

# WE-Heraeus

## Green function workshop 2023

### Athens

*First-principles Green function formalisms:  
algorithms, method developments and  
applications to spinorbitronics and magneto-  
superconductivity*



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## General Information

### About the workshop

#### **First-principles Green function formalisms: algorithms, method developments and applications to spinorbitronics and magneto-superconductivity**

4 September -7 September 2023, Athens, Greece

Generously supported by the [WE-Heraeus Foundation](#) and the [Psi-k charity](#).

#### **Objectives**

This workshop aims to bring together the community in the field of first-principles approaches to magnetism, spintronics and superconductivity. The plan is to discuss fundamental challenges at the method development level, and promote the exchange of ideas and stimulating new research directions with a focus on:

- Method developments for first-principles approaches using Green functions
- Superconductors interfaced with magnetic and topological materials
- Open issues in simulation of complex magnetic materials, chiral and topological concepts
- Magneto-transport properties and dynamics in the presence of superconductivity
- High-performance computing algorithms and codes for data science and exascale

Workshop website: <https://go.fzj.de/gf2023>

#### **Organisation Committee**

- Dr. Philipp Rüßmann, University of Würzburg and Forschungszentrum Jülich, Germany
- Dr. Manuel dos Santos Dias, STFC Daresbury Laboratory, United Kingdom
- Prof. Samir Lounis, Forschungszentrum Jülich, and University of Duisburg-Essen, Germany
- Prof. Phivos Mavropoulos, National and Kapodistrian University of Athens, Greece

### Code of Conduct

Adapted from the [code of conduct of the carpentries](#).

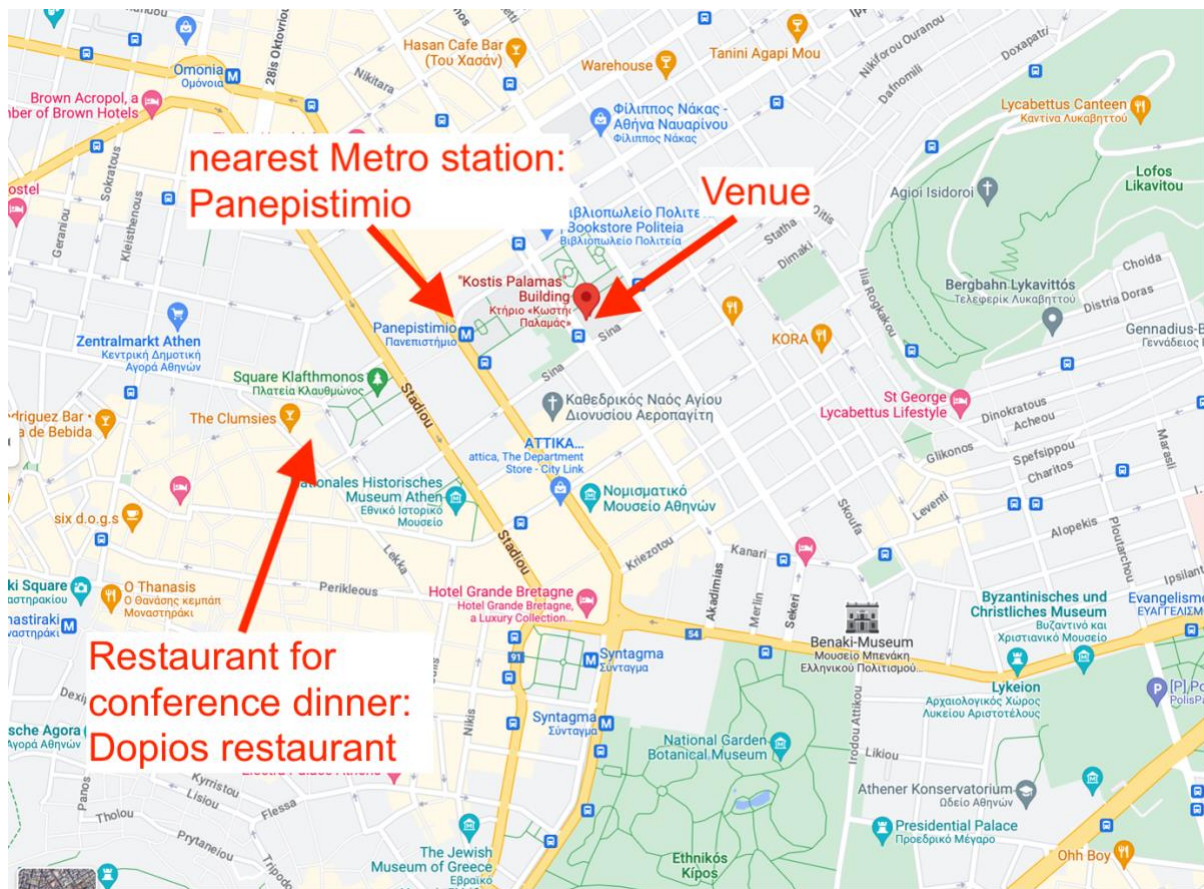
We are dedicated to providing a welcoming and supportive environment for all people, regardless of background or identity. By participating in this workshop, participants accept to abide by the Code of Conduct and accept the procedures by which any Code of Conduct incidents are resolved. Any form of behaviour to exclude, intimidate, or cause discomfort is a violation of the Code of Conduct. In order to foster a positive and professional workshop environment we encourage the following kinds of behaviours:

- Use welcoming and inclusive language
- Be respectful of different viewpoints and experiences
- Gracefully accept constructive criticism
- Focus on what is best for the community
- Show courtesy and respect towards other community members

If you believe someone is violating the Code of Conduct, we ask that you report it to the workshop organizers, who will take the appropriate action to address the situation.

## Venue

The workshop takes place at the [Kostis Palamas Building, 48 Akadimias & Sina Str, 10562 Athens, Greece](https://en.uoa.gr/about_us/services_units/kostis_palamas_building) ([https://en.uoa.gr/about\\_us/services\\_units/kostis\\_palamas\\_building](https://en.uoa.gr/about_us/services_units/kostis_palamas_building)).



## Conference Dinner

The conference dinner (Wednesday evening) takes place in the [Dopios restaurant](#).

## Program

|                                       | Monday, 4.9.2023       |                  | Tuesday, 5.9.2023  |            | Wednesday, 6.9.2023 |              | Thursday, 7.9.2023      |            |
|---------------------------------------|------------------------|------------------|--------------------|------------|---------------------|--------------|-------------------------|------------|
| 09:00 - 11:00 am                      |                        |                  | Ultrafast Dynamics | Delin      | Complex Magnetism   | Mankovskyy   | SC + Magnetism          | Saunderson |
|                                       |                        |                  |                    | Ebert      |                     | AbuAwwad     |                         | Ujfalussy  |
|                                       |                        |                  |                    | Henk       |                     | Bouaziz      |                         | Aceves     |
|                                       |                        |                  |                    | Ziolkowski |                     | Palotas      |                         | Nyári      |
| coffee break<br>11:00 - 11:30 am      |                        |                  | coffee break       |            | coffee break        |              | coffee break            |            |
| 11:30 am - 1:00 pm                    | arrival & registration |                  | Beyond DFT I       | Jackson    | Spin-orbitronics    | Belashchenko | Beyond DFT II           | Biermann   |
|                                       |                        |                  |                    | Aguilera   |                     | Szunyogh     |                         | Minar      |
| lunch & discussions<br>1:00 - 2:30 pm |                        |                  | lunch              |            | lunch               |              | lunch                   |            |
| 2:30 pm - 4:00 pm                     | Spin-orbitronics       | Opening          |                    | Wasmer     |                     | Paischer     | Round table discussions |            |
|                                       |                        | Kioussis         | Poster session I   |            | Poster session II   |              |                         |            |
|                                       |                        | Sipr             |                    |            |                     |              |                         |            |
| coffee break<br>4:00 - 4:30 pm        | coffee break           |                  | coffee break       |            | coffee break        |              | departure               |            |
| 4:30 - 6 pm                           | Superconductivity      | van Schilfgaarde | Towards Exascale   | Zeller     |                     | Bajaj        |                         |            |
|                                       |                        | Park             |                    | Eisenbach  | Marrazzo            |              |                         |            |
|                                       |                        |                  |                    |            | conference dinner   |              |                         |            |

