AB INITIO MODELING OF ADVANCED MATERIALS (AMM-2019)

PSI-K WORKSHOP
SATELLITE TO VII EASTMAG SYMPOSIUM

Ekaterinburg
10 – 13 September 2019

Organizers

Ural Branch of Russian Academy of Science

Institute of Metal Physics Ural Branch RAS

Ural Federal University

Institute of Quantum Materials Science, Ltd

Organizing Committee

Yuri Gornostyrev (Ekaterinburg, Russia)
Mikhail Katsnelson (Nijmegen, Netherlands)
Joerg Neugebauer (Dusseldorf, Germany)
Vladimir Anisimov (Ekaterinburg, Russia)

The conference AMM-2019 will focus on the recent progress in the development and application of ab-initio based methods of calculation and thermodynamic/kinetic modelling for microstructure and finite-temperature properties of a wide range of materials, from steel and alloys up to modern functional compounds. The special topics of this, already second AMM conference, will be problems related to magnetism and magnetic materials.

The conference brings together prominent scientists from the area of theoretical modelling to assess the state of the art in applications of the electronic structure theory for the knowledge-based design of advanced materials. Development of any strategy for design of the materials requires combined multi-disciplinary efforts. The aim of the conference is to provide a fruitful atmosphere and framework for development and dissemination of novel ideas and concepts in order to resolve the present challenges in the field.

Master class by Alexander I. Poteryaev the “Application of the AMULET code for DFT+DMFT calculations of realistic compounds” will be held during the conference.

Conference Venue: Onegin Hotel Conference center, 10 – 13 September

The conference is supported and financed by

PSI-K NETWORK

SVERDLOVSK REGION ADMINISTRATION

IMP UB RAS Ekaterinburg

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RTC AUSFERR Magnitogorsk

AMM-2019 conference program

10 September

9:00 –9:55	**Registration. Coffee is served**
9:55 –10:00	**Opening. Welcome talk Yuri Gornostyrev**
SESSION 1: MAGNETIZM AND MAGNETIC MATERIALS	
10:00–13:05	**Chair Joerg Neugebauer**
10:00 –10:40 *Key-note talk*	**Olle Eriksson**, **Attila Szilva,** Uppsala University, Uppsala, Sweden *Spin-lattice simulations; formalism and some initial results*
10:40 –11:20 *Key-note talk*	**Tamio Oguchi,** Osaka University, Osaka, Japan *Materials Design of Heusler Alloys for Spintronics*
11:20 – 11:50	**Coffee break**
11:50 –12:15	**Andrey Katanin**, IMP Ural Branch RAS, Ural Federal University, Ekaterinburg, Russia *Local magnetic moments and their interaction in alpha- and gamma-iron*
12:15 –12:40	**Alexander Yaresko**, Max Planck Institute for Solid State Research, Stuttgart, Germany *Band structure study of anisotropic magnetic interactions in Iridium oxides*
12:40 –13:05	**Peter Igoshev,** Valentin Irkhin, IMP Ural Branch RAS, Ekaterinburg, Russia *Giant van Hove singularities in the density of states of cubic lattices and anomalies of electronic properties*
13:05 –14:00	**Lunch**
14:00-17:55	**Chair Tamio Oguchi, Eva Pavarini**
14:00 –14:40 *Key-note talk*	**Sergey Savrasov,** University of California Davies, USA *Weyl semimetals*
14:40 –15:05	**Yaroslav Kvashnin**, Uppsala University, Uppsala, Sweden *Emergent magnetism at the surface of Heusler semiconductors*
15:05 –15:30	**Attila Szilva**, Uppsala University, Uppsala, Sweden *Beyond the Heisenberg exchange interaction. Theory for non-collinear spin systems*

15:30 –16:00	**Coffee break**
16:00 –16:40 *Key-note talk*	**Ryotaro Arita**, T. Nomoto, Department of Applied Physics, The University of Tokyo, Japan *Anomalous transverse transport and domain wall motion in non-collinear antiferromagnets*
16:40 –17:05	**Luca de' Medici**, Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris (ESPCI), Paris, France *Electronic compressibility and high-Tc superconductivity: new links*
17:05 –17:30	**Nikita Pavlov,** I. Nekrasov, D. Evtushinsky, Institute of Electrophysics UB RAS, Ekaterinburg, Institute of Physics, Ecole Polytechnique Federale, Lausanne, Switzerland *LDA+DMFT spectral properties of $BaNi_2As_2$ and $K_{1-x}Fe_{2-y}Se_2$ superconductors comparison with ARPES*
17:30 –19:00	**Poster session**

