Workshop and hands-on school on the FP-LMTO method and DMFT

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Abstract Booklet

An introduction to FP-LMTO and RSPt

John Wills

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In this talk I will present a brief history of the full-potential linear muffin-tin orbital method (FP-LMTO), in relation to the electronic structure code RSPt. I will illustrate the motivations that led to RSPt and focus on the development of new functionalities through the last two decades. I will also illustrate how FP-LMTO can be used as a tool to extract materials-tailored pseudopotentials.

A density based Electron Localization Function

Ann Mattsson

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The subsystem functional scheme (SSF) for constructing Density Functional Theory (DFT) functionals uses two types of ingredients: a) one specialized functional for every type of subsystem that we want to accurately treat with the final functional, and b) an interpolation index that decides how much of each specialized functional is used in a point in the real system. The SSF was successfully used to create the AM05 exchange-correlation functional, where a) the uniform electron gas (UEG) and Airy gas (AG) surface systems provided the specialized functionals, and b) the interpolation index was based on the dimensionless gradient of the density, s. At small values of s, a functional based on the UEG (LDA) is used, while for large s the specialized functional created from the AG surface system is successively used more. In our current work of creating an exchange-correlation functional accurate also for systems with a mix of localized and itinerant electrons, we will add a) a specialized functional for confined systems based on the harmonic oscillator (HO) gas, and b) use the Electron Localization Function (ELF) as interpolation index. Since the ELF is using the kinetic energy density, this will result in a meta-GGA type functional. I will discuss our efforts to parametrize the ELF as a function of s and the dimensionless Laplacian, q, to instead obtain an ordinary GGA type functional.

Single molecule magnets: spin manipulation, intermolecular interactions and electronic structure. An overview by ab-initio calculations and beyond

Barbara Brena

Uppsala University

Organic molecules like 3*d* transition metal phthalocyanines and porphyrins are among the most promising candidates for applications in molecular electronics and spintronics. It has been shown that the electronic structure and the spin of these compounds can be affected by factors such as ligands and adsorption configurations. In search of a practically feasible magnetic switching mechanism, we have previously studied how the molecular spin in porphyrins and phthalocyanines is affected by the interaction with magnetic substrates as well as by the adsorption of gases [1]. Our studies are based on ab-initio calculations in collaboration with soft x-ray spectroscopy. Aiming to understand the magnetic behavior in novel supramolecular architectures, we have also analyzed the magnetic coupling and moment in molecular sandwiches of these compounds like FePc and MnPc. It is known that Density functional theory (DFT) in the generalized gradient approximation (GGA) and in the local density approximation (LDA) has big limitations in properly describing highly correlated and localized d-electrons. We have therefore thoroughly studied the effect of the Hubbard U method, which accounts for the intra-atomic Coulomb interactions [2], on the electronic structure of several 3*d* phthalocyanines [3]. In addition, with the goal to reveal in detail the still debated electronic structure of such molecules, we have developed a computational scheme for the first-principles modeling of the L2,3 edges X-ray Absorption Spectra (XAS), based on the combination of Density Functional Theory plus Dynamical Mean Field Theory (DFT+DMFT) and Multiplet Ligand Field Theory (MLFT). The method has been so far successful in the simulation of the L2,3 edge XAS of transition Metal Oxides, and the coming developments will address several different materials including 3*d* metal phthalocyanines [4].

[1] S. Bhandary, et al., Phys. Rev B 88, 024401 (2013); D. Klar, et al., Phys. Rev. B 88, 224424 (2013); H. C. Herper, et al., Phys. Rev. B 89, 085411 (2104); H. Herper and B. Brena, DOI: 10.1063/1.4917242
[2] A. I. Liechtenstein, et al., Phys. Rev. B 52, R5467 (1995); S. L. Dudarev, et al., Phys. Rev. B 57, 1505 (1998)
[3] I.E. Brumboiu, et al., J. Chem. Theory Comput. 12, 1772 (2016); I.E. Brumboiu, et al., in manuscript
[4] Johann Lüder, et al., Phys. Rev. B 96, 245131 (2017)

A density based Electron Localization Function

Diana Iuşan

Uppsala University

In this talk I will present a general method for simulating spin-lattice dynamics. The methodology is built upon the atomistic spin dynamics framework, as implemented in the UppASD code. The interactions between the spin and lattice degrees of freedom are described using a general Hamiltonian. The parameters entering the Hamiltonian are computed within density functional theory, using the full-potential linear muffin-tin orbital method as implemented in the RSPt code. I will exemplify this methodology with simulations for bcc Fe and clusters.