## Presentation Abstracts – Monday

### Opportunities and Challenges in Spintronics: A first principles perspective

Nicholas Kioussis ([nick.kioussis@csun.edu](mailto:nick.kioussis@csun.edu))

*California State University Northridge, USA*

I will review our computational developments during the past decade to explore several open questions and provide guiding rules for the design of ultra-low energy spintronic devices. (1) Exploit the large spin orbit coupling and emergence of magnetism in ultrathin heavy-metal-based ferromagnetic (FM) or antiferromagnetic (AFM) heterostructures to achieve large perpendicular magnetic anisotropy and high voltage-controlled magnetic anisotropy efficiency, the two major challenges for ultralow-power and high density nonvolatile MeRAM devices; (2) Employ the effect of alloying or phonons to enhance the charge-to-spin current conversion efficiency in nonmagnetic heavy metals; (3) Dynamically control both the direction and amount of current-induced spin accumulation at heavy metal/FM interface using an electric field in an oxide capped spin orbit torque device; and (4) Search and identify novel two-dimensional van der Waals Dirac half-metal magnets characterized by a band structure with a large gap in one spin channel and a Dirac cone in the other with carrier mobilities comparable to those in graphene. This research was supported by NSF-PREM Grant No. DMR-1205734 and NSF Grant No. ERC TANMS-116050.

### Comparing magnetotransport properties of doped alloys and doped crystals

Ondrej Sipr ([sipr@fzu.cz](mailto:sipr@fzu.cz))

*FZU - Institute of Physics, Czech Acad. of Sci., Czech Republic*

The description of magnetotransport has so far focused on how doping influences clean crystals. However, interest is turning also to substitutional alloys as hosts. Our aim is to investigate to what extent the approaches that proved to be useful for doped crystals can be applied to doped alloys. Calculations are performed for permalloy  $\text{Fe}_{19}\text{Ni}_{81}$  doped with V, Co, Pt, and Au impurities, relying on the Kubo-Bastin equation implemented using the KKR-Green function method.

The dependence of the anomalous Hall and spin Hall conductivities on the dopant concentration is nonmonotonic and strongly influenced by the temperature. The fact that the host is disordered and not crystalline has profound influence on how the conductivities depend on the dopant concentration. In particular, off-diagonal anomalous Hall and spin Hall conductivities are not proportional to the diagonal charge conductivity for low dopant concentrations. Consequently, the dependence of the anomalous Hall effect and spin Hall effect on the dopant concentration cannot be ascribed unambiguously to skew scattering, side-jump scattering, or intrinsic contributions in the same way as it can be done when investigating the effect of doping for a crystalline host, i.e., the standard scaling laws do not apply.

## Ab initio description of unconventional superconductivity

Mark van Schilfgaarde ([mark.vanschilfgaarde@nrel.gov](mailto:mark.vanschilfgaarde@nrel.gov))

*National Renewable Energy Laboratories, MCCS, USA*

Approaches to Green's function methods largely divide into two tracks: low-order many-body perturbation theory (MBPT), applicable to systems with weak or moderate correlations, and nonperturbative methods such as Dynamical Mean Field Theory (DMFT), where the independent particle picture is no longer adequate but the vertex is assumed to be local.

I show recent progress in joining MBPT with DMFT to characterize one- and two- particle spectral functions with much higher fidelity than either separately, or with DFT+DMFT. Within the DMFT framework, a nonlocal vertex is constructed from the local two-particle Green's function generated from DMFT. This yields momentum-dependent response functions and provides a path to examine instabilities towards spin- or charge- mediated superconductivity.

One finding the two tracks that evolved historically corresponds to a natural division among phenomena between high-energy charge fluctuations and low-energy spin fluctuations. Provided a sufficiently good starting point is taken, low-order MBPT can describe with remarkable accuracy a wide range of materials provided spin fluctuations are not strong. When they become strong, as in the unconventional superconductors, spin fluctuations drive low-energy, mostly local correlations that give rise to exotic phenomena.

These points are illustrated by describing a range of properties in different classes of materials, including some unconventional superconductors.

## First-principles studies of proximity superconductivity and Yu-Shiba-Rusinov states

Kyungwha Park ([kyungwha@vt.edu](mailto:kyungwha@vt.edu))

*Virginia Tech, Department of Physics, USA*

Superconductivity combined with topology in the reciprocal space has brought many interesting ideas including topological or triplet superconductivity and Majorana zero modes. Spin-orbit coupling plays a key role in inducing topological superconductivity. So far, most of theoretical studies on this have been carried out using effective models based on a single band with artificial parameters. Recently, the Dirac-Bogoliubov-de Gennes equations have been solved considering first-principles band structures and relativistic effects including spin-orbit coupling, within the multiple scattering Green's function methodology [Csire et al., Phys. Rev. B 97, 024514 (2018); Nyari et al., Phys. Rev. B 104, 235426 (2021)]. We apply this first-principles approach to topological-insulator superconductor heterostructure, finding several induced superconducting (SC) gaps in the topological insulator (TI) at different momenta when the chemical potential crosses the TI conduction band region [Park et al., Phys. Rev. B 102, 134504 (2020)]. The induced SC gap arising from the top TI surface state is almost zero, and the induced SC gap size depends on degree of hybridization with the SC substrate. Furthermore, we apply the first-principles approach to single magnetic adatoms on a strongly spin-orbit coupled s-wave superconductor such as Pb, showing a strong dependence of the Yu-Shiba-Rusinov (YSR) states on the orientation of the adatom magnetic moment [Park et al., New J. Phys. 25, 033022 (2023)]. We find that the deepest YSR states can merge into a zero-energy state with strong spin polarization, although the zero-energy state is topologically trivial. The calculated YSR states are compared to experimental data.



## Presentation Abstracts – Tuesday

### Ultrafast spin dynamics and spin-lattice interactions

Anna Delin ([annadel@kth.se](mailto:annadel@kth.se))

*KTH, Applied Physics, Sweden*

The interaction of ultrafast laser pulses with magnetic materials can induce complex spin dynamics, both during and after the laser pulse. One example is the recently demonstrated ultrafast Einstein-de Haas effect, in which angular momentum lost from the spin system upon laser-induced demagnetization of ferromagnetic iron is transferred to the lattice on sub-picosecond timescales. Another example is the optical intersite spin transfer (OISTR) effect. In this talk, I will give a brief overview of ultrafast spin dynamics, discuss the role of angular momentum transfer between the spin and lattice subsystems, and present our recent work on computing spin-lattice couplings from first principles.