11 September

SESSION 2: STRONGLY CORRELATED MATERIALS	
10:00-13:05	**Chair Vladimir Anisimov**
10:00 –10:40 *Key-note talk*	**Leonid Pourovskii**, CPHT-Ecole Polytechnique, Palaiseau, France *Multipolar superexchange interactions and low-temperature ordered phases in actinide dioxides*
10:40 –11:20 *Key-note talk*	**Eva Pavarini**, Forschungszentrum, Jülich, Germany *Spin-orbit effects and magnetism in strongly correlated t_{2g} materials*
11:20 –11:45	**Igor Nekrasov**, Institute of Electrophysics UB RAS, Ekaterinburg, Russia *Magnetocaloric effect: Hartree-Fock vs. DMFT*
11:45 – 12:15	**Coffee break**
12:15 –12:40	**Malte Rösner**, Radboud university, Nijmegen, The Netherlands *Competition of strong charge and spin fluctuations in monolayer NbS_2*
12:40 –13:05	**Jindrich Kolorenc**, Institute of Physics, Czech Academy of Sciences, Prague, *Modeling resonant x-ray emission and resonant inelastic x-ray scattering in the LDA+DMFT framework*
13:05 –14:00	**Lunch**
14:00-16:50	**Chair Igor Abrikosov, Sergey Savrasov**
14:00 –14:40 *Key-note talk*	**Ivan Leonov**, Institute of Metal Physics, Ekaterinburg, Russia *Interplay of electronic structure, magnetic state and lattice stability in iron oxides under extreme conditions*
14:40 – 15:05	**Viktor Pardo,** Universidade de Santiago de Compostela, Spain *Low-valence layered nickelates: a close analogue to the electronic structure of cuprate high-temperature superconductors*
15:05 – 15:30	**Sergey Skornyakov**, V. Anisimov, I. Leonov, Institute of Metal Physics, Ural Federal University, Ekaterinburg, National University of Science and Technology “MISIS”, Moscow, Russia *Electronic structure and phase stability of the superconducting chalcogenides: the case of the parent compounds FeSe and FeS*
15:30 –16:00	**Coffee break**
16:00 – 16:25	**Josef Kaufmann,** Klaus Steiner, Karsten Held, Oleg Janson, TU Wien, Austria, IFW Dresden, Germany, UC Davis, USA

	Dynamical vertex approximation for the Kagome-lattice Hubbard model
16:25 – 16:50	**Lyudmila Tikhonova**, Yu. Mikhalev, Siberian Federal University, Krasnoyarsk, Russia *New nanoscale VTe_2/graphene and VTe_2/graphene/VTe_2 heterostructures for spintronic applications*
17:00 –18:30	**Alexander Poteryaev**, Institute of Metal Physics UB RAS, Ekaterinburg, Russia **Master class** *Application of the AMULET code for DFT+DMFT calculations of realistic compounds*

12 September

SESSION 3: ADVANCED MATERIALS I	
10:00-13:10	**Chair Pavel Korzhavyi, Yuri Gornostyrev**
10:00 –10:40 *Key-note talk*	**Igor Abrikosov**, Linköping University, Linköping, Sweden *Metastable states of matter: a path towards new advanced materials*
10:40 –11:20 *Key-note talk*	**Tilmann Hickel,** Halil Sözen, Fritz Körmann, Jan Janssen, Jörg Neugebauer, Max-Planck-Institut für Eisenforschung, Dusseldorf, Germany *Ab initio based finite temperature phase stabilities of hard-magnetic materials*
11:20 –11:50	**Coffee break**
11:50 –12:30 *Key-note talk*	**Pavel Korzhavyi**, Royal Institute of Technology, Stockholm, Sweden *Ab initio based models of disordered materials*
12:30 –13:10 *Key-note talk*	**Vladimir Mazurenko,** Ural Federal University, Ekaterinburg, Russia *Neural network approaches for material science and quantum computing*
13:10 –14:00	**Lunch**
15:00 –17:00	**City excursion**
19:00	**Conference diner**

13 September

SESSION 4: ADVANCED MATERIALS II	
10:00-13:05	**Chair Mikhail Katsnelson, Leonid Pourovskii**
10:00 –10:40 *Key-note talk*	**Alexander Lichtenstein**, University of Hamburg, Germany *Electron correlations in Magnetic and Superconducting Materials*
10:40 –11:20 *Key-note talk*	**Tony Paxton**, King's College, London, UK *Microscopic origins of plastic anisotropy in magnesium*
11:20 –11:45	**Andrey Sobolev,** South Ural State University, Chelyabinsk, Russia *Interplay between structure and magnetism in (Fe, Cr)7C3 ternary system*
11:45 – 12:15	**Coffee break**
12:15 –12:40	**Alexander Tsirlin**, University of Augsburg, Germany *Kitaev magnetism and dimerization instability in honeycomb iridates*
12:40 –13:05	**Grigory Astretsov**, G. Rohringer, A. Rubtsov, Russia Quantum Center, Moscow State University, Moscow, Russia *Phase diagram of High-Tc cuprates calculated within a multi-scale scheme with controllable approximations*
13:05 – 14:00	**Lunch**
14:00-17:55	**Chair Vladimir Mazurenko, Tilmann Hickel**
14:00 –14:40 *Key-note talk*	**Igor Solovyev**, S. Nikolaev, National Institute for Materials Science, Tsukuba, Tokyo Institute of Technology, Tokyo, Japan *Electric polarization induced by skyrmionics order in GaV4S8: from first-principles calculations to microscopic models*
14:40 –15:20 *Key-note talk*	**Sergey Streltsov**, I. Solovyev, S. Nikolaev, A. Ignatenko, V. Irkhin, Institute of Metal Physics UB RAS, Ekaterinburg, Russia, National Institute for Materials Science, Tsukuba, Tokyo Institute of Technology, Tokyo, Japan *Spin-orbit coupling and Jahn-Teller effect: friends or foes?*
15:20 –15:45	**Alexey Golovchan,** V. Valkov, U. Aparajita, O. Roslyak, V. Koledov, Donetsk Institute for Physics and Engineering, Donetsk, Ukraine, BMCC, CUNY, Fordham University, New York, USA, IREE RAS, 125009 Moscow, Russia *Antiferromagnetic phase transition in Cr_2As via anisotropy of exchange interactions*
15:45 –16:10	**Alexander Edstrom**, Xiangzhou Zhu, Claude Ederer Eidgenössische Technische Hochschule (ETH), Zürich, Switzerland *New Insights into the Magnetic Exchange Interactions of Multiferroic $SrMnO_3$*

