provides a microscopic foundation for the proposed interorbital pairing state, validating its relevance to Sr_2RuO_4's unconventional superconducting phase.

Real-space mapping of Yu-Shiba-Rusinov states around magnetic defects on superconducting surfaces

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Interfacing magnetic impurities with superconductors generally gives rise to Yu-Shiba-Rusinov (YSR) bound states. Using first-principles, we study the case of Mn impurities deposited on a superconducting Ta (110) surface. We explore both the orbital nature and amplitude of the induced YSR states while investigating their spatial extent, which is characterized by an oscillatory and anisotropic behavior as function of distance with respect to the Mn impurities.In particular, we study the interplay of intrinsic electronic structure properties of the hosting superconductor and that of the impurities, which impacts the resulting "cloud" of YSR states.

We employ the Kohn-Sham Bogoliubov-de Gennes method within the all-electron full-potential relativistic Korringa-Kohn-Rostoker Green function method interfaced with the AiiDA infrastructure for high-throughput automation.

First principles analysis of Gd nanostructures on superconducting Nb(110)

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Yu-Shiba-Rusinov (YSR) states arising from magnetic atoms on superconducting surfaces can lead to Majorana zero modes (MZMs) at the end of magnetic chains, which offer the possibility for fault-tolerant quantum computing via topological qubits [1].

While magnetic transition metal (TM) chains on superconductors have been widely studied [2-4], rare-earth (RE) chains remain mostly unexplored, although partially filled 4f orbitals in RE elements can produce significantly stronger magnetic moments. This is particularly true for gadolinium (Gd), which exhibits a fully occupied 4f down spin channel and empty 4f up spin channel, maximising the magnetic moment. This strong magnetic moment can be used as a lever to influence the coupling between Gd atoms and the superconducting Nb substrate, offering unique opportunities to tune the YSR interactions towards the realisation of MZMs.

In this work, we used the Bogoliobov-de Gennes (BdG) formalism implemented in the Korringa-Kohn-Rostoker (KKR) method [5] to analyse Gd nanostructures - such as dimers and chains - on Nb(110) surface and study the underlying mechanism of the emergence of YSR states and zero modes. We explored the influence of Hubbard U correction, spin texture, and chain geometries on the YSR states profiles, and compared the results with experimental data [6].

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Spin and Orbital Polarization in WSe_2: Insights from Layer-Resolved Analysis

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Transition metal dichalcogenides (TMDs) such as WSe_2 exhibit strong spin-orbit coupling (SOC), leading to significant spin and orbital polarization effects. In this study, we investigate the band splitting and the contributions of spin and orbital magnetic moments at different energies and k-points in WSe_2, employing a layer-resolved approach.

Our results indicate that while the total signal remains weak, summing over individual layers reveals a strong polarization in both Sz and Lz. Furthermore, we explore how circularly polarized light interacts differently with spin states, and how light carrying orbital angular momentum (OAM) couples selectively to electronic states based on their orbital magnetic moment Lz [1,2,3]. This observation is crucial for understanding the role of (OAM) in TMDs and its potential impact in spintronic applications.

Controlling the electronic and magnetic properties of graphene superlattices

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Graphene is one of the 2D materials with excellent properties due to the presence of the Dirac cone. However, the lack of a band gap and intrinsic spin polarization limits its applications. The patterned vacancies with various symmetries were introduced periodically in the graphene superlattice. The intervalley coupling is needed in order to open the gap in graphene. The graphene with A=B vacancy can only open the gap if the superlattice size is 3n x 3n where n is the number of the repeating unit cell, and the vacancy contains C3 symmetry, such as C3, D3, D6. Other types of vacancy, like C1 and C2 cannot open the gap, but only cause the shift of the Dirac cone to the lower symmetry point. The band gap of a graphene with patterned vacancy is increasing with the defect concentration. On the other hand, the A ≠ B vacancy in graphene superlattices can induce a flat band, which is a sign of the presence of magnetic properties. The electronic and magnetic properties of graphene superlattice can be controlled by the rational guidelines that we established.

Realistic modelling of transport properties at finite tempeature in magnetic materials by local quantization of a Heisenberg model

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The quantitative description of the electrical resistivity of a magnetic material remains challenging to this day. Qualitatively, it is well understood that the temperature-induced lattice and spin disorder determines the temperature dependence of the resistivity. While prior publications reached good agreement with experiment in the so-called supercell or direct approach for non-magnetic materials where the spin-disorder contribution to the resistivity is negligible, an accurate, purely theoretical description of magnetic materials remains elusive. This shortcoming can be attributed to the missing accuracy in the description of the temperature-dependent spin-disorder itself. In this

work, we employ a joint approach from ab-initio transport calculations and atomistic modeling of the temperature-dependent spin-disorder. Using the example of α-Fe, we demonstrate that the inclusion

of quantum mechanical effects using a semiclassical local quantization of the Heisenberg model significantly improves the description of the spin-disorder component to the electrical resistivity. Compared to previous approaches, this model includes the description of magnetic short-range order effects, enabling us to study temperature effects around and above the Curie temperature, where prior mean-field theory-based approaches inevitably predicted a constant contribution.