### Variation of magnetic model parameters during ultrafast demagnetisation

Hubert Ebert ([Hubert.Ebert@cup.uni-muenchen.de](mailto:Hubert.Ebert@cup.uni-muenchen.de))

*Ludwig-Maximilians-University Munich, Department of Chemistry, Germany*

Recent developments in time-dependent density functional theory (TD-DFT) paved the way towards investigating the ultrafast demagnetisation caused by a strong laser pulse on an ab initio level. However, the relaxation processes after a pump pulse still require to use phenomenological models that allow to account for different types of relaxation mechanisms on the basis of model parameters, that can be calculated from first principles. A stumbling block for such schemes is that the electronic structure is strongly out of equilibrium after the laser pulse and changes with time due to the relaxation. In the present work, we explore whether the parameters which determine the magnetization dynamics in this time regime can indeed be described on a first-principles level. This concerns first of all the exchange coupling, magnetic anisotropy and the Gilbert damping parameters that have been calculated for several transition metals using the spin-polarized relativistic Korringa-Kohn-Rostoker method. To account for the time evolution of the system, the calculations have been performed employing the TD-DFT potentials and occupation numbers generated by the Elk code [<http://elk.sourceforge.net>] for different time steps during the laser pulse and shortly after it, i.e. in the non-relaxed situation. In all cases a strong modification of the parameters compared to the equilibrium situation is found.

### Ultrafast Orbital Hall Effect in Metallic Nanoribbons

Jürgen Henk ([juergen.henk@physik.uni-halle.de](mailto:juergen.henk@physik.uni-halle.de))

*Martin Luther University Halle, Institute of Physics, Germany*

The orbital Hall effect in metals has been extended into the femtosecond time domain. In this theoretical study, we investigate the orbital angular momenta and their currents induced by a femtosecond laser pulse in a Cu nanoribbon. Our numerical simulations provide detailed insights into the laser-driven electron dynamics on ultrashort timescales with atomic resolution. The ultrafast orbital Hall effect described in this work is consistent with the familiar pictorial representation of the static orbital Hall effect, but we also find pronounced differences between physical quantities that carry orbital angular momentum and those that do not. For example, there are deviations in the time

series of the respective currents. This study lays the foundations for investigating ultrafast Hall effects in confined metallic systems.

## Exploring Pathways to Ultrafast Demagnetization: Simulations with a Real-Space Tight-Binding Model

Franziska Ziolkowski ([franziska.ziolkowski@physik.uni-halle.de](mailto:franziska.ziolkowski@physik.uni-halle.de))  
*Martin Luther University Halle, Institute of Physics, Germany*

Ultrafast demagnetization (UFD) is a highly promising and rapidly evolving field of research, characterized by the rapid quenching of magnetization upon excitation with a femtosecond laser pulse. This phenomenon encompasses diverse underlying processes and theoretical approaches that are crucial for understanding UFD. To bridge the gap between various time and length scales as well as between microscopic and empirical approaches we introduce EVOLVE, our novel real-space tight-binding model. EVOLVE provides a powerful framework for investigating microscopic processes and spin transport within inhomogeneous samples. In this study, we delve into the dynamics of demagnetization and examine the spin currents generated by inhomogeneous excitations, particularly at interfaces between ferromagnetic and nonmagnetic regions. Additionally, we incorporate a method to simulate initial disorder by introducing static noncollinearity. Through our comprehensive analysis, we shed light on the intricate mechanisms governing UFD in various magnetic materials.

## Quasiparticle self-consistent GW in Questaal

Jerome Jackson ([jerome.jackson@stfc.ac.uk](mailto:jerome.jackson@stfc.ac.uk))  
*STFC Daresbury Laboratory, Scientific Computing, United Kingdom*

Quasiparticle self-consistent GW (QSGW) provides a reliably accurate single-particle description of a wide range of materials, ranging from simple semiconductors to strongly correlated transition metal oxides. Quasiparticle self-consistency avoids the starting point dependence inherent in single-shot GW by building a single-particle potential as close as possible to the true GW self-energy. This obviates the need for empirical methods based on correcting density functional theory such as DFT+U. A recent extension of QSGW by the inclusion of ladder diagrams in the evaluation of the screened Coulomb interaction, thereby adding the most important diagrams missing in GW, will be shown to yield extremely accurate results. The talk will give an introduction to the Questaal code project and a discussion of the strengths and limitations of QSGW.

## Quasiparticle methods for functional materials with heavy elements

Irene Aguilera ([i.g.aguilera@uva.nl](mailto:i.g.aguilera@uva.nl))  
*University of Amsterdam, Institute for Theoretical Physics, The Netherlands*

Many-body perturbation theory (MBPT) has proven track record of predictive power for properties of topological materials. In this class of materials, an intricate interplay of crystal field effects, electronic correlations, and strong spin-orbit coupling (SOC) is key for the richness of physical effects they present.

I will discuss the relativistic quasiparticle self-consistent GW method (QSGW) and I will illustrate the method using the example of the elementary (non-radioactive) crystal with strongest spin-orbit coupling: Bi. I will concentrate on topological phase transitions (TPT) that are specially challenging for ab initio methods because the well-known underestimation of band gaps in DFT translates into an

overestimation of the inverted band gaps of non-trivial materials. I will outline our current theoretical and experimental efforts to induce not only a TPT in Bi, but also a semimetal to semiconductor (SMSC) transition by a combination of strain and Sb doping.

The SPEX code uses time-reversal symmetry to improve the efficiency of the calculations. However, in systems with non-collinear magnetism, such as *magnetic* topological insulators, the time-reversal symmetry is broken. As an outlook, I will discuss the consequences and challenges for an implementation.

## Benchmark study of symmetry-adapted ML-DFT models for magnetically doped topological insulators

Johannes Wasmer ([j.wasmer@fz-juelich.de](mailto:j.wasmer@fz-juelich.de))

*Forschungszentrum Jülich, Institute of Advanced Simulation, Germany*

We present a benchmark study of surrogate models for impurities embedded into crystalline solids. Using the Korringa-Kohn-Rostoker Green Function method [1], we have built databases of several thousand calculations of single impurities (monomers) embedded into different elemental crystals, as well as magnetic transition metal impurity dimers embedded in the topological insulator Bi<sub>2</sub>Te<sub>3</sub>. We predict the converged monomer impurity electron potential and the isotropic exchange interaction of the impurity dimer in the classical Heisenberg model. From these surrogates, we intend to build transferable models for larger systems in the future, which will accelerate the convergence of our DFT codes. The study compares various recent E(3)-equivariant models such as ACE and MACE [2] in terms of performance and reproducible end-to-end workflows.

[1] P. Rüßmann *et al.*, npj Comput Mater **7**, 13 (2021)

[2] I. Batatia *et al.*, arXiv:2206.07697 (2022)

## Green-function density-functional calculations for a million atoms: algorithmic developments

Rudolf Zeller ([ru.zeller@fz-juelich.de](mailto:ru.zeller@fz-juelich.de))

*Forschungszentrum Jülich, Institute for Advanced Simulations, Germany*

In my talk I will show that the Korringa-Kohn-Rostoker Green-function method is suitable in density-functional calculations for supercells with more than 100000 atoms if modern supercomputers are used. I will describe our massively parallel code KKRnano developed in Jülich, the mathematical basis of the code and the solution of problems encountered when approaching exascale computing. I will argue that such calculations require pronounced speedups for the self-consistency iterations and for the calculation of the Hartree (Coulomb) potential and show how this is achieved. As an example I will present total-energy results for a vacancy in Cu investigating the convergence in supercells with up to a million atoms.