Localized systems within DFT+Hubbard-I approach: multiplets, crystal-field effects and inter-site exchange interactions

Leonid Pourovskii

Ecole Polytechnique, Palaiseau

The DFT+DMFT framework in conjunction with the quasi-atomic (Hubbard-I) approximation for the quantum impurity problem represents a computationally efficient, though simplified, approach to correlated materials. We review its applications to strongly-localized rare-earth and transition-metal systems focusing on several topics: crystal-field (CF) and exchange-field effects as well as intersite exchange interactions. A modified DFT+Hubbard-I approach suppressing the LDA self-interaction for localized states is applied to evaluate crystal and exchange fields in rare-earth-based hard magnetic intermetallics. We obtain a good agreement with experiment for the well-known hard magnet SmCo5; the same approach is applied to perspective hard magnets of the *R*Fe12*X* family (*R*=Nd or Sm) to evaluate the impact of interstitials *X*=N, Li on the CF on rare-earth ions. The effect of hybridization on the CF splitting can be effectively included within DFT+Hubbard-I by using extended Wannier orbitals to represent 4*f* states in solids as shown for the rare-earth oxychlorides series *R*OCl. Finally, we discuss a technique for evaluating intersite exchange interactions within the the DFT+Hubbard-I framework. Such interactions are extracted from a linear response of DFT+Hubbard-I grand potential to fluctuations on two neighboring localized shells around their symmetric paramagnetic configuration.

High throughput calculations applied to double perovskites

Anna Delin

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Double perovskite oxides are a versatile class of systems with, sometimes, unusual combinations of electronic, magnetic and electrochemical properties, including half metallicity and multiferroicity. The general formula of a double perovskite oxide is A2B’B’’O6. Structurally, they consist of oxygen octahedra, centered around metal cations (B’ and B’’), plus larger atoms (A) in the voids in between the oxygen octahedra. The octahedra may be tilted visavi each other and they can also be slightly distorted. Among the double perovskite oxides, several half-metals are well known, for example Sr2FeMoO6. Furthermore, the compound Sr2CrOsO6 has a unique electronic structure, as it has a completely filled 5*d* t2g minority-spin orbital, while the majority-spin channel is still gapped. This means that this system is at the end point of an ideal fully spin-polarised metal-insulator transition. A large number of double perovskites have been synthesized and characterized, but it is apparent that the space of possibilities is still very far from exhausted. In this project, the aim is to complete the map using high-throughput DFT-based computations and predict new, stable double perovskites. In this presentation, I will focus in particular on iridium-based double perovskites, where only a few systems have been synthesized. Our results agree well with available experimental data.

XAS for strongly correlated systems

Johan Schött

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X-ray absorption spectroscopy measured at the L edge of transition metals (TMs) is a powerful element-selective tool providing direct information about the correlation effects in the 3*d* states. The theoretical modeling of the $2p \rightarrow 3d$ excitation processes remains to be challenging for contemporary *ab initio* electronic structure techniques, due to strong core-hole and multiplet effects influencing the spectra. In this work, we present a realization of the method combining the density-functional theory with multiplet ligand field theory, proposed by Haverkort *et al.* [Phys. Rev. B **85**, 165113 (2012)]. In this approach, a single-impurity Anderson model (SIAM) is constructed, with almost all parameters obtained from first principles, and then solved to obtain the spectra. In our implementation, we adopt the language of the dynamical mean-field theory and utilize the local density of states and the hybridization function, projected onto TM 3d states, in order to construct the SIAM. The developed computational scheme is applied to calculate the L-edge spectra for several TM monoxides. A very good agreement between the theory and experiment is found for all studied systems. The effect of core-hole relaxation, hybridization discretization, possible extensions of the method as well as its limitations are discussed.