16:10 –16:40	**Coffee break**
16:40 –17:05	**Evgeny Stepanov,** A. I. Lichtenstein, M. I. Katsnelson, Ural Federal University, Ekaterinburg, Russia; University of Hamburg, Germany; Radboud university, Nijmegen, The Netherlands *Consistent description of collective electronic fluctuations beyond dynamical mean-field theory*
17:05 –17:30	**Mikhail Petrik**, Yu. Gornostyrev, P. Korzhavyi, Institute of Metal Physics Ural Branch RAS; Institute of quantum materials science, Ekaterinburg, Russia, Royal Institute of Technology, Stockholm, Sweden *Vacancy mediated Guinier-Preston zones to θ'-phase transformation in Al-Cu based alloys*
17:30 – 17:55	**Vladimir Chernyshev**, V. Ryuimshin, Ural Federal University, Ekaterinburg, Russia, *Lattice dynamics and pressure influence on MeF_2 (Me=Ca, Sr, Ba): ab initio calculation*
17:55	**Closing Mikhail Katsnelson, Joerg Neugebauer**

Poster Session and Reception
10 September, 18:00 – 19:30

1	Juan M. Guerra, M. Giar, C. Mahr, M. Czerner, and C. Heiliger, Institute of Theoretical Physics, University of Giessen, Giessen, Germany *Ab initio calculations of electronic properties of thermoelectric Mg_2X-Mg_2Y (X,Y=Si,Ge,Sn) alloys*
2	Sergey Sozykin, Valery Beskachko. South Ural State University, Russia *Optical properties of defective carbon nanotube (11,0)*
3	Alexander Mirzoev, Anastasiia Verkhovykh, South Ural State University, Chelyabinsk, Russia *Ab initio modeling of p, s and c interaction with the grain boundaries in α -iron*
4	Danis Badrtdinov, Vladimir Mazurenko, Alexander Tsirlin, Ural Federal University, Russia, University of Augsburg, Germany *Unusual collinear magnetic order at spinel-type Cu_2GeO_4 system*
5	Arsenii Gerasimov, Y.O. Kvashnin, L. Nordström, V.V. Mazurenko. Ural Federal University, Russia, Uppsala University, Sweden *Wannier functions in ELK code for DFT+DMFT solver*
6	Alexander V. Serdtsev, N. I. Medvedeva, Institute of Solid State Chemistry Ural Branch RAS, Russia, Ural Federal University, Russia *Effect of Hubbard correlations on the sodium diffusion and redox properties of molybdates with alluaudite structure*
7	D. A. Prishchenko, V. G. Mazurenko, M. I. Katsnelson and A. N. Rudenko. Ural Federal University, Ekaterinburg, Russia, Radboud University, The Netherlands, Wuhan University, China *Gate-tunable infrared plasmons in electron-doped single-layer antimony*
8	Dmitriy Nazipov, A. Nikiforov. Ural Federal University, Ekaterinburg, Russia *Raman spectrum and elastic properties of rare-earth oxyorthosilicates R_2SiO_5: Ab initio calculation*
9	Ilya V. Kashin, V. V. Mazurenko, A. N. Rudenko, Ural Federal University, Ekaterinburg, Russia, Radboud University, Nijmegen, The Netherlands. *First-principles investigation of ferromagnetism in chromium triiodide monolayer*
10	Alexander Belozerov, S. Skornyakov, I. Leonov, Institute of Metal Physics UB RAS, Ekaterinburg, National University of Science and Technology 'MISIS', Moscow, Russia *Pressure-induced insulator-to-metal transition in $BiNiO_3$ controlled by lattice effects*
11	Dmitrii Korotin**,** I. Leonov**,** Institute of Metal Physics UB RAS, Ekaterinburg, National

	University of Science and Technology 'MISIS', Moscow, Russia *Mott insulator-metal transition and melting of charge ordering in YNiO3 under pressure*
12	Lyudmila Dobysheva, Physics-Technical Institute, UdmFRC, UB RAS, Izhevsk, Russia *First-principles calculation for alloyed cementite (Fe-Ni-Cr)$_3$C*
13	Ayaz Abdullin, E. Voronina and L. Dobysheva, Kazan Federal University, Russia Physical-Technical Institute of UdmFRC UB RAS, Izhevsk, Russia *First-principles calculations for ternary alloys based on Fe–Al*
14	Svetlsna Krylova, A. Krylov, E. Roginskii, Kirensky Institute of Physics, Krasnoyarsk, Ioffe Institute, Sankt-Petersburg State University, Sankt-Peterburg, Russia *Structural and optical properties of $HoGa_3(BO_3)_4$*
15	Tagir Nuretdinov, A. Volkov, A. Povzner, Ural Federal University, Yekaterinburg, Russia *Electronic structure and zero spin fluctuation in quantum ferromagnets*
16	Andrey Kuznetsov, Yu. Gornostyrev, I. Shmakov, Institute of Metal Physics UB RAS, Institute of Quantum Materials Science Ltd, Institute of Physics and Technology, Ural Federal University, Ekaterinburg, Russia. *Short-range order in advanced soft magnetic alloys*
17	P.I. Bezotosnyy, K.A. Dmitrieva, I.A. Nekrasov, N.S. Pavlov, A.A. Slobodchikov, Lebedev Physical Institute RAS, Moscow, Institute for Electrophysics, UB RAS, Ekaterinburg, Russia *Electronic structure of SnAs: DFT and ARPES study*
18	Vitaly Ryumshin, V. Chernyshev, Institute of natural sciences and mathematics, Ural Federal University, Ekaterinburg, Russia *Crystal structure and lattice dynamics of $Gd_2Ge_2O_7$ crystal: ab initio calculation*
19	Aleksandr Deviatov, I. A. Iakovlev, V. V. Mazurenko, Ural Federal University, Ekaterinburg, Russia, *Recurrent network classifier for ultrafast skyrmion dynamics*
20	Oleg Sotnikov, V. Mazurenko, J. Colbois, F. Mila, M. Katsnelson, E. Stepanov, Ural Federal University, Ekaterinburg, Russia, Institute of Physics, École Polytechnique Fédérale de Lausanne, Switzerland, Radboud University, Nijmegen, The Netherlands, University of Hamburg, Germany *Quantum nanoskyrmion*
21	Ilia Iakovlev, A. A. Bagrov, M. I. Katsnelson, V. V. Mazurenko, Ural Federal University, Ekaterinburg, Russia, Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands *Neural network solution of the kagome problem*
22	Georgiy Pushkarev, V. G. Mazurenko, V. V. Mazurenko D. W. Boukhvalov, Ural Federal University, Ekaterinburg, Russia. College of Science, Institute of Materials Physics and Chemistry, Nanjing Forestry University, China S*tructural phases transition in VSe_2: energetics, electronic structure and magnetism*