## Large scale first principles materials calculation using multiple scattering theory

Markus Eisenbach ([eisenbachm@ornl.gov](mailto:eisenbachm@ornl.gov))

*National Center for Computational Sciences, Oak Ridge National Laboratory, USA*

The effect of disorder in materials is of great fundamental and technological interest. 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 (Locally-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  $O(10,000 - 100,000)$  atoms on current high performance computing architectures. For exascale systems, we have extended the use of accelerators to enable the efficient calculation for embedding methods and forces. Currently ongoing work focuses on the calculation of electric conductivity in the presence of disorder and defects. We will present first results of our LSMS in calculating resistivities in solid solution alloys and in metallic glasses.

While DFT calculations have proven to be a useful tool in the study of ground state properties of many materials, we will go beyond the ground state by describing an approach to utilize machine learning methods to combine first principles density functional calculations with classical Monte-Carlo simulations to investigating the statistical mechanics of materials. The investigation of finite temperature properties relies on the possibility of a large number of evaluations of the system's Hamiltonian that are required to sample the phase space needed to obtain physical observables. We have demonstrated a solution to this problem that harnesses the computational power of large massively parallel computers by combining classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) by employing Machine Learning techniques. The combination of LSMS with a machine learning workflow, that can consider both classical interaction models and artificial neural network based models, allows us to investigate alloy ordering transitions for increased simulation cell sizes. Our approach is able to sample both magnetic or chemical order, allowing the first principles calculation of order/disorder phase transitions and phase separations in alloys.

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 and by the Laboratory Directed Research and Development (LDRD) Program of Oak Ridge National Laboratory. 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.

## Presentation Abstracts – Wednesday

### Multi-site expansion of the Heisenberg Hamiltonian within the KKR Green function formalism

Sergiy Mankovsky ( [Sergiy.Mankovsky@cup.uni-muenchen.de](mailto:Sergiy.Mankovsky@cup.uni-muenchen.de) )  
*Ludwig-Maximilians-University of Munich, Chemistry, Germany*

The higher-order terms of the extended Heisenberg Hamiltonian accounting for the multi-spin multi-site exchange interactions can lead to new physical effects. The corresponding parameters can only be provided by first-principles electronic structure calculations. Various approaches have been suggested for their estimation. I will discuss a scheme to map the exchange interactions based on spin-density-functional theory onto the extended Heisenberg Hamiltonian making use of the multiple-scattering Green's function formalism. In general, this approach gives access to all types of multi-spin interactions, while I will focus on three- and four-site interactions. Another type of the multi-site interactions I will discuss are the so-called spin-lattice interactions, which may be seen as a correction to the spin-spin interactions accounting for lattice distortions. The corresponding parameters give access to the magnon-phonon interactions, and their first-principles calculations may contribute for instance to the understanding of an angular momentum transfer between the spin and lattice degrees of freedom, properties of geometrically frustrated antiferromagnets, etc.

### Two-dimensional materials as a layer for topological magnetism in complex heterostructures

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The discovery of two-dimensional (2D) van der Waals magnetic materials and their heterostructures provided an exciting platform for emerging phenomena with intriguing implications in information technology.

Here, based on a multiscale modeling approach that combines first-principles calculations and a Heisenberg model, we demonstrate that interfacing a CrTe<sub>2</sub> layer with various Te-based layers enables the control of the magnetic exchange and Dzyaloshinskii-Moriya interactions as well as the magnetic anisotropy energy of the whole heterobilayer, and thereby the emergence of topological magnetic phases such as skyrmions and antiferromagnetic N'eel merons. The latter are novel particles in the world of topological magnetism since they arise in a frustrated N'eel magnetic environment and manifest as multiples of intertwined hexamer-textures. Our findings pave a promising road for proximity-induced engineering of both ferromagnetic and long-sought antiferromagnetic chiral objects in the very same 2D material, which is appealing for new information technology devices employing quantum materials.

### From magnetic frustration to novel spin textures and their magneto-transport signatures

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Itinerant magnets exhibit complex magnetic phases and can host exotic topological spin textures such as skyrmions. These spin textures are generally promoted by the Dzyaloshinskii-Moriya interactions. Recently, it was shown that long-range competing isotropic exchange interactions in centrosymmetric

Rare-earth intermetallic (REI) systems stabilize skyrmion lattices [1]. First, we investigate two prototypical REI,  $\text{GdRu}_2\text{Si}_2$  and  $\text{Gd}_2\text{PdSi}_3$  using a first principles approach, and show that Ruderman-Kittel-Kasuya-Yosida interactions between the Gd moments generate a helical single-Q state. Using atomistic spin-dynamical simulations, we study the effects of magnetic anisotropy and construct a general magnetic phase diagram that explains the stabilization of the 2Q-skyrmion lattice observed experimentally with applied magnetic fields [2]. Second, skyrmions imprint a characteristic signature on the Hall signal known as the topological Hall effect, allowing their detection using magnetotransport measurements. Relying on perturbation theory, we disentangle the multiple contributions to the Hall signal originating from non-collinear magnetism in presence of relativistic effects and breaking of inversion symmetry. We unveil a new contribution, the non-collinear Hall effect (NHE) [3], whose angular form is determined by the magnetic texture, the spin-orbit field of the electrons, and the underlying crystal structure. The NHE together with other components of the Hall resistivity enables the decoding of exotic non-collinear magnetic textures that have been observed in itinerant magnets.

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## Real-space nonlocal Gilbert damping from exchange torque correlation implemented into the KKR formalism

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The energy-dissipative damping process plays an important role in magnetization dynamics. The in-depth understanding of the magnetization damping is crucial for the development of spintronic applications in the future. For this reason, in this work we present an ab initio scheme based on linear response theory of exchange torque correlation, implemented into the real-space Screened Korringa-Kohn-Rostoker (SKKR) framework to calculate diagonal elements of the Gilbert damping tensor. The method is applied to bcc iron and fcc cobalt bulk systems and their (001)-oriented surfaces.

## Spin-orbit torques in disordered metallic bilayers and trilayers

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Current-induced spin-orbit torques enable electric control and switching of the magnetization which can be utilized in spintronic devices such as nonvolatile memory and tunable nano-oscillators. This talk will present the results of first-principles calculations of spin-orbit torques based on the nonequilibrium Green's function formalism [1]. Combined with supercell disorder averaging, this technique amounts to a computational experiment treating all transport mechanisms on equal footing. In Co/Pt bilayers such calculations revealed a large interfacial contribution to the dampinglike torque and a higher-order torque with a planar-Hall-like angular dependence [2]. In Co/Cu/Co trilayers with a Cu layer whose thickness is below the mean-free path, novel effects beyond the spin-diffusion theory were found, including the giant magneto-torque effect and a nonlocal torque with an unconventional angular dependence [3].

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## Electrically Driven Singlet-Triplet Transition in Triangulene Spin-1 Chains

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Simple spin models have played a key role in the formulation and comprehension of the basic principles of magnetism and statistical mechanics since the early days of quantum theory. The interest in these models and in the systems realizing them persists today due to their connection to many topological properties of matter, as well as their potential to become the building blocks of viable and robust quantum computers.

Recently, graphene triangulene (GT) chains have been synthesized and their magnetic response has been analyzed by STM methods by Mishra and coworkers [1]. Motivated by this study, we determine the exchange bilinear and biquadratic constants of the triangulene chains by calculating two-spin rotations in the spirit of the magnetic force theorem. We then analyze open-ended, odd-numbered chains, whose edge states pair up forming a triplet ground state. We propose three experimental approaches that enable us to trigger and control a singlet-triplet spin transition. Two of these methods are based on applying a mechanical distortion to the chain. We finally show that the transition can be controlled efficiently by the application of an electric field. [2]

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## First principles theory of electron-magnon scattering and the spin polarized electron energy loss spectroscopy

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Magnetic solids constitute a very important class of materials as they are extensively used in everyday life, e.g. in the electric energy generation and propulsion, medical imaging, and information storage, and are essential to many new technologies currently under development. In spite of their high relevance, some of the basic properties of magnetic materials still remain a mystery. One of those topics not fully understood is the interaction between the magnetic and electronic degrees of freedom in such materials. It leads to spin dependent lifetimes of electronic states and inelastic electron transport to name but a few.