Theory of resonant x-ray emission spectra at the L and M edges in compounds with localized f electrons

Jindrich Kolorenc

Czech Academy of Sciences

I discuss a theoretical description of the resonant x-ray emission spectroscopy (RXES) that is based on the Anderson impurity model. The parameters of the model are determined with the aid of the material-specific LDA+DMFT method. The full calculation of RXES from the Kramers-Heisenberg formula is demanding but under certain simplifying assumptions about the shape of the core-hole potentials the computational complexity can be reduced to the complexity of the single-photon core-level spectroscopies like the x-ray photoelectron spectroscopy (XPS) or the x-ray absorption spectroscopy (XAS). Recently, this simplified approach was shown [1] to accurately reproduce the L-edge RXES measured in lanthanides [2,3,4]. Here, the method is extended to the spectroscopy at the M edge and it is applied to selected uranium and plutonium compounds, mostly oxides. Depending on the progress with implementation of further generalizations, the resonant inelastic x-ray scattering (RIXS) will be discussed as well.

[1] J. Kolorenc, Physica B 536, 695 (2018)
[2] J. A. Bradley, et al., Phys. Rev. B 85, 100102 (2012)
[3] K. Hamalainen, et al., Phys. Rev. Lett. 67, 2850 (1991)
[4] K. O. Kvashnina, et al., J. Electron. Spectrosc. Relat. Phenom. 194, 27 (2014)

Spin-orbit interaction in light element K-edge XMCD

Akihiro Koide

Rennes University

The X-ray magnetic circular dichroism (XMCD) spectra have been used in order to obtain local information of the magnetic properties on absorbing atoms. Although the L2,3 edge XMCD has been useful by the aid of

the sum-rule analysis for the spin and orbital moments of *d* orbitals, the *K*-edge XMCD has attracted an attention to extract an information in light element magnetic materials. From a view point of experiments, the *K* edge XMCD of light elements is measured by the same way as the L2,3-edge XMCD of 3*d* transition metals. However, this similarity may make misleading. In terms of the spin orbit interaction (SOI), the core SOI works on 2*p* state for L2,3 edges but not on 1*s* state for K edge. A question is whether the SOI at the absorbing atom is also important for the *K* edge XMCD as the case of the L2,3 edges or not. To investigate the SOI, we calculated oxygen K edge XMCD for CrO2 as a prototype of light element magnetic materials. The calculated spectra were obtained by taking the first perturbed SOI into account. This perturbation scheme enables us to represent the XMCD spectra by sum of the contribution of each site SOI. The site-resolved XMCD analysis shows that the nearest neighbour Cr ions have the dominant contribution to the oxygen *K* edge XMCD for CrO2. The total XMCD spectra has same energy dependence of the orbital-momentum density. We concluded that the absorbing light element just borrows not only the spin but also orbital moments of the surrounding magnetic ions by the hybridization. This differs from the scenario of the L2,3 edge XMCD.

From an LMTO to a PAW basis set: a GW implementation

Mebarek Alouani

Strasbourg University

In this talk we will discuss how to transform the LMTO basis set to a projector augmented wave (PAW) basis set. We will show that this transformation facilitates the GW implementation in the RSPt code, which is based on the full-potential LMTO method.

Understanding of dynamics of excited states by means of static one-step model of ARPES

Jan Minar

Plzen University

Spectroscopy can be seen as an important experimental tool providing information about the electronic structure the probed correlated materials and therefore works as a stringent benchmark for the success of any electronic structure theory. The investigations of ground state properties have been complemented with corresponding spectroscopical investigations with an emphasis on angle-resolved photo-emission (ARPES). The commonly used comparison between calculated density of states or pure spectral functions to the corresponding stereoscopic experiments ignores the influence of specific spectroscopical aspects like matrix elements, surface effects etc. In our studies performed within this research unit we included all these effects as far as possible. For example, in the case of ARPES our approach combines coherently the KKR+DMFT method with the one step model of photo-emission that allows to account properly for all relevant issues [1,2]. In last decade, pump-probe ARPES gain a lot of interest. This technique can be theoretically described by time dependent one-step model of photoemission [3]. Our approach is based on a general treatment of the photo emission process 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. However, until now within this approach we can deal only with simple sistems. In my presentation I will show three examples where [3,4,5] where simple stationary one step model of ARPES can deliver important informations concernig dynamics of the ARPES process. These examplese covers femtosecond dynamics of topological insulators as well as attosecond dynamics of the excitation process measured by spin-polarised ARPES.