23	Sergei Andreev, V.V. Mazurenko, Ural Federal University, Ekaterinburg, Russia *Magnetic interactions in $Sr_3Ir_2O_7$*
24	Anton Filanovich, A.A. Povzner, Ural Federal University, Ekaterinburg, Russia *Ab initio based modelling of the lattice properties of superconducting 115 compounds*

ABSTRACTS
INVITED AND CONTRIBUTED TALKS

SPIN-LATTICE SIMULATIONS; FORMALISM AND SOME INITIAL RESULTS

*Olle Eriksson[1,2], Attila Szilva[1]**

Uppsala University[1], Örebro University[2], Uppsala, Sweden

In this presentation coupled spin- and lattice dynamics will be presented, with details provided both concerning the formalism, as well as the implementation. Examples of spin-lattice dynamics simulations will be presented for bulk and cluster systems. The examples involve influence of spin-lattice coupling on both phonon- and magnon modes, as well as coupled modes. The relevance of spin-lattice simulations for ultrafast magnetization dynamics, e.g. as studied in pump-probe experiments will also be reported. The usefulness of these types of simulations for studying complex alloys, e.g. steel will be discussed.

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MATERIALS DESIGN OF HEUSLER ALLOYS FOR SPINTRONICS

Tamio Oguchi

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Center for Spintronics Research Network, Osaka University, Japan
Institute for Datability Science, Osaka University, Japan

For several decades, Heusler alloys have continuously provided an interesting playground with novel electronic properties applicable to spintronic, thermoelectric, and shape-memory devices. Half-metallicity is well recognized as the most remarkable property among them originating from peculiar electronic states, placing Heusler alloys on the list of promising materials for spintronic applications. General formula of Heusler alloys is a ternary X_2YZ, where X and Y are transition-metal d-electron elements while Z is an *sp*-electron one, leading to a vast number of possible combinations for their composition. Furthermore, two X sites may accommodate different kinds of element (quaternary Heusler alloys: XX'YZ) or one of them may be vacant (half-Heusler alloys: XYZ), resulting in even more possibility of the combinations for designing and/or optimizing properties required by particular applications. In this talk, I shall introduce our recent works by means of first-principles density-functional-theory calculations to explore Heusler alloys with novel electronic properties such as spin gapless states and antiferro-magnetism with high Néel temperatures targeted for spintronic applications.

This work was done in collaboration with F. Kuroda, H. Fujii, and T. Fukushima.

LOCAL MAGNETIC MOMENTS AND THEIR INTERACTION IN ALPHA- AND GAMMA-IRON

A. A. Katanin[1], A. S. Belozerov[1,2], V. I. Anisimov [1,2]*

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[2] Ural Federal University, Ekaterinburg, Russia

Investigations of ferromagnetism of iron attracts a lot of attention in spite of both, theoretical and practical interest to this substance. It was shown in Ref. [1] that alpha-iron possesses local magnetic moments. To explain physical properties of iron it is important to obtain magnetic interaction between these local moments. While major part of previous approaches considered symmetry-broken state, unbiased evaluation of magnetic interaction requires treatment of the symmetric state. We use the ab initio LDA + supercell DMFT approach to determine magnetic interaction between local moments [2,3].

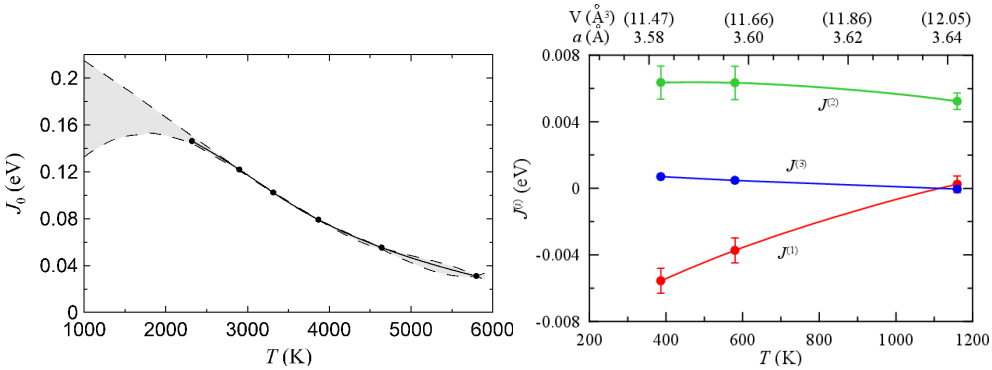

Fig. 1. Temperature dependence of magnetic interaction in alpha (left, reproduced from Ref. [2]) and gamma (right, reproduced from Ref. [3]) iron.