In our current study we investigate the impact of magnetic excitations on the electronic spectrum of solids as well as the scattering of high energy electrons with magnetic materials to formulate an ab initio theory for the spin polarized electron energy loss spectroscopy (SPEELS). We model the electron-magnon scattering as interaction between electrons and an effective dynamical field associated with bosonic magnons. Our approach is formulated in the framework of the formally exact many body GW theory. The novelty in our approach is that quantities from linear response time dependent density functional theory (LRTDDFT) calculations will be used to approximate an effective interaction between electrons and magnons. As our LRTDDFT calculations are based upon the Korringa-Kohn-Rostocker method, bulk systems as well as complex geometries can be accounted for.



## First-principles studies on quantification and modulation of intrinsic spin transport in 5d transition metals

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Spin-Hall effect (SHE) enables charge-to-spin conversion in heavy transition metals, such as Ta and Pt, with strong spin-orbit coupling (SOC) strengths. It has been extensively studied as a viable mechanism for the development of next-generation spintronics-based non-volatile memory devices. Numerous experimental and first-principles approaches have been devised to quantify the charge-to-spin conversion efficiency i.e., the spin-Hall angle (SHA) or the spin-Hall conductivity (SHC), for the SHE. However, such approaches unavoidably involve interface contributions and, in general, extrinsic effects such as disorder and impurities, which are known to be less dominant than the bandstructure-only intrinsic contribution in such heavy metals. In this work, we use Density Functional Theory combined with the non-equilibrium Green's functions approach to quantify the intrinsic SHAs/SHCs of bulk elemental and thin-film models of 5d transition metals. We then computationally demonstrate a strategy for modulating the SHA within the same device, using Pt and Au as contrasting examples. Our computational work not only provides a quantitative estimation of the intrinsic SHAs for these materials, but also enables its theoretical understanding aimed towards the development of higher performance and power-efficient spintronic-based non-volatile memory devices.

## Twist-resilient and robust ferroelectric quantum spin Hall insulators driven by van der Waals interactions

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In this talk, I will show how an emergent ferroelectric quantum spin Hall insulating (QSHI) phase can spontaneously occur—or be engineered—in van der Waals heterostructures. I will illustrate the general idea by considering a heterostructure made of a well-known ferroelectric material,  $\text{In}_2\text{Se}_3$ , and a suitably chosen, easily exfoliable trivial insulator,  $\text{CuI}$ . In one polarization state the system is trivial, while it becomes a QSHI with a 50 meV band gap upon polarization reversal. Remarkably, the topological band gap is mediated by the interlayer hybridization and allows to maximize the effect of intralayer spin-orbit coupling, promoting a robust ferroelectric topological phase that could not exist in monolayer materials and is resilient against relative orientation and lattice matching between the layers.

A. Marrazzo and M. Gibertini, Twist-resilient and robust ferroelectric quantum spin Hall insulators driven by van der Waals interactions, *npj 2D Materials and Applications* **6**, 30 (2022)



## Presentation Abstracts – Thursday

### Impurity scattering and gap anisotropy in multiband superconductors from a first principles Green's function technique

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### Topology in superconducting surface nanostructures

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In this talk we apply relativistic multiple scattering theory to analyze edge states of chains of magnetic atoms deposited on the surface of superconductors. We find, that a broad range of spin spirals can be identified with a robust zero energy state displaying signatures of a Majorana Zero Mode. For these spirals, we explore the structure of various superconducting order parameters, where we find a new tool to determine the topological nature of the induced gap in the Shiba bands. Furthermore, we also discover from first principles that the topological edge states form an exotic type of state: an internally antisymmetric triplet. Through additional computer experiments, their robustness is also demonstrated, representing a huge step toward potential experimental realizations.

### Magnetic exchange interactions in proximity to a superconductor

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Magnetic exchange interactions (MEI) play a crucial role in advancing technologies, particularly in collinear and non-collinear magnetism. Understanding MEI within realistic electronic descriptions is essential. Our focus lies on analyzing magnetic impurities and nanostructures on superconductors, which exhibit intriguing in-gap phenomena such as Yu-Shiba-Rusinov states and Majorana zero modes. We employ a multi-orbital tight-binding model based on DFT calculations, incorporating superconductivity via the Bogoliubov-de Gennes method. By expanding the bilinear MEI tensor to include electron-hole coupling, we explore the impact of superconductivity strength on Heisenberg exchange and Dzyaloshinskii-Moriya interaction (DMI). Our self-consistent calculations on a Mn/Nb(110) system at 4.2K reveal that, for small gap values, the presence of superconductivity has negligible effects on the magnetic ground state. However, when MEI approaches the superconducting gap magnitude, the magnetic ground state transitions significantly from antiferro- to ferromagnetic. Additionally, we observe that the correction term in DMI exhibits opposite chirality to the non-superconducting contribution. These findings hold promise for technological advancements, particularly in quantum computing and magnetic storage devices, by providing insights into manipulating magnetism-superconductivity interaction

## Sihba bands in magnetic chains on s-wave superconductors based on the relativistic Bogoliubov-de Gennes KKR theory

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A magnetic impurity placed on an s-wave superconductor leads to the formation of Yu-Shiba-Rusinov (YSR) bound states. Bringing these impurities close to each other the YSR states are hybridize which results in band formation in the case of atomic chains, called Shiba bands. If the band structure is topologically non-trivial, then topologically protected Majorana zero modes (MZMs) appear localized to the ends of the chain. In quantum computing these states are of high interest due to the proposed applications as fault tolerant quantum bits.

In the present work we introduce how the Screened Korringa-Kohn-Rostoker method, together with Green's function embedding, can be applied for the study of MZMs by solving the Dirac-Bogoliubov-de Gennes equations, providing a material specific ab initio based framework. We present results for Mn chains on Nb(110) and Fe chains on Au/Nb(110) compared to recent experiments. Then we utilize the capabilities of my approach and present computer experiments. We show the topological phase transition as a function of spin spiral rotation angle together with the effect of spin-orbit coupling. We also show the calculated spin singlet and spin triplet anomalous densities proving that the zero energy states are corresponding to induced triplet pairing. With further manipulation of the spin configuration we show that MZMs are localized to the boundaries of topologically non-trivial segments within the chain.

Based on the previous results we conclude that our theory is capable of predicting the existence of MZMs in an arbitrary superconductor magnet heterostructure and can provide suggestions for experimentalist what are the suitable materials and geometries for the formation of MZMs.

## Formation of zero energy states and topological bands in magnetic chains on superconductors

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In magnetic chains on superconductors, so-called Shiba bands are formed within the superconducting gap of the host. Inside the Shiba bands, a minigap can be induced around zero energy by forming a magnetic spin spiral state by a large the spin-orbit coupling in the system. In the spirit of the bulk-edge correspondence principle, if the band structure is topological, then zero energy bound states (Majorana states) can be found at both ends of finite chains. 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. With examples, we show that physical quantities that are antisymmetric with respect to the Fermi energy, e.g., the singlet order parameter, can be used to prove band inversion of the system. Moreover, through the manipulation of the direction or the magnitude of the magnetic moments, we explore the conditions for the formation of topological phases in the chains and compare this to the change of Shiba state energies in single adatoms.

