MA 7: Computational Magnetism

Time: Monday 15:00–18:00 Location: HSZ 02

MA 7.1 Mon 15:00 HSZ 02

Quantitative theories of magnetic interactions in solids — •Attila Szilva[1], Yaroslav Kvashnin[1], Evgeny A. Stepanov[2], Lars Nordström[1], Olle Eriksson[1], Alexander I. Lichtenstein[3], and Mikhail I. Katsnelson[4] — [1]Uppsala University — [2]Institut Polytechnique de Paris — [3]Universität Hamburg — [4]Radboud University

The talk will summarize the review paper Quantitative theories of magnetic interactions in solids, by focusing on the derivation of the LKAG formula and the extension of the formalism for the case of non-collinear magnets. A first version of the paper can be read here: https://arxiv.org/abs/2206.02415. The paper reviews the method of explicit calculations of interatomic exchange interactions of magnetic materials. This involves exchange mechanisms normally refereed to as Heisenberg exchange, Dzyaloshinskii-Moriya interaction and anisotropic symmetric exchange. The connection between microscopic theories of the electronic structure, such as density functional theory or dynamical mean field theory, and interatomic exchange, is given in detail.

MA 7.2 Mon 15:15 HSZ 02

Magnetic Anisotropy and Ground States of α-RuCl$_3$ — •Seung-Ju Hong[1] and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, South Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, South Korea

In this talk, I will talk about the magnetic anisotropy of the Kitaev candidate α-RuCl$_3$. This material gained much attention due to its proximity to Kitaev spin liquid. Thus, there are many kinds of research that computed the anisotropic exchange parameters from first principles.

However, in our work, we conducted an unprecedented number of *ab initio* calculations with constrained density functional theory and total energy fitting. We both examined the monolayer and multilayer systems and computed the intra/inter-layer exchange parameters. Then, from Monte Carlo simulations, we compute the thermodynamical quantities. From these computations, we obtained a non-trivial results.

MA 7.3 Mon 15:30 HSZ 02

Modification of Magnetic Anisotropy at Organic-Inorganic Interfaces — •Anita Halder, Sumanta Bhandary, David O'Regan, Stefano Sanvito, and Andrea Droghetti — School of Physics and CRANN, Trinity College, Dublin 2, Ireland

The adsorption of nonmagnetic organic molecules on ferromagnetic materials offers an opportunity to tune their magnetic properties for promising applications in high-density data storage and spintronic devices. In this work, we report the manipulation of the magnetocrystalline anisotropy (MCA) of Co slabs through the adsorption of small molecules, such as benzene, cot etc. We consider a simple model based on 2nd-order perturbation theory to explain the modification of MCA due to molecular adsorption in a qualitative way. Further, we have used Density Functional Theory and the magnetic force theorem to calculate magnetic anisotropy. The results indicate that molecular adsorption tends to favour perpendicular MCA at surfaces by reducing in-plane MCA of the slab. A detailed analysis of various atom-resolved quantities demonstrates that the underlying physical mechanism is the metal-molecule interfacial hybridization, and, in particular, it is related to the chemical bond between the molecular p_z and the surface d_{z^2} orbitals. Generalizing the same argument, we also show that the complex molecules C_{60} and Alq_3 deposited on fcc-Co induce a similar modification of the in-plane MCA, and we related the results to recent experimental observations.

MA 7.4 Mon 15:45 HSZ 02

Strain dependence of magnetism in transition-metal phosphorus trichalcogenides — •Yang-Jun Lee[1,2,3], Tae Yun Kim[2], and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Few-layer transition-metal phosphorus trichalcogenides (TMPX3) are two-dimensional (2D) antiferromagnetic materials, which have recently attracted attention because they can realize interesting 2D magnetic phenomena; they are considered materials whose magnetism can be described by the Heisenberg model, Ising model, or XY model depending on the transition metal ion. In this talk, we present the strain effects on the magnetism of TMPX3 compounds obtained from first principle calculations. Also, we will talk about the change in the symmetry and the magnetic model due to the strain.

MA 7.5 Mon 16:00 HSZ 02

Microscopic Insights for Beyond Room-Temperature Ferromagnetism in Two-Dimensional Fe5-xNixGeTe2 — •Sukanya Ghosh[1], Soheil Ershadrad[2], and Biplab Sanyal[3] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

The FenGeTe2 (n=3-5) (FGT) systems belong to the class of two-dimensional (2D) van der Waals (vdW) materials, promising candidates to explore magnetism in low-dimension with potential applications in spintronics. These systems are special due to their tunable structural, electronic and magnetic properties. Among the existing members of FGT family, Fe5GeTe2 has room temperature ferromagnetism with several intriguing properties. With the inclusion of dynamic electron correlation effect, our DFT+DMFT study shows how the spin moments, exchange interactions and Curie temperature (TC) of 2D Fe5-xGeTe2 can be varied significantly by substitutional doping with Ni. More importantly, the highest TC ~400 K is achieved for 20% doping concentration, beyond which the ferromagnetic order gets gradually suppressed. Our DFT+DMFT results are in good agreement with the experimental reports on bulk Fe5-xNixGeTe2 [1]. Moreover, we investigate the microscopic mechanisms responsible for the observed trend of TC in Fe5-xNixGeTe2 monolayer as an interplay between specific magnetic exchange interactions.