In alpha-iron we find dominating nearest neighbor ferromagnetic exchange, whose magnitude at low temperatures ~0.20 eV is close to previous estimates in the renormalized magnetic force and DLM approaches allowing to reproduce experimental value of the spin stiffness. In gamma-iron we find that nearest neighbor magnetic exchange changes sign at T~1000K, see Fig. 1, such that at low temperatures the antiferromagnetic order with the wavevector $(0,0,2\pi)$ is preferable, while at higher T the ferromagnetic correlations dominate. Close competition of ferro- and antiferromagnetic correlations at high temperatures in γ-iron is in agreement with the experimental data [4].

[1] Katanin A. A., Poteryaev A. I., et al., Phys. Rev. B 2010; 81: 045117.
[2] A. S. Belozerov, A. A. Katanin, V. I. Anisimov, Phys. Rev. B 2017; 96: 075108.
[3] A. A. Katanin, A. S. Belozerov, V. I. Anisimov, Phys. Rev. B 2018; 98: 045138.
[4] P. J. Brown, et al., J. Magn. Magn. Mater. 1983; 30: 335.

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BAND STRUCTURE STUDY OF ANISOTROPIC MAGNETIC INTERACTIONS IN IRIDIUM OXIDES

Alexander Yaresko [1*]

[1] *Max Planck Institute for Solid State Research, Stuttgart, Germany*

Because of strong spin-orbit coupling of Iridium magnetic interaction in Ir^{4+} oxides cannot be described by an isotropic Heisenberg-like model and anisotropic exchange interactions become important. In Sr_2IrO_4 and $Sr_3Ir_2O_7$ with corner sharing octahedra the dominant magnetic interactions are isotropic nearest neighbor coupling *J* and anti-symmetric Dzyaloshinskii-Moriya (DM) interactions. In α-Na_2IrO_3 and other honeycomb iridates with edge sharing IrO octahedra magnetic interaction were suggested to be bond-dependent and to be described by the Kitaev model. I present results of LSDA+U band structure calculations performed for a number of iridates with corner or edge sharing IrO octahedra. The strength of Coulomb repulsion *U* was fixed by comparing calculated optical spectra to experimental data [1]. Effective magnetic interactions were estimated by mapping the total energy differences between various magnetic configurations with constrained Ir moment directions onto a model which includes isotropic Heisenberg-like as well as bond-dependent anisotropic magnetic interactions. In Sr_2IrO_4 and pyrochlore $Y_2Ir_2O_7$ the dominant anisotropic exchange is the anti-symmetric DM interaction. In α-Na_2IrO_3 and some other honeycomb iridates symmetric anisotropic terms are at least as strong as the isotropic ones.

[1] *Proepper D, Yaresko A, Hoeppner M,.Matiks Y, Mathis Y-L, Takayama T, Matsumoto A, Takagi H, Keimer B, Boris AV Phys Rev B 2016; 94:035158.*

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GIANT VAN HOVE SINGULARITIES IN THE DENSITY OF STATES OF CUBIC LATTICES AND ANOMALIES OF ELECTRONIC PROPERTIES

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Starting from the correspondence with the square lattice, we investigate the density of states (DOS) $\rho(\varepsilon;\tau)$ for the simple (sc), base-centered (bcc) and face-centered (fcc) cubic lattices with account of nearest- and next-nearest-neighbor hopping. t and t'. for different ratios $\tau = t'/t$. The corresponding analytical expressions in terms of elliptic integrals and singular power-law DOS asymptotics for peculiar τ values are obtained. The singular contributions owing to Van Hove (vH) point and lines are treated. The change of topology of isoenergy surfaces with τ is considered.

For the sc lattice, such a change takes place at τ=1/4 when a giant van Hove singularity occurs (the vH singularity line Λ is formed) due to merging of energy levels of band bottom (Γ) and saddle-type (X) **k** points are present at τ<0.25, which results in the singularity $\rho \sim (\varepsilon+3t)^{-1/4}$. For $\tau \gtrsim 0.25$ the structure formed by **k** points with low velocity induces a narrow plateau between two van Hove saddle points energies w_{Λ^*} and w_{Σ^*} (points on Σ and Λ lines, corresponding to vH singularity point) where DOS is strongly enhanced and varies only weakly (the situation at small τ is different: here a broad plateau is present between X and M points). This Σ-Λ feature is rather stable (see examples in Fig. 1a at $\tau = 0.4$, 0.75) and decays weakly when τ moves away from τ=0.25 upwards: $\rho(w_{\Lambda^*};\tau) \approx \rho(w_{\Sigma^*};\tau) \sim (4\tau-1)^{-1/2}$, whereas its width is $4(\tau-1/4)^2 t/\tau$.