[1] J. Braun, J. Minar, H. Ebert, Phys. Reports **740,** 1 (2018)
[2] H. Ebert, D. Ködderitzsch and J. Minar, Rep. Prog. Phys. **74,** 096501 (2011).
[3] Cacho, et al., Phys. Rev. Lett. 114, 097401 (2015)
[4] Fanciulli, et al., Phys. Rev. Lett. 118, 067402 (2017)
[5] Barriga, et al., Phys. Rev. B 95, 125405 (2017)

Valence photoionization beyond the electric dipole approximation: the case of [Ni(H2O)6]2+

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Photoelectron spectroscopy of the valence band (VB-PES) is a powerful technique to investigate the electronic structure of materials, from single molecules to solids. The strength of the technique lies in the fact that different atomic states are ionized with different probabilities by photons of different energies and, therefore, the changes in relative peak intensities with photon energy may be used to disentangle atomic contributions to the valence photoelectron spectrum. Computationally, photon energy dependent valence spectra may be calculated by multiplying the projected densities of states (PDOS) with the corresponding atomic phtoionization cross-sections, calculated within the dipole approximation. This method has two limitations: (1) it assumes that the photoionization probability of an electron in an isolated atom can be directly used to compute the photoionization probability from a molecular orbital and (2) the atomic photoionization cross-sections are computed within the dipole approximation, valid for low photon energies, but arguably not valid for the case of hard x-rays in combination with highly delocalized initial states, such as in conjugated organic molecules or the valence bands in solids. In this work we aim to go beyond limitations (1) and (2) by directly using Khon-Sham orbitals, the full field operator and a plane-wave final state to compute the photoionization cross-sections of transition metal complexes. The methodology is applied to the nickel complex [Ni(H2O)6]2+, which represents a molecular model for the NiO crystal.

Itinerant or localized?

How we can predict the nature of 4f states in Ce-compounds

Heike Herper

Uppsala University

With the steadily growing dependence on technology and technical devices in every part of our lives the search for new functional materials is a vital task. Increasing computer power together with new developments in materials informatics has opened up the possibility to classify properties of materials in which one studies the aggregate properties of a large body of materials within the same class in addition to detailed investigations of the single compounds in that class. Here, we present the first large scale study of electronic properties in Ce-based compounds which is accompanied by a systematic study of the analysis of the 4*f*-localization via the hybridization function. Cerium is the most abundant rare earth and its compounds are used in many applications such as catalysis, glass manufacturing, and recently it has also been discussed in view of permanent magnets. Depending on the application different materials properties are needed. Since the localization of the 4*f* electrons mainly determines the materials properties an understanding of the degree of localization is essential for materials classification and prediction. Aiming to classify a large body of data (> 360 sets) according to the degree of localization of the 4*f* states we made use of the hybridization function which has been derived from ab initio calculations using the full-potential LMTO code RSPt. We demonstrate that the strength of the hybridization function allows conclusions about the level of 4f localization. Our results are consistent with the available experimental information. The calculated information entropy for this set of data clearly hints to a high predictability. As an example we discuss the transition from CeO2 to Ce2O3 is believed to correspond to a transition from a completely itinerant system to a fully localized one.

Magnetic anisotropy of Fe3Sn-based magnets: a first-principles RSPT study

Olga Vekilova

Uppsala University

The increasing importance of permanent magnets to the modern society has resulted in renewed interest in the design of new magnetic materials that are cheap and abundant. A good permanent magnet must have a high Curie temperature, high saturation magnetization and uniaxial anisotropy energy. Fe-rich systems like the hcp Fe3Sn compound are promising candidates. However, it is a magnet whose magnetization easy axis is in-plane, rather than uniaxial. One of the possibilities for changing the easy axis direction is by doping with other elements. Using the highly accurate FP-LMTO RSPT code we study from first principles the electronic structure of Fe3Sn-based alloys that naturally exhibit ferromagnetic properties, in combination with a set of phase stabilizers, such as Si, P, Ga, Ge, As, Se, In, Sb, Te, and Bi. We aim at understanding of the origin of the magnetic properties and find new ferromagnetic phases with uniaxial anisotropy that can be used to develop advanced permanent magnets. The stability of the phases is elucidated theoretically by the calculation of formation enthalpies. The experimental comparison is provided. The trends in the calculated magnetocrystalline anisotropies and Curie temperatures of these compounds are analyzed and suggestions for better permanent magnets are formulated.