MT6Z6 Kagome Compounds: phonon instabilities, CDW, flat bands, and magnetism

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Kagome materials exhibit a variety of rich physical properties due to the emergence of diverse electronic phases. AV3Sb5 has garnered substantial interest for its coexisting charge orders, superconductivity, and controversial time-reversal symmetry breaking. More recently, the bilayer kagome ScV6Sn6 has also drawn attention as it exhibits a charge density wave (CDW) with a distinct wave vector without superconductivity. This raises the question: What is occurring in bilayer kagome ScV6Sn6? Our work aims to unravel the mysteries of bilayer

kagome ScV6Sn6 and beyond, highlighting the rich physical properties induced by flat bands, potential CDW transitions, as well as their interplay with magnetism.

Strain engineering of magnetic exchange interaction in CrI_3 monolayer

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Monolayer CrI_3 has gained significant attention as a potential candidate for spintronic and topological magnonic technologies due to its inherent ferromagnetism and adaptable electronic characteristics. In this study we performed detailed ab initio simulations using density functional theory to explore how biaxial strain influences the magnetic properties of CrI_3 monolayer. The calculated exchange interactions reveal a strain-induced magnetic phase transition from a ferromagnetic to an antiferromagnetic ground state. Importantly, we demonstrate that biaxial strain affects the Dzyaloshinskii–Moriya interaction (DMI) both in magnitude and orientation. Overall, our findings shed light on strain-driven modulation of magnetism in CrI_3 monolayer and highlight the potential of strain engineering of future spintronic devices.

Ab-initio Investigation of YSR States of Fe Adatoms Interacting with Rashba-Split Surface States on BiAg2

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One of the most sought after topics in modern condensed matter physics research, has been the creation of topological superconductivity systems that are able to host Majorana states. A plethora of material configurations have been proposed to that end, with emphasis on the interplay between magnetism, SOC and superconductivity. Here, we investigate the behaviour of Fe adatoms deposited on a BiAg2 surface with a superconducting Nb substrate, using the Bogoliubov-de-Gennes full-potential relativistic Korringa-Kohn-Rostoker Green function method [1]. We explore the emergence of Yu-Shiba-Rusinov (YSR) states and their dependence on the adatom deposition site and magnetic moment rotation, as well as the effect of the strong spin-orbit coupling from the substrate. We construct chains of Fe adatoms and study the YSR state behaviour with an increasing chain length and its correlation with the magnetic ground state. Finally we explore the possibility of non-trivial end-states emerging on the Fe chain.

Ab-initio study of transition metal-superconductor interfaces

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The realisation of Majorana-based topologically protected qubits requires a careful design and optimization of material interfaces for superconductor (SC) / topological insulator (TI) heterostructures. To this end, we perform ab-initio simulations to investigate the superconducting properties at the interface of transition metal overlayers (M = Os, Ir, Pt, Au) deposited on a Nb(110) film. Our density functional theory calculations are based on the full-potential Korringa-Kohn-Rostoker (KKR) Green function method and its Kohn-Sham Bogoliubov-de Gennes (KS-BdG) extension [1, 2]. In our study we explore the possibility to control the work function mismatch through the overlayer, which is essential to overcome spurious band bending effect at typical SC/TI interfaces. Furthermore, we uncover the proximity induced superconductivity in the metal overlayers and discuss related details in their electronic structure. Our findings show that some of these structures might be promising material candidates for interfacing a TI with a superconductor without unwanted band bending effects at SC/M/TI interfaces.

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Quest for topological bands in magnetic chains on superconductors

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In magnetic chains placed on superconductors, Shiba bands are formed within the superconducting gap. Spin-orbit coupling or a spin-spiral configuration can lead to the hybridization of Shiba bands which can open a topologically non-trivial gap around the Fermi energy. Simple models are suitable to understand which effects assist the formation of topological band structure, but provide no recipe how this works out in real situations. To have a quantitative and realistic description of these systems, we solve the Kohn-Sham-Dirac Bogoliubov-de Gennes equations within the Korringa-Kohn-Rostoker multiple scattering theory. Elementary superconducting surfaces rarely support the appearance of a topological superconducting state, since either the superconducting gap or the spin-orbit coupling strength is small. By adding a non-magnetic overlayer between the superconductor and the chain, we explore the topological properties of a large variety of systems in terms of changing the crystallographic direction of the chain and the magnetic configuration.