## Non-local correlations in transition metal oxides

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## Time and spin resolved photoemission: recent developments and applications

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Quantum technologies is a new and very pulsing multidisciplinary research area on the border between physics, chemistry, mathematics, informatics and materials science with a very high technological impact. In order to understand the physical properties of quantum materials on a fundamental level, one needs to explore the corresponding electronic states in detail and disentangle the role of the various interactions. In the past years we saw a big progress in the quantum mechanical description of topological systems and their properties at ideal conditions which are relatively easy to simulate but very hard to achieve in practice, such as, e.g., at zero absolute temperature or ideal structure. However, to directly promote technological progress it is necessary to deepen the theoretical understanding of specific quantum phenomena and/or materials under real conditions such as finite temperatures, structural and chemical disorder, presence of impurities and under the influence of ultrafast light pulses. This way it is important further to develop flexible, material specific theoretical methods which do allow to describe properties of real systems beyond the ground state. In this presentation I will show that fully relativistic multiple scattering Green function KKR theory [1] is the method of choice to include most of these effects as for example correlation effects by means of dynamical mean field theory [2] or the alloy analogy model for the description of spin fluctuations under finite temperatures [3]. Furthermore I will focus on extending our capabilities of performing quantitative calculations of excitations by light ranging from 10 eV up to 10 keV [4]. As an example I will concentrate on the angle-resolved photoemission spectroscopy (ARPES) which is a leading experimental probe for studying the electronic structure and complex phenomena in topological 3D and 2D quantum materials [5,6,7]. As the latest development a theoretical frame for the description of pump-probe photoemission is presented. The approach is based on a general formulation using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives the system out of equilibrium [10].

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## Poster Abstracts – Session I

### Materials for quantum computing : Magnetic impurities embedded in superconductors from first principles

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Due to the physical limits of classical processor architectures, future progress in scientific computing is expected to come from the realization of quantum computers, that requires to overcome challenges of decoherence and dephasing of the qubits. Materials that combine magnetism, spin-orbit interaction and conventional s-wave superconductivity are a suitable platform to study Majorana zero modes (MZM) [1], that can be used as building blocks for fault-tolerant topological qubits. In general, magnetic impurities in superconductors lead to localized Yu-Shiba-Rusinov (YSR) states bound to the impurities [2]. Understanding their interplay with MZMs is crucial to achieve topological quantum computers in the future.

In our work, we implemented the Bogoliubov-de Gennes (BdG) formalism in the juKKR Korringa-Kohn-Rostoker Green function impurity code [3] to allow material-specific description of defects perfectly embedded in superconductors from first principles. We apply it to magnetic transition metal adatoms placed on a superconducting Nb(110) surface to observe the emergence of YSR states, and discuss the influence of the impurity-substrate distance on the energy of the YSR states.

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### Nanoscale Electron Transport in Magnetic Proximitized Two-Dimensional van der Waals Quantum Systems

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Two-dimensional (2D) materials beyond graphene constitute a 2D flatland, which has become one of the active and emerging current research field. As 2D layers are held together by a van der Waals (vdW) force, the realization of vertical structures based on these layers is an approach that offers a rich platform to study fascinating vdW force-driven properties, like, commensurate lattice coincidence, electronic structure and band structure, magnetic and transport properties, spin-orbit coupling or exchange coupling induced by proximity effect and inversion symmetry breaking. In this aspect, the integration of intrinsic 2D ferromagnets with vdW semiconductors can become fertile ground for fundamental science as well as of great practical interest toward the seamless integration of electron transport. The primary focus will be on elucidating the impact of magnetically doped MX<sub>2</sub> and intrinsic 2D ferromagnets on the electronic structure and quantum transport properties with stable and large valley and spin polarization. All the simulation will be performed using appropriate first principle based ab initio simulation tools using advanced exchange correlation functional. Moreover, channel transport in nanoscale and spectral function projection techniques have been performed using large supercell

calculations to reconstruct the primitive-cell band structure to determine the electron device functionality of the heterostructure system with an expectation of experimental realization.

## Spin-dependent transport properties through $\text{Fe}_4\text{GeTe}_2/\text{GaTe}/\text{Fe}_4\text{GeTe}_2$ van der Waals heterostructures

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Quantum transport through two-dimensional (2D) magnetic structures has emerged as a fascinating field of research with promising implications for spintronics and quantum computing. Charge, energy, and spin behavior in nanoscale systems is studied by quantum transport, where quantum mechanical effects play a dominant role. Unlike classical transport, which adheres to deterministic laws, quantum transport is governed by probabilistic behavior and wave-particle duality. The comprehension and manipulation of quantum transport are vital for advancing next-generation electronic devices, quantum computing, and spintronics.

Moreover, 2D magnetic structures, such as atomically thin ferromagnetic films and magnetic heterostructures, possess distinct spin-dependent properties that enable efficient control and manipulation of electron spins. Understanding spin transport in these systems is crucial for the development of spin-based electronic devices and spintronic circuits. A magnetic junction can be achieved by utilizing van der Waals (vdW) heterostructures with 2D magnets. The weak vdW forces facilitate the formation of a clean and atomically sharp interface between layers, enabling efficient transfer of spin-polarized electrons between the magnetic materials. This magnetic junction exhibits intriguing properties, including spin injection, spin accumulation, and spin transport, which positions it as a promising candidate for next-generation spintronic devices and magnetic sensors.

Recent discoveries of  $\text{Fe}_n\text{GeTe}_2$  ( $n=3, 4, 5$ ), a class of 2D itinerant ferromagnets with a Curie temperature approaching room temperature (ranging from 150-220 K depending on Fe occupancy), provide exciting prospects for 2D spintronic advancements.

Here, we will present our study on the spin-dependent transport properties of vdW magnetic tunnel junctions comprising 2D  $\text{Fe}_4\text{GeTe}_2$  electrodes and a 2D GaTe barrier layer as a spacer. Moreover, through first-principles calculations and employing the nonequilibrium Green's function technique, we will demonstrate the spin-polarized ballistic transport through single- or bi-layer  $\text{Fe}_4\text{GeTe}_2$  connected to  $\text{PtTe}_2$  electrodes. We will also show a comparison between the electronic and magnetic properties of a 2D  $\text{Fe}_4\text{GeTe}_2$  monolayer sandwiched between two  $\text{PtTe}_2$  electrodes and the freestanding one.

## Dynamics of non-collinear magnets from first principles

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On my poster, I would like to present the current state of my Phd project, in the course of which I am developing and implementing a method to describe the dynamics of non-collinear magnets from first principles. Our approach is based on the Korringa-Kohn-Rostoker (KKR) Green's function method and the linear response method of Buczek et al.. Once the implementation is completed, we will be able to describe various excitations, such as magnons, Stoner excitations and density fluctuations on an equal, first principles, footing

## Ab initio study of magnetic doping in an Ising superconductor

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The transition-metal dichalcogenide NbSe<sub>2</sub> is a layered superconducting material that exhibits unconventional Ising superconductivity which is particularly robust against directions of external magnetic fields [1]. We combined the Bogoliubov-de-Gennes formalism in the Korringa-Kohn-Rostoker Green function method with the Coherent Potential Approximation [2-4], to study superconducting NbSe<sub>2</sub> in the presence of dilute concentrations of magnetic transition-metal impurities.