For the bcc lattice, at τ=0 we have the vH singularity line D (PN) with $\rho \sim \log^2(t/\varepsilon)$ when the energy levels $w_{\rm P}$, $w_{\rm N}$, w_{Λ^*} at small positive τ merge. When τ increases from 0 to 1, the maximum of DOS is achieved at $\varepsilon = w_{\Lambda^*} = 2\tau(2\tau^2 - 3)t$. Its energy level corresponds to vH point Λ^* which is split off from P point and migrates to Γ point along the Λ line as τ increases. At $\tau = 1$ the change of spectrum topology occurs, and $\rho(\varepsilon;\tau)$ has two-side giant VH singularity $\sim (\varepsilon+2t)^{-1/4}$ produced by vH line Σ (ΓN), which originates from merging of vHS levels w_Γ , $w_{\rm N}$, w_{Λ^*} (w_{Δ^*}). When τ is close to 1, the vH structure is determined by three levels: at $\tau < 1$ it is formed by a wide asymmetric plateau between $w_{\rm N}$ and w_{Λ^*} (width $\sim (\tau-1)$) and sharp drop between levels w_{Λ^*} and w_Γ (width $\sim (\tau-1)^2$); at $\tau > 1$, a asymmetric plateau between the levels $w_{\rm N}$ and w_{Δ^*} (width $\sim (\tau-1)$) and sharp drop between levels w_{Δ^*} and w_Γ (with much smaller width, $\sim (\tau-1)^2$) occur. For vH points Γ, Σ^* and Λ^* all three masses diverge as $(\tau-1)^{-1}$, whereas for N only one mass has such a divergence. Such a complicated structure of VH points considerably distinguishes the bcc and sc lattices and leads to peculiar thermodynamic properties. The treatment of the DOS singularities in the ferromagnetic state can be relevant for the α-γ-δ transformation in the bcc iron.

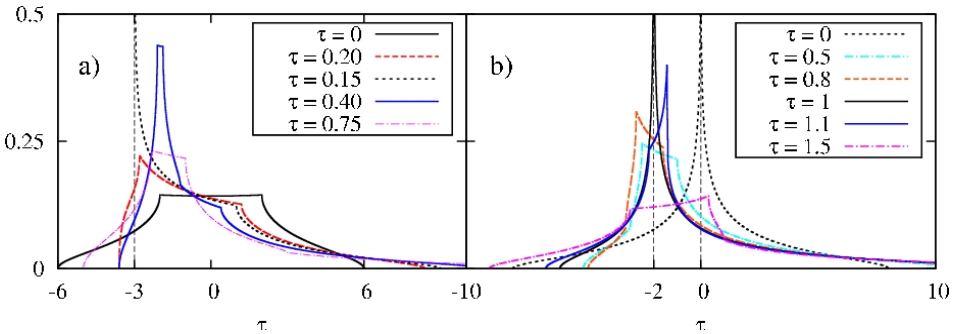

Fig. 1 Density of states at van Hove singularity points at different τ (a) sc lattice, (b) bcc lattice.

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WEYL SEMIMETALS

Sergey Savrasov[1]

[1]*University of California Davies, United States*

Weyl semimetals, a three-dimensional analog of graphene with linearly dispersing excitations, has become an active research arena with 1000s of published articles for the last 8 years. In this talk I will overview the state of the field, starting from the main physical properties of Weyl semimetals such as chiral anomaly and existence of disconnected Fermi arcs surface states. A variety of materials that have recently been proved to exhibit Weyl semimetal behavior will be discussed both from theoretical and experimental standpoints, including their high throughput screening in infinite space of chemically allowed compounds as well as angle resolved photoemission results uncovering topological surface states. Finally, most recent developments on ultra-high conductivities in Weyl semimetal nanostructures and searches for Weyl semimetal states in correlated electron systems will be presented.

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EMERGENT MAGNETISM AT THE SURFACE OF HEUSLER SEMICONDUCTORS

Yaroslav Kvashnin[1], Samara Keshavarz[1], Igor Di Marco[1,2,3], Danny Thonig[1], Liviu Chioncel[4,5], Olle Eriksson[1,6]*

[1] Department of Physics and Astronomy, Uppsala University, Sweden
[2] Asia Pacific Center for Theoretical Physics, Pohang, South Korea
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[4] Theoretical Physics III, University of Augsburg, Germany
[5] Augsburg Center for Innovative Technologies, Germany
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The Heusler compounds seem to never exhaust the possibility to surprise and challenge the materials science community. In this work we investigate a relatively new class of Heusler semiconductors with a general formula XX'YZ. Bulk and interface properties of these materials have been previously studied in detail by means of first-principles calculations [1,2,3].

Here, we make a prediction that these non-magnetic bulk semiconductors host metallic magnetic states, which appear spontaneously at the surface. Such a drastic modification of the electronic and magnetic properties is extremely rare if not unique and is thoroughly investigated in our work.

We have found pronounced magnetic moments at the surface of several systems of this family of compounds. A special attention is paid to CoMnVAl, for which we also compute and analyse the Heisenberg exchange interactions. Based on the obtained coupling constants, we performed Monte Carlo simulations, which suggest that magnetism should persist up to temperatures at least as high as 170 K. Adiabatic magnon spectrum also suggests a stable magnetic order, where Co and Mn spins at the surface are aligned parallel to each other and antiparallel with respect to V moment, located in the layer below.

We also discuss experiments, which could confirm the suggested effects as well as their possible technological applications.

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BEYOND THE HEISENBERG EXCHANGE INTERACTION. THEORY FOR NON-COLLINEAR SPIN SYSTEMS

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We show for a simple noncollinear configuration of the atomistic spins (in particular, where one spin is rotated by a finite angle in a ferromagnetic background) that the pairwise energy variation computed in terms of multiple-scattering formalism cannot be fully mapped onto a bilinear Heisenberg spin model even in the absence of spin-orbit coupling. The non-Heisenberg terms induced by the spin-polarized host appear in leading orders in the expansion of the infinitesimal angle variations. However, an e_g and $t2_g$ symmetry analysis based on the orbital decomposition of the exchange parameters in bcc Fe leads to the conclusion that the nearest-neighbor exchange parameters related to $t2_g$ orbitals are essentially Heisenberg-like: they do not depend on the spin configuration, and can, in this case, be mapped onto a Heisenberg spin model even in extreme noncollinear cases. We show the symmetry resolved interatomic exchange for other 3*d* materials and, finally, we mention the concept of a non-collinear direct Weiss-field calculation.