Magnetic Anisotropy in CoPd Alloys and Ordered Structures: A First-Principles Study

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Understanding the magnetic anisotropy in magnetic materials is crucial for designing devices like sensors or data storages. In this work, we present ab initio density functional theory calculations of the magnetocrystalline anisotropy of Co_xPd_(1-x) alloys with varying concentrations and CoPd L1_0 ordered structures with different thicknesses of Co and Pd layers. For our calculatios, we employ the relativistic screened Korringa-Kohn-Rostoker Green's function method. The alloys are treated within the coherent potential approximation. Additionally, we explore the magnetic anisotropy of thin Co_xPd_(1-x) layers, considering both the magnetocrystalline and shape anisotropy. Our results provide valuable insights into the composition- and thickness-dependent magnetic properties of CoPd structures.

Ab-initio studies of chirality induced spin & orbital selectivity in linear response

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Relativistic KKR-GF calculations are used to gain insight on features of the electronic structure that are compensated in the ground state, but can manifest physical effects upon applying perturbations such as an electric field, in the regime of linear response or beyond it. The role of spin-orbit coupling and finite temperature are also examined, highlighting effects from the orbital degree of freedom and its robustness, stemming from the low-symmetry lattice structure of specific materials' families.

Electric polarization driven by non-collinear spin alignment in type II multiferroics based on first principles calculations

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We are going to discuss first principles calculations of the electric polarization induced by non-collinear magnetic order in insulating materials. While the electric polarization requires broken inversion symmetry, different mechanisms can be responsible for magnetically induced dipole moments in these materials, involving the relativistic spin–orbit coupling (SOC) or not, depending on the symmetry of the material (see, e.g., references in Refs. [1,2]). On a phenomenological level, this can be described by the expression for the polarization $\vec{P}$, ${P}^\nu = \sum_{ij,k}' [{P}^{0,\nu}_{ij,k} (\hat{s}_i\cdot \hat{s}_j) + {\vec P}^{1,\nu}_{ij,k} \cdot (\hat{s}_i\times \hat{s}_j)] +\sum_{i,k} \hat{s}_i {\underline \Pi}^{\nu}_{ii,k} \hat{s}_i$, with $\hat{s}_{i(j)}$ unit vectors along the magnetic moments on sites $i(j)$, symmetric and anti-symmetric polarization parameters, ${P}^{0,\nu}_{ij,k}$ and $\vec{P}^{1,\nu}_{ij,k}$, respectively, and 'single-site' polarization tensor ${\underline \Pi}^{\nu}_{ii,k}$.

However, in order to clarify the dominating mechanism of the induced polarization, first principles electronic structure calculations are required [2]. In our contribution we represent an approach for a calculation of the phenomenological parameters ${P}^{0,\nu}_{ij,k}$ and $\vec{P}^{1,\nu}_{ij,k}$, that gives information on the origin of the polarization in a particular material. We will discuss several examples using as prototype systems materials which belong to the family of triangular lattice antiferromagnets (TLA), as for instance CuFeO$_2$ and ACrO$_2$ with A = Li, Na, Cu, Ag, considering polarization as a consequence of different types of spin spirals. We present also the results of calculations on spin lattice interactions for these materials, which are responsible for the stabilization of the helimagnetic structure in frustrated TLA and are closely connected with the polarization caused by the atomic displacements [3].

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Reconstruction of NiO's Electron Momentum Density via Compton Scattering

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NiO is the poster-child for strongly correlated oxide materials. Despite the partially filled Ni 3d shell, NiO exhibits insulating anti-ferromagnetic behaviour. Conventional electronic structure methods, such as Density Functional Theory (DFT), fail to capture its insulating ground state, often predicting a metallic phase instead. This has prompted the application of beyond-DFT methods such as DFT+U and DFT + Dynamical Mean Field Theory (DFT+DMFT). Although these approaches ameliorate some of the predictions, such as getting the correct band gap, experimental data which captures the essence of the ground state many-body wavefunction is vital. Compton Scattering is a unique experimental technique as it directly probes the electron momentum density, offering a direct probe of the ground state many-body wave function. Here we present the electron momentum density for NiO reconstructed from a series of profiles measured at the SPring-8 synchrotron in Japan and consider how closely the different computational frameworks match the experiment, and highlight the challenges which remain.

Spin model of graphene triangulenes embedded in hexagonal boron nitride

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We are investigating triangulene shaped substitutional defects in hexagonal boron nitride filled with carbon atoms. We show how the triangulene shaped defects encompass magnetic moments and with ab initio methods we build Heisenberg like classical spin models representing their interactions. We show how different lattice terminations and sizes impact the magnetic properties of the system.