Electronic structure, magnetism, and exchange integrals in transition-metal oxides: Role of the spin polarization of the functional in DFT+U calculations

Samara Keshavarz

Uppsala University

Density functional theory augmented with Hubbard-U corrections (DFT+U) is currently one of the most widely used methods for first-principles electronic structure modeling of insulating transition-metal oxides (TMOs). Since U is relatively large compared to bandwidths, the magnetic excitations in TMOs are expected to be well described by a Heisenberg model. However, in practice the calculated exchange parameters Jij depend on the magnetic configuration from which they are extracted and on the functional used to compute them. In this work we investigate how the spin polarization dependence of the underlying exchange-correlation functional influences the calculated magnetic exchange constants of TMOs. We perform a systematic study of the predictions of calculations based on the local density approximation plus U (LDA+U) and the local spin density approximation plus U (LSDA+U) for the electronic structures, total energies, and magnetic exchange interactions Jij extracted from ferromagnetic (FM) and antiferromagnetic (AFM) configurations of several transition-metal oxide materials. We report that for realistic choices of Hubbard U and Hund’s J parameters, LSDA+U and LDA+U calculations result in different values of the magnetic exchange constants and band gap. The dependence of the band gap on the magnetic configuration is stronger in LDA+U than in LSDA+U and we argue that this is the main reason why the configuration dependence of Jij is found to be systematically more pronounced in LDA+U than in LSDA+U calculations. We report a very good correspondence between the computed total energies and the parametrized Heisenberg model for LDA+U calculations, but not for LSDA+U, suggesting that LDA+U is a more appropriate method for estimating exchange interactions.

Currents and spin-currents in non-collinear magnets

Lars Nordström

Uppsala University

In magnetically ordered systems it is well known that there exist currents, as e.g. manifested in orbital moments. For collinear magnets these currents only exist in the presence of spin orbit coupling (SOC), but for non-coplanar order currents can exist also without SOC. In a similar way spin-currents, i.e. transport of spin rather than charge, have to be induced by SOC in collinear magnets but not in any non-collinear order. I will discuss the origin of these currents, explain their symmetry properties, discuss possible manifestations and present some first principles calculations of such currents.

Chiral Spin Texture in the Charge-Density-Wave Phase of the Correlated Metallic Pb/Si (111) Monolayer

Gianni Profeta

L’Aquila University

We investigate the 1/3 monolayer alpha-Pb/Si(111) surface by scanning tunneling spectroscopy (STS) and fully relativistic first-principles calculations. We study both the high-temperature 3X3 and low-temperature 3X3 reconstructions and show that, in both phases, the spin-orbit interaction leads to an energy splitting as large as 25% of the valence-band bandwidth. Relativistic effects, electronic correlations, and Pb-substrate interaction cooperate to stabilize a correlated low-temperature paramagnetic phase with well-developed lower and upper Hubbard bands coexisting with 3X3 periodicity. By comparing the Fourier transform of STS conductance maps at the Fermi level with calculated quasiparticle interference from nonmagnetic impurities, we demonstrate the occurrence of two large hexagonal Fermi sheets with in-plane spin polarizations and opposite helicities.

Enhancing low quality crystal structures and predicting new crystal structures with solid state calculations

Lars Eriksson

KTH, Stockholm

Some crystal structure investigations do not enable accurate conclusions about for example hydrogen bonding patterns, coordination geometries or superstructures. In many cases a combination with quantum chemical calculations on solid state structures could reveal a great deal of information. Successful prediction and verification of hydrogen bond structures and molecular conformations indicated by both single crystal X-ray diffraction and solid state NMR methods have been done. Furthermore we have used theoretical methods for elucidating mechanism and geometrical characterization of carbon dioxide adsorption in Prussian Blues. Both these investigations have been done with pseudopotential calculations using plane waves. We hope to be able to use more theoretical methods in the future in order to gain more insight into different processes and structures.