The superconducting gap of NbSe<sub>2</sub> achieved in this study is in agreement with the experimental measurements and is utilized for further impurity simulations. We investigated the effects of magnetic impurities at different concentrations in the host system, NbSe<sub>2</sub>. The theoretical expectation of the suppression of superconductivity at higher magnetic impurity concentration is satisfied, in agreement with the Abrikosov-Gorkov theory. We find the critical concentration of the breakdown of superconductivity and analyze the dependence of the critical impurity concentration with respect to magnetic ordering in the disordered local moments approach. Furthermore the role of SOC is discussed.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 – 390534769.

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## Disorder effects on superconductors

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Impurity effects, particularly those of magnetic nature, have held a central role, prompting investigations into their influence on superconductivity. Magnetic impurities disrupt the phenomenon, as observed through the linear reduction of critical temperature due to exchange interactions. Theoretical models and computational methods, such as the KKR-BdG approach, have emerged to comprehend these effects. This study examines the repercussions of 3d-transition magnetic impurities on the s-wave superconductor Pb, probing pair-breaking mechanisms and the intricate interplay between magnetism and superconductivity. These endeavors contribute to a more comprehensive understanding, encompassing theoretical underpinnings and computational strategies.

## Topological Hall effect caused by magnetic skyrmions in Pd/Fe/Ir(111)

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The topological Hall effect (THE) provides a way of electrically detecting magnetic skyrmions. This work comprises an ab-initio computational study of the THE arising from stable magnetic skyrmions [1], which are formed in the Fe atomic layer of the ultrathin films Pd/Fe/Ir(111) [2]. Our simulations are performed employing the non-collinear spin-density-functional theory within the full-potential relativistic Korringa-Kohn-Rostoker (KKR) Green function method combined with the semiclassical Boltzmann transport equation [3,4]. We analyze the resistivity and the Hall angle of the system, and we discuss the dependence of the THE on disorder, modelled by an additional electron scattering term. The effect of the skyrmion size on the Hall angle is also examined.

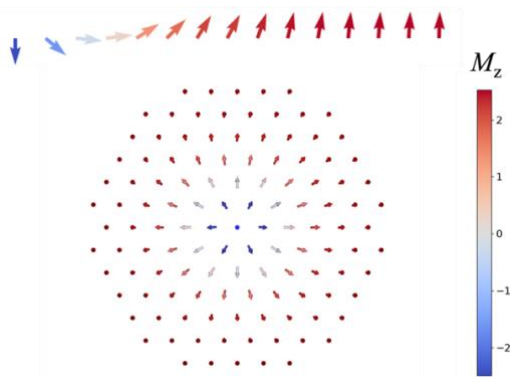


Figure 1: Magnetic skyrmion formed in ultrathin film Pd/Fe/Ir(111).

### Acknowledgements

AK and PR acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy -- Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 – 390534769. AK acknowledges financial support by the Hellenic Foundation for Research and Innovation (HFRI) for this research work under the HFRI PhD Fellowship grant (No. 1314). AK and PM acknowledge computational support from the Greek Research & Technology Network (GRNET). This work has additionally been performed under the Project HPC-EUROPA3 (HPC17CTZOF), with the support of the EC Research Innovation Action under the H2020 Programme, with computer resources and technical support provided by HLRS.

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## Yu-Shiba-Rusinov states in small Fe clusters on Pb(111)

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Using band-theoretical methods, we investigated the Yu-Shiba-Rusinov (YSR) states in various systems that comprised single, double, and triple magnetic Fe adatoms positioned on the Pb(111) surface. The formation of these states within the superconducting gap was examined by solving the fully relativistic Bogoliubov-de Gennes equations. Moreover, we explored the influence of different atomic arrangements, lattice relaxations, and spin configurations on the YSR states. Additionally, we analyzed the density of states (DOS) resolved by orbitals for these systems.

To ensure accurate comparison between our theoretical results and experimental observations, we implemented several measures. Firstly, we convoluted the calculated density of states with the instrumental broadening function, accounting for the resolution effects of the scanning tunneling microscope (STM) utilized in the experiments. This convolution process allowed us to simulate the experimental measurements accurately.

One calculation of experimental relevance involved examining the spatial distribution of the Yu-Shiba-Rusinov (YSR) states both within the surface plane and perpendicular to it. Furthermore, we took into consideration various aspects of the STM experiment, modeling these details to facilitate a comprehensive comparison between our theoretical predictions and the experimental data.

## Antiferromagnetism and proximity-induced Rashba interaction at inversion asymmetric heterojunctions

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Rashba-like spin-orbit interaction at oxide heterostructures emerges as a much sought-after feature in the context of oxide spintronics and spin-orbitronics.  $\text{KTaO}_3$  (KTO) is one of the best substrates available for the purpose, owing to its strong spin-orbit interaction and alternating  $+1| - 1$  charged layers along the (001) direction. Employing first-principles calculations within density functional theory (DFT) and proposing a possible electrostatic model for charge transfer to the surfaces of KTO slabs, we comprehensively analyze Rashba-like spin-orbit interaction with the help of three-dimensional band dispersion, isoenergetic contours, and projected spin textures – all directly obtained from our DFT results – in a thin insulating slab and a conducting thick slab of KTO.

Our results reveal reasonably strong linear Rashba interaction with no signature of Dresselhaus or higher-order Rashba interactions in the KTO slabs considered here [1]. We propose the interface between 3d cubic  $\text{BaMnO}_3$  is an antiferromagnetic insulator and 5d band insulator KTO as a substrate to study the electronic and magnetic properties at the 3d-5d interfaces. The proximity of strong spin-orbit coupling and strong magnetism from different parts of a heterostructure may offer a promising playground for exploring novel spintronics technology. We use ab initio DFT to examine the asymmetric  $\text{BaMnO}_3 | \text{KTaO}_3$  (BMO|KTO) oxide heterostructure where the inequivalent bottom and top interfaces break the inversion symmetry due to their opposite polar discontinuities.

We observe Rashba-like splitting for the bands of Mn-3d near the Fermi level of C-type antiferromagnetic BMO|KTO owing to the proximity to Ta atoms from the 5d series. We critically study Rashba-like spin-orbit interaction with the help of three-dimensional band dispersion, isoenergetic contours, and projected spin textures for Rashba-like Mn-3d bands. The results for asymmetric BMO|KTO report reasonably strong linear Rashba interaction in the heterostructure. The rigorous analysis of spin textures of the antiferromagnetic heterostructure presented here may be crucial for future developments in spintronics.



## Poster Abstracts – Session II

### Electronic structure and model Hamiltonian study of the polar-polar $\text{LaVO}_3/\text{KTaO}_3$ interface

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Interfaces of perovskite oxides of  $\text{ABO}_3$  type have growing advantages over the other interfaces in terms of physical applications due to their abundant accessibility in the nature and easily producible. The higher density and large localization of two-dimensional electron gas (2DEG) is a result of the polar discontinuity at the polar-polar (001) interface of the Mott insulators,  $\text{LaVO}_3$ , and the band insulator  $\text{KTaO}_3$ . In this work we perform thorough electronic structure calculations with different layers of LVO and KTO. At the Fermi level, mainly  $d_{xy}$  orbital of the Ta, which resides at the interface of  $(\text{LVO})_n/(\text{KTO})_m$  heterostructure, and the V atoms from the different layers of LVO unit-cells contribute. We report the 2DEG at the (001) interface of  $\text{LaVO}_3/\text{KTaO}_3$  (LVO/KTO) undergoes a Lifshitz transition (LT) due to the carrier doping at the interface. The LT has also been reported previously for the  $\text{LaAlO}_3/\text{SrTiO}_3$  (LAO/STO) interface. We further adopt the  $(\text{LVO})_4/(\text{KTO})_4$  heterostructure for our theoretical analysis, and interestingly, our extensive first-principles study demonstrate that unlike the LAO/STO, where the LT develops between the  $t_{2g}$  manifold of the Ti at the interface, in LVO/KTO it emerges from the Ta12- $d_{xy}$  and V14- $d_{yz/xz}$ . We employ a model Hamiltonian with six  $t_{2g}$  spin-orbit coupled orbitals taken from our DFT calculations and extract the hopping and on-site energy parameters of all three orbitals. The strengths of the atomic and Rashba spin-splitting are measured to be small. With the obtained Hamiltonian we aim to study the transport properties in the presence of interorbital electron-electron correlations using the dynamical mean field theory (DMFT).