Probing the semiconductor-to-Dirac semimetal transition in Na-Sb-Bi alloys via Compton scattering

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We investigate the semiconductor-to-Dirac semimetal transition in Na-Sb-Bi alloys using x-ray Compton scattering experiments, combined with first-principles modeling of the electronic structure using the coherent potential approximation within the fully relativistic, full potential Korringa-Kohn-Rostoker method implemented in the SPRKKR package. A robust signature of the semiconductor-to-Dirac semimetal transition is identified in the spherically averaged Compton profile. We demonstrate how the number of electrons involved in this transition can be estimated to provide a descriptor for quantifying the strength of spin-orbit coupling responsible for driving the transition. Our study also shows the sensitivity of the Compton scattering technique toward capturing the spillover of Bi relativistic states onto Na sites.

Ab-initio exploration of complex magnetism of frustrated Mn and Cr films on hexagonal metallic surfaces

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We employ ab initio first-principles simulations to explore the complex magnetic behavior in antiferromagnetic (AFM) systems. Specifically, we investigate Mn films on an Ag(111) substrate, where spin-polarized STM experiments established Néel order as the ground state for a single Mn layer [1,2] in contrast to previous predictions. Our focus extends to the interplay of Heisenberg exchange interactions, leading to magnetic frustration, and higher-order magnetic interactions when increasing the thickness of Mn films, which can host complex three-dimensional AFM spin-textures. Additionally, we examine the magnetic properties of multiple AFM Cr layers deposited on a PdFe bilayer supported by an fcc Ir(111) substrate. Instead of being in a Néel state, a single Cr layer prefers a row-wise AFM state, which hosts single and catenated intrinsic AFM skyrmions [3]. For thicker Cr films, we monitor the emergence of new topological magnetic objects.

Neutron scattering spectra of dinuclear copper compounds from first principles

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Dimeric compounds with their antiferromagnetically coupled pairs of spins have been of fundamental interest in solid-state magnetism during the past century, recently revived by the discovery of their bosonic state with a high-temperature quantum phase transition. Experimentally, the exchange coupling between dimeric atoms can be unambiguously probed by inelastic neutron scattering (INS). In this work, we calculate the ground-state electronic structure of the prototypical dimer copper acetate monohydrate and derive its INS spectra, showing an excellent agreement with experiment. We provide the tools for the calculation of first-principles neutron scattering spectra as an open-source python package which can be applied to any dimeric compound in general.

Magnetism and its impact on atomic arrangements in substitutional alloys: Concentration wave analyses within the KKR-CPA

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Alloy phase diagrams—describing the equilibrium phase(s) of mixtures of two or more elements as a function of temperature and composition, usually at ambient pressure—are indispensable in materials science. This is because the nature of atomic arrangements in an alloy plays a key role in determining nearly all physical properties for applications. Considerable effort has been exerted into developing robust theories and computational methodologies capable of predicting the equilibrium phase(s) of an alloy within the framework of first-principles electronic structure calculations. In such models, it is routinely assumed that alloys containing magnetic elements such as Ni, Fe, and Co can be modelled in their (ordered) magnetic ground state. In reality, however, much materials processing takes place at temperatures well above many alloys' Curie temperatures, meaning this assumption is not well-justified. Here, using a novel analysis technique based on the KKR-CPA and using 'concentration waves' to describe atomic-scale chemical fluctuations [1], we demonstrate that the magnetic state of an alloy can have a profound impact on predicted phase diagrams. Using both binary systems such as FeNi [2], as well as multicomponent systems such as CrCoNi [3] as test cases, we compare results of concentration wave analyses performed on the alloys simulated in non-magnetic, ferromagnetic, and paramagnetic states, where the paramagnetic state is described via application of the disordered local moment (DLM) picture. We demonstrate that the nature of predicted chemical ordering, as well as the temperature at which it emerges, is significantly affected by the simulated magnetic state. These results have profound implications for the materials simulation community, as well as for experimentalists, by suggesting that atomic ordering in some alloys may by 'tunable' following application of a magnetic field during the annealing process.

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Ab initio study of magnetic and transport properties of compensated ferrimagnetic Heusler alloys at finite-temperatures

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Fully compensated ferrimagnets are promising materials for spintronics applications from the viewpoints of suppressing stray magnetic fields and high-density integration for memory applications due to net zero magnetization. In particular, Heusler alloys with 24 valence electrons per unit cell have been attracting attention because they can simultaneously achieve a half-metallic electronic structure with nearly 100% spin polarization at the Fermi level and fully compensated ferrimagnetism at a finite temperature.

For practical use in spintronics devices, it is important to exhibit such excellent magnetic properties at room temperature or above. In this study, we developed ab initio spin fluctuation theory at finite-temperatures based on the coherent potential approximation and disordered local moment and we applied this theory to fully compensated Heusler alloys and investigated the temperature dependence of the electronic structure, magnetic properties, and electrical conductivity from the first-principles approach.

In this presentation, we will report these results and discuss future prospects.