Probing the topological nature of SmB6 using DFT+DMFT in RSPt

Patrik Thunström

Uppsala University

The electronic structure of the strongly correlated topological insulator candidate material SmB6 has been investigated using DFT+DMFT. Through a symmetry analysis of the Pole Expanded (PE) Hamiltonian, and a parity decomposition of the k-resolved spectral density, we confirm that the electronic structure has a non-trivial topology also when a local self-energy is present. The topological surface states are probed in a set of slab calculations, and their robustness to perturbations is explicitly shown. The presentation includes a small tutorial on how to perform the symmetry decomposition of the spectral density in RSPt.

Scaling behavior of the Compton profile of elemental metals

Michael Sekania

Augsburg University

The contribution of the valence electrons to the Compton profiles of the crystalline alkali metals is calculated using density functional theory. We show that the Compton profiles can be modeled by a q-Gaussian distribution, which is characterized by an anisotropic, element dependent parameter q. Thereby we derive an unexpected scaling behavior of the Compton profiles of all alkali metals [1].

[1] M. Sekania, et al., Physica A 489, 18-27 (2018)

Two-particle self-consistent method (TPSC) for the Hubbard model on the honeycomb lattice

Arya Subramonian

APCTP, Pohang

The two-particle self-consistent method (TPSC) was introduced to study the Hubbard model on the square lattice. TPSC satisfies many physical constraints like conservation laws, the Pauli principle, local sum rules for susceptibilities, and the Mermin-Wagner theorem. It captures the physics of the long-ranged antiferromagnetic fluctuations at low temperatures as the interaction is increased, and describes the crossover to the renormalized classical regime and the appearance of a pseudogap. The debate over the existence of an intermediate spin liquid phase in the half-filled Hubbard model on the honeycomb lattice demands a study using a technique which aptly captures the effects of antiferromagnetic fluctuations. We generalize TPSC to the two-band case of the Hubbard model on the honeycomb lattice. Upon lowering the temperature, and increasing the value of interaction, the antiferromagnetic correlation length increases. As the correlation length exceeds the thermal de Broglie wavelength, the system enters a renormalized classical regime. This 'crossover' can be extrapolated to zero temperature to obtain an estimate of the critical interaction strength for the semimetal to antiferromagnet transition. The estimates of the interaction strength for a Mott transition are larger, hence the intermediate spin liquid phase is ruled out. For the tight-binding model on the honeycomb lattice, when a uniaxial strain is applied along the zigzag direction, the Dirac point shifts from the K point to the M point, and at a critical strain a bandgap opens. The possibility of the application of reversible strains up to 20% and the sizable electron-electron interactions in graphene motivate the use of TPSC to investigate the interplay of strain and antiferromagnetic fluctuations. TPSC is implemented taking into account the modified hopping parameters under zigzag strain. Close to critical strain, at large values of interaction, the nematic susceptibility diverges as the temperature is lowered, signaling a quantum phase transition. This can be observed by studying the magnetovolume, thermal expansion and magnetic Gruneisen coefficients.

Scaling behavior of the Compton profile of elemental metals

Saleem Ayaz Khan

Plzen University

In our recent work [1], we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

[1] S. A. Khan, et al, Phys. Rev. B, 94, 144436 (2016)

Electrical control of spin-texture in non-magnetic ferroelectrics

Silvia Picozzi

Chieti University

Upon inversion symmetry breaking, spin-orbit coupling allows for spin-dependent electronic structures, even in the absence of long-range magnetic ordering. Given the prerequisite of showing a polar axis, ferroelectrics are not only natural candidates for this kind of phenomena, but they also offer intriguing perspectives to control/induce/switch spin-textures with an electric field that switches the ferroelectric polarization. I will focus on several types of mechanisms to achieve the goal, ranging from Rashba spin-splitting to spin-valley coupling. Based on density functional simulations, I will show several realizations of ferroelectric materials (chalcogenides, hyperferroelectrics, oxide-based systems, …), where the k-dependent spin texture is one-to-one linked to polarization.