### Complex magnetism of Gd intermetallics

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Using an ab-initio electronic structure theory which includes disordered local moments and strong f-electron correlations, we have investigated the magnetic ordering and critical temperatures of a range of Gd intermetallics, and compared the results to experiment.

## Magnetic ordering and spin-lattice interactions in $\text{MCrO}_2$ and $\text{MCrS}_2$ (with $\text{M} = \text{Li, Na, K, Cu, Ag}$ )

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We discuss the first-principles calculations of the spin-lattice coupling (SLC) parameters, considering the properties of the contributions linear and quadratic with respect to displacements. As a particular example of the SLC calculations, we discuss two groups of compounds, treated in the literature as the geometrically frustrated triangular-lattice antiferromagnets,  $\text{MCrO}_2$  and  $\text{MCrS}_2$  (with  $\text{M} = \text{Li, Na, K, Cu, Ag}$ ), exhibiting strong impact of the SLC on their magnetic properties. First-principles calculations of their electronic structure, exchange coupling and SLC parameters demonstrate the difference between the properties of these two groups of compounds. We discuss the role of the SLC for the ferro-elastic transition observed in these materials, as well as different contributions to the spin-lattice interaction which can have impact on their phonon spectra. In addition, we discuss a relationship between the origin of the spin-lattice interaction and the magnetically driven ferroelectricity observed in these compounds.

## Ab-initio exploration of complex magnetism of frustrated Mn Layer on Ag(111) surface

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Utilizing ab-initio simulations we explore the complex magnetism emerging in Mn films deposited on Ag(111) surface. The antiferromagnetic nature of Mn and the fcc(111) triangular lattice give rise to magnetic frustration which was explored both theoretically [1,2,3] and experimentally [4]. Here we investigate the inconsistency between the experimentally identified Néel-state [4] and the row-wise antiferromagnetic state predicted theoretically to be the ground state [1,2,3]. By employing the full-potential Korringa-Kohn-Rostoker Green function method, we extract the underlying tensor of magnetic exchange interactions and proceed to an in-depth analysis. Notably, we find the free-standing Mn layer to host a spin spiraling state as the ground state, while the Néel state is promoted to be the lowest in energy once Mn is deposited on Ag(111).

Project funded by the Deutsche Forschungsgemeinschaft (DFG) through SPP 2137 “Skyrmionics” (Project LO 1659/8-1).

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## Magnetic anisotropy energy of 3d adatoms and 3d–O molecules on the bilayer of MgO

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Designing systems with large magnetic anisotropy energy [MAE] is desirable and critical for nanoscale magnetic devices. Thus far, the MAE per atom in single-molecule magnets and ferromagnetic films remains typically one to two orders of magnitude below the theoretical limit imposed by the atomic spin-orbit interaction. Experimentally Rau et al. realized the maximum MAE for a 3d transition metal atom by coordinating a single Co atom to the O site of a MgO(100) surface [1].

Theoretically, simple density functional theory (DFT) calculations do not recover the large MAE of this system. Here, including a Hubbard U correction and spin-orbit coupling, we reproduce the large MAE of an individual Co adatom on a MgO (001) surface. More importantly, we take one step further by investigating the possibility of enhancing the MAE of 3d transition metal adatoms by considering various structural geometries of 3d–O molecules deposited on MgO. In one of the structures, where the molecules are perpendicular to the surface, the MAE can be enhanced while reducing the interaction with the substrate, which should minimize spin fluctuations and enhance the magnetic stability. Moreover, we evidence the ability to substantially modify the MAE by atomic control of the location of the 3d–O molecules on the substrate.

### Acknowledgements

This work was supported by the Federal Ministry of Education and Research of Germany in the framework of the Palestinian-German Science Bridge (BMBF grant number 01DH16027).

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## Magnetic Skyrmions in thin films

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Magnetic skyrmions exhibit intriguing and novel phenomena due to their topologically non-trivial spin textures. Their exceptional stability makes them possible candidates for information carriers for future spintronic devices.

We have determined the parameters appearing in a classical spin model from first principle for a FePd bilayer on Ir(111) and Pt<sub>95</sub>Ir<sub>05</sub>/Pd(111) overlayer and performed various magnetic simulations to explore the finite temperature behavior of the two skyrmionic systems.

The magnetic structure of a single skyrmion under different magnetic fields has been optimized and its diameter is compared to the results of spin polarized STM measurements.

The interaction energies between a pairs of skyrmions have also been calculated and exponential decay has been found with the separation.

We investigated the thermal evolution of magnetic skyrmions in the two thin film systems by means of metadynamic Monte Carlo simulations. In the case of Pt<sub>95</sub>Ir<sub>05</sub>/Pd(111) there is no skyrmion lattice ground state and the thermal average of the topological charge drops rapidly after achieving a maximum at 60K. For FePd/Ir(111) double layer skyrmion lattice exists at a certain range of the external

magnetic field perpendicular to the surface and the skyrmion number remains finite at zero temperature. At low temperature hedgehog skyrmions with topological charge of -1 are the dominant magnetic structure but increasing the temperature skirmonic objects with various topological charges are also present.

## All-electrical readout of three-dimensional spin-textures enabled by electron holography

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Three-dimensional (3D) spin-textures, similarly to their 2D counterpart (skyrmions), are attracting widespread interest, especially because of their potential application as magnetic bits for energy-efficient storage devices. Thereby, a major challenge is their identification. To address this problem, we have investigated the electronic properties of different topological spin-textures using a simple model. By combining multiple scattering theory with a tight-binding scheme, the influence on the local density of states can be expressed in terms of the orientation of the spins. Accordingly the local density of states carries non-trivial magnetic information induced by spin-mixing and spin-orbit mechanisms. Electron holography provides access to this new information by reconstructing phase-images. Therefore, we calculate and compare systematically the strength of the new and the conventional contributions to the phase-image. We explore the impact of spin-orbit interaction, exchange splitting, hopping and position of the d-electron states with respect to the Fermi energy.

## Structural transitions of magnetic thin films induced by two-dimensional materials

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Interfaces of magnetic thin films play a key role in determining magnetic behaviors and implementations of spintronic devices. In the last decade, the increased availability of high-quality two-dimensional (2D) materials has helped to broaden the scope of interfaces, leading to the discovery of novel electronic and magnetic properties.

Here, we explore with density functional theory calculations the impact of hexagonal boron nitride (h-BN) on the magnetism and structural properties of magnetic monolayers placed on heavy metal surfaces. We found that h-BN induces various structural transitions, and we investigate how magnetic interactions, such as the Heisenberg exchange interaction and the Dzyaloshinskii-Moriya interaction (DMI), are influenced by these reconstructions. These results contribute to new avenues for stabilizing complex spin-textures.