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UNRAVELING THE GLASSY NATURE OF THE MAGNETIC STATE OF ND

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Spin glasses are a fascinating but poorly understood magnetic state of matter, appearing in complex alloys like iron-based superconductors and magnetically-doped metals, like Mn-doped Cu. Intricately linked to spin frustration and disorder, spin glasses exhibit no long-range magnetic order upon cooling. Likewise, spin glasses exude the distinguishing phenomenon known as aging, where the magnetic state is dependent on the history of the material, unlike quantum spin liquids. Here we show a new type of non-collinear spin glass order, or so-called spin-Q glass, observable in elemental Nd(0001) in the absence of disorder. Using spin-polarized scanning tunneling microscopy down to mK temperature, we visualize the competing local non-collinear order at the atomic-scale and probe the subsequent aging phenomena in response to variable magnetic field and temperature. We relate the resultant glassy behavior to the crystalline symmetry, which leads to competing magnetic interactions. Results from ab initio calculations will also be discussed.

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ANOMALOUS TRANSVERSE TRANSPORT AND DOMAIN WALL MOTION IN NON-COLLINEAR ANTIFERROMAGNETS

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Recently, Mn_3Sn has attracted considerable attention as a magnetic Weyl semimetal [1] exhibiting a large anomalous Hall effect [2,3,4] and anomalous Nernst effect [5,6]. While these effects are usually observed in ferromagnets, the net (uniform) magnetization is vanishing small in the non-collinear antiferromagnetic structure of Mn_3Sn. Interestingly, this magnetic structure can be viewed as ferroic ordering of cluster magnetic octupoles. In fact, this octupole can induce anomalous transverse transport, since its irreducible representation is the same as that of the magnetization (magnetic dipole) [7]. More recently, Higo *et al*. have observed a large magneto-optical Kerr effect in Mn_3Sn, and succeeded in visualizing magnetic octupole domains and their reversal [8].

Motivated by this experiment, we perform numerical simulations with the atomistic Landau-Lifshitz-Gilbert (LLG) equation and investigate the dynamics of a domain wall in Mn_3Sn. We show that the spin-orbit torque drives the domain wall much faster than that in ferromagnets. Next, we rewrite the LLG equation in terms of cluster multipoles and derive an equation of motion for the magnetic octupole, which can be solved analytically. The analytical solution reproduces the numerical simulation very accurately. This result indicates that the cluster magnetic octupole is a useful order parameter to describe the domain wall motion and spin dynamics in non-collinear antiferromagnets.

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ELECTRONIC COMPRESSIBILITY AND HIGH-TC SUPERCONDUCTIVITY: NEW LINKS

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In multi-orbital Hubbard models including strong intra-atomic exchange a so-called "Hund's metal" phase is realized that, among other hallmarks, typically shows a strong differentiation in the degree of correlation of the conduction electrons based on their orbital character. This selective physics is also a key player in Iron-based superconductors (FeSC), where a wealth of experimental evidences validates this theoretical picture.

We here show that at the frontier between this Hund's metal phase and a conventional metal, the electronic compressibility is strongly enhanced or even divergent, and that among the FeSC, those that have a high Tc are placed in our simulations on this frontier. This same theoretical evidence of enhanced compressibility at the frontier between a phase with selective correlations and a more conventional metal is found in cuprates, and we will outline the main indications for a common scenario of high-Tc superconductivity.

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LDA+DMFT SPECTRAL PROPERTIES OF $BaNi_2As_2$ AND $K_{1-x}Fe_{2-y}Se_2$ SUPERCONDUCTORS COMPARISON WITH ARPES

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The $BaNi_2As_2$ superconductor was investigated using the angle-resolved photoemission spectroscopy (ARPES) and the dynamical mean-field theory (LDA+DMFT). The results showed a weak manifestation of correlations. The effective mass is about 1.2. The experimental resolution and mainly the final-state lifetime effects mask the unchanged LDA electronic structure, by prefacing it in a manner similar to the electronic structure formed by the correlation effects. The main result is that LDA+DMFT analysis of ARPES data is very important for distinguishing correlation effects from the experimental resolution and the final-state lifetime effects (see Fig. 1).

Also, we provide theoretical LDA+DMFT support of recent ARPES experimental observation [1] of the so called hidden hole like band and corresponding hidden Fermi surface sheet near Γ-point in the $K_{0.62}Fe_{1.7}Se_2$ superconductor. To some extent this is a solution to the long-standing riddle of Fermi surface absence around Γ-point in the $K_xFe_{2-y}Se_2$ class of iron chalcogenide superconductors. In accordance with the experimental data the Fermi surface was found near the Γ-point within LDA+DMFT calculations [2].

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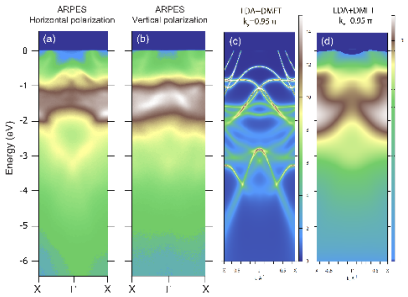

Fig. 1 (a,b) ARPES, (c) LDA+DMFT spectral function map and (d) with a experimental resolution and the final-state lifetime effects for $BaNi_2As_2$.

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MULTIPOLAR SUPEREXCHANGE INTERACTIONS AND LOW-TEMPERATURE ORDERED PHASES IN ACTINIDE DIOXIDES

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Localized *f*-shells in lanthanide and actinide compounds may give rise not only to conventional dipole magnetic moments, but also to higher rank multipole ones [1]. Intersite interactions between such high-rank multipoles may either impact the magnetic order or induce purely multipole-ordered phases. Such ordered states are not seen by the neutron diffraction; hence, they are often named "hidden-order" phases.