1. X. Chen et al, Phys. Rev. Lett. 128, 217203 (2022).

MA 7.6 Mon 16:15 HSZ 02

Efficient calculation of exchange interactions in magnetic materials — •Tae Yun Kim[1,2,3] and Cheol-Hwan Park[1,2,3] — [1]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea

Accurate description of the total energy of a magnetic system as a function of the local magnetic moments has always been a matter of importance, since it allows one to access the relevant low-energy excitation of the system, i.e. the magnon, which governs the low-temperature thermodynamics and remains important even at temperatures as high as the Curie temperature [1]. In this contribution, I will talk about an efficient way of calculating exchange interactions based on a constrained density functional theory method that captures accurately the magnetic total energy surface. As a concrete example, our ab-initio results on a magnetic system with substantial Dzyaloshinskii-Moriya interactions will be presented and be compared with that reported from previous studies to confirm the validity of our scheme.

[1] S. V. Halilov et al., Phys. Rev. B 58, 293 (1998)

MA 7.7 Mon 16:30 HSZ 02

Magnetic phases and stability of MPS4 — •Beatriz Costa Guedes[1], Thomas Brumme[2], Andrea Leon[3], and Thomas Heine[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Chair of Theoretical Chemistry, Technische Universität Dresden, Dresden, Germany — [3]Physics Faculty, Pontificia Universidad Católica de Chile, Santiago,Chile

The discovery of magnetic van der Waals materials provided a new playground for studying different aspects of magnetic interactions in reduced dimensions. Some interesting materials in this regard are the transition metal phosphorous chalcogenides MPS3 and CrPS4 (M = Mn, Fe, Co, and Ni), which are semiconductors exhibiting novel magnetic properties such as an intriguing dependence of the magnetic or-

dering on the transition metal (M). CrPS4 is particularly interesting because it exhibits a magnetic transition from antiferromagnetic (AFM) to ferromagnetic (FM) ordering in the monolayer limit, analog to the CrI3 compound, which is, in contrast, not stable in air. In this research, we study the stability and the electronic properties of the whole MPS4 family using density functional theory with a special focus on magnetic properties. Our results reveal a rich magnetic phase diagram with a complex electronic and magnetic dependence on M. They can be semiconductors, metals, or half-metals with AFM, FM, and non-magnetic configurations. We explain this behavior by discussing the interplay among structure, magnetism, and Coulomb interaction. By comparing it with the MPS3 system, we find some keys to understanding the magnetic properties of the MPS4 family.

MA 7.8 Mon 16:45 HSZ 02

Effect of Coulomb interaction on the magnetic properties of orthorhombic monolayer CrSBr — •Alexander Rudenko — Radboud University, Nijmegen, The Netherlands

Two-dimensional CrSBr is a recently discovered semiconducting spin-3/2 ferromagnet with the Curie temperature around 140 K. Unlike many other known 2D magnets, CrSBr has an orthorhombic lattice, giving rise, for instance, to spatial anisotropy of the magnetic excitations within the 2D plane. Theoretical description of CrSBr within the spin Hamiltonian approach turns out to be essentially nontrivial due to the complex character of the magnetic anisotropy resulting from low crystal symmetry. Here, we employ the Green's function formalism combined with first-principles calculations to systematically study magnetic properties of monolayer CrSBr. We find that the magnetic anisotropy and thermodynamical properties of CrSBr depend strongly on the Coulomb interaction and its external screening. In the free-standing limit, the system is close to an easy-plane magnet, whose long-range ordering is partially suppressed. On the contrary, in the regime of large external screening, monolayer CrSBr behaves like an easy-axis ferromagnet with more stable magnetic ordering. Our findings suggests that 2D CrSBr is an excellent platform for studying the effects of substrate screening on magnetic ordering.