Complexities at oxide interfaces

Biplab Sanyal

Uppsala University

In this talk, I will discuss the properties of interfaces of oxide heterostructures, studied by ab initio theory. In the first example, the experimental observation of the vertical shift in the exchange bias will be explained for YMnO3/LSMO heterostructures. In the next example, I will show results of SrRuO3/SrTiO3 interfaces, where ab initio density functional theory can qualitatively explain the experimental transport characteristics of the heterostructures. Finally, some results from the ongoing work on graphene/SrTiO3 interfaces will be shown.

The theoretical path of uncovering new stackings in 2D-Mo2C and their electronic and vibrational properties

Weiwei Sun

Oak Ridge National Laboratories

The variations of stacking of 2D materials attract increasing interests due to their potentially wide applications. In this talk, I will give insights into the theoretical path of discovering the new stacking of 2D transition metal carbides, BiXenes showing 1H symmetry in contrast to the 1T symmetry shown in MXenes. The predicted series of 2D carbides have formation energies close to that of germanene and comparable cleavage energies with respective to 2D Ca2N, TcSe2 or TcS2. The structure prediction of M2C (M=Mo, Ru, Rh, Os) at ambient conditions is motivated by recently reported hydrostatic quench of a new phase of Ru2C from high pressure. By the aid of mechanical exfoliation of the bulk structure, one can obtain the 2D monolayer of M2C. One of the predicted Mo2C is subsequently synthesized by molten copper-catalyzed chemical vapor deposition (CVD), and a few more Bernal stackings and a variety of interfaces combing distinct stackings are identified by scanning transmission electron microscopy (STEM).

Spin-spiral dispersion and magnon-phonon interactions in gamma-Fe

Duo Wang

Uppsala University

Unlike α-Fe, some theoretical studies show that γ-Fe is a weak magnet exhibiting magnetovolume instability and non collinear magnetic structure under compression. We did calculations for volume dependence of spin-spiral dispersion in fcc-Fe, the approach implemented in the Vienna Ab initio Simulation Package (VASP) package. It is shown that at low volumes, the magnetic configuration corresponding to the ground state is a spin-spiral at q2 = 2π/a(0.2, 0, 1), whereas for higher volumes the ground state is at q1 = 2π/a(0,0,0.6). We found VASP package is a reliable tool for the calculation of spin-spiral structure because almost all the results we got are consistent with the data from full-potential linearized augmented-plane-wave method (FP-APW+lo) study [1]. Besides that, such system may also show some structural instability depending on the magnetic structure indicating magnon-phonon interactions. We are trying to find out how different magnetic structures affect the lattice vibration.

[1] Elisabeth Sjöstedt and Lars Nordström, Phys. Rev. B 66, 014447 (2002)

Monolayer platinum dichalcogenides with promising applications in solar cell

Hamid Ullah

Ulsan University

The electronic and optical properties of monolayer platinum dichalcogenides, PtX2 (*X*=S,Se,Te), family have been investigated using the density functional theory. We found that the PtS2, PtSe2, and PtTe2 are indirect band gap semiconductor with bandgaps of 2.70 eV, 1.94 eV, and 0.82 eV, respectively. The monolayer platinum dichalcogenides family have strong absorption with very sharp absorption edges, confirming the direct transition from the valence to the conduction band. Their optical absorption spectra show strong optical absorption for these materials is below 4.0 eV, which make them an efficient candidate for solar energy applications. PtS2 and PtSe2 show strongest absorption in the wide range from infra-red to the ultra-violet region of the light spectrum. Furthermore, due to their wider band gap and strong device absorption efficiency make them an excellent candidate for the top cell in the tandem architecture. PtTe2 is considered to be an excellent candidate for bottom cell in the tandem architecture due to its narrow band gap and strong absorption efficiency. Moreover, the band-edge potentials are estimated using Mulliken electronegativity and compared to the redox potential of water to evaluate their possible applications in photocatalysis, we found that PtX2 family can be used to oxidize H2O into O2 but failed to reduce H+ to H2.