We study the effect of superexchange interactions between high-rank multipole local moments in the prototypical example of actinide dioxides AO_2. These interactions are evaluated on the basis of ab initio density-functional+dynamical mean-field theory (DFT+DMFT) in conjunction with a quasi-atomic approximation to local correlations on the actinide 5f shell. Starting from the high-temperature local-moment paramagnetic state described within this DFT+DMFT framework, we derive the exchange interactions by evaluating the response of DFT+DMFT functional to small fluctuations in atomic configurations on two neighboring sites [2]. The method is shown to correctly reproduce the intersite exchange in the insulating regime of simple one-band and two-band Habbard models. Applying this approach to UO_2 we evaluate the superexchange coupling between the dipole and quadrupole moments of the U 5*f* shell [3]. The calculated superexchange Hamiltonian has a non-collinear 3**k** antiferromagnetic (AFM) ground state, in agreement with the experimental magnetic structure of UO2. We find that the stabilization of 3k AFM is due to a subtle anisotropy of the quadrupolar superexchange lifting the degeneracy between various AFM structures on the frustrate fcc U sublattice. The exotic 3**k**-AFM order in UO_2 can thus be accounted for by a purely electronic superexchange mechanism. Applying the same approach to NpO_2 we predict a purely multipolar low-temperature ordered state with no dipole magnetic moments and a primary triakontadipole rank-5 order parameter.

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SPIN-ORBIT EFFECTS AND MAGNETISM IN STRONGLY CORRELATED t2g MATERIALS

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Strong-correlation effects in systems with low symmetry, non-spherical Coulomb vertex and spin-orbit interaction are particularly difficult to describe. The core of the problem is that, in QMC-based LDA+DMFT calculations, these terms sizably increases the computation time. This has two reasons. The first is the increase in the number of degrees of freedom that have to be considered and the second the fact that a strong sign problem might appear. Recently it has been shown that, with specific basis choices, calculations for t2g materials are feasible down to experimental temperatures [1]. In this talk, I will apply this technique to explain the electronic properties of representative t2g materials [1-5]. For the unconventional superconductor Sr_2RuO_4 I will clarify the key role played by spin-orbit coupling and tetragonal Coulomb terms in determining the topology of the Fermi surface. For the Mott insulator Ca_2RuO_4, I will show that the spin-orbit interaction plays a little role in the metal-insulator transition. For the magnetic phase, two different scenarios have been proposed, the local spin-moment (S = 1) scenario and the zero total-angular-momentum (or van-Vleck) picture. I will show that magnetic order and spin-wave spectra are well described in the perturbative spin-orbit limit, thus excluding the van-Vleck scenario. For Sr_2RuO_4 I will discuss the range of validity of the resilient quasi particle scenario.

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MAGNETOCALORIC EFFECT: HARTREE-FOCK VS DMFT

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In this work we investigated change of entropy within magnetocaloric effect (MCE) for metallic strongly correlated systems. We consider case of second order magnetic phase transitions such as ferromagnet-paramagnet.

Here we systematically study MCE within the framework of the dynamical mean-field theory (DMFT) [1] for the one band doped Hubbard model and compare it with our previous results for the mean-field solution of the Hubbard model [2]. It is shown that the temperature profile of the DMFT obtained entropy change has quine universal behavior and is very close to the mean-field results, although has some peculiarities (see Fig. 1).

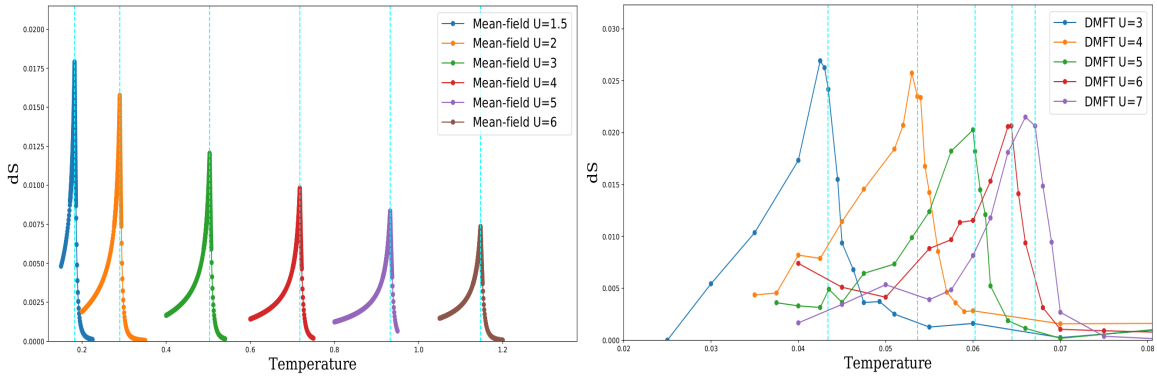

Fig. 1 Isothermal entropy change (under magnetic field change Δh = 0.001D) calculated within mean-field approximation for one band Hubbard model (left panel) and DMFT (right panel). Cyan vertical lines correspond to Curie temperatures at given Coulomb interaction U.

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COMPETITION OF STRONG CHARGE AND SPIN FLUCTUATIONS IN MONOLAYER NBS_2

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Single-layers of transition metal dichalcogenides have rich phase diagrams featuring metallic, insulating and charge/spin density wave phases. Competing interactions lie beneath these competing phases. Theoretical descriptions have so far focused on the