MA 7.9 Mon 17:00 HSZ 02

Cu(VO)2(AsO4)2 with ferromagnetic V-V and antiferromagnetic Cu-V interactions — •Victoria Ginga[1,2], Alexander Tsirlin[1], and Oleg Siidra[2] — [1]Universität Leipzig, Felix Bloch Institute for Solid State Physics, Linnestraße 5, 04109 Leipzig — [2]St. Petersburg, Russia

Recent years have seen an increased interest in studying the magnetic properties of mineral-like compounds. The Cu(VO)2(AsO4)2 obtained by the CVT reaction method reproducing exhalative conditions has a new type of structure, which is characterized by layers formed by two [1+4+1]V4+-tOeq-[1+4+1]V4+ and one [1+4+1]V4+-vOeq-[1+4+1]V4+ linkages of V-centered octahedra. Arsenate groups decorate vanadate layers via corner-sharing with the VO6 octahedra, while single CuO6 octahedra are connecting vanadate layers into a framework via edge-sharing. Our ab initio calculations show that the magnetism of Cu(VO)2(AsO4)2 is dominated by the antiferromagnetic Cu-V coupling JCu-V = 257 K and the ferromagnetic V-V coupling JV-V =-277 K. This high energy scale is not uncommon in both Cu2+ and V4+ oxide compounds with the edge-shared octahedral geometry. Our results show the formation of unusual interaction geometries through the mixing of different spin-1/2 ions in the crystal structure. Experimental and computational results of the study of the Cu(VO)2(AsO4)2 with two distinct spin-1/2 magnetic ions will be presented.

MA 7.10 Mon 17:15 HSZ 02

SU(4) magnetism on a triangular moiré superlattice — •Lasse Gresista[1], Dominik Kiese[2], Michael Scherer[3] und Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Center for Computational Quantum Physics, Simons Foundation Flatiron Institute, New York, USA — [3]Institute for Theoretical Physics III, Ruhr- University Bochum, Germany

The discovery of correlated insulating states in several graphene based moiré heterostructures such as trilayer graphene aligned with hexagonal boron nitride (TG/h-BN) has renewed the interest in strongly coupled electron systems where spin and orbital (or valley) degrees of freedom are intertwined. Considering the strong coupling limit, the localized degrees of freedom in such systems may be described by generators of SU(4) instead of the conventional SU(2) spin operators. Here, we study such an SU(4) 'spin-valley' model on a triangular lattice at a filling of two electrons (or holes) per moiré unit cell, with interactions that strongly break the SU(4) symmetry down to $SU(2)_{spin} \otimes U(1)_{valley}$. This is, e.g., relevant for the flat band physics of TG/h-BN within the topologically trivial regime. Using a pseudo-fermion functional renormalization group approach and semi-classical Monte Carlo calculations, we are able to distinguish parameter regimes showing no magnetic order, suggesting a spin-valley liquid or other quantum disordered ground state, and a multitude of classically ordered phases including ferromagnetic, antiferromagnetic, incommensurate and stripe order that manifests in different sectors of the coupled spin-valley space.

MA 7.11 Mon 17:30 HSZ 02

$YSrFeCrO_6$ as a Robust Ferromagnetic Semiconductor with Large Photovoltaic Efficiency — •Avijeet Ray, Paresh C. Rout, and Udo Schwingenschlögl — Physical Sciences and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

Semiconducting ferromagnetic transition metal oxides play a key role in spintronics applications. Employing first-principles calculations, we predict the existence of the double perovskite Y_2FeCrO_6 and study its properties. While both rock-salt (RS) and layered (L) structures are found to be dynamically stable, the L structure turns out to be energetically favorable. We determine the magnetic phase diagram under hydrostatic pressure. We find that the RS structure is dynamically stable and energetically favorable over the L structure in the case of $YSrFeCrO_6$ (hole doping by substitution of Y by Sr). $YSrFeCrO_6$ realizes a ferromagnetic ordering with a magnetic moment of 7 μ_B per formula unit, which is promising for spintronics applications. In addition, the ferromagnetic ordering is not compromised by hydrostatic pressure from −10 to 16 GPa. While the L structure of Y_2FeCrO_6 is an indirect bandgap semiconductor, the RS structure of $YSrFeCrO_6$ shows a direct bandgap of 0.90 eV (spin-orbit coupling taken into account in the calculation). We obtain a large spectroscopic limited maximum efficiency of 26% for $YSrFeCrO_6$, which is suitable for photovoltaic applications.

MA 7.12 Mon 17:45 HSZ 02

Magnetic Anisotropy of α-$RuCl_3$ — •Seung-Ju Hong[1], Tae Yun Kim[2], and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, South Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, South Korea

α-$RuCl_3$ has gained much attention due to its proximity to Kitaev spin liquid. In this talk, we will discuss the magnetic anisotropy of α-$RuCl_3$. We performed first-principles calculations on the magnetic anisotropy of α-$RuCl_3$. We will compare the results of our first-principles calculations with available previous experimental and theoretical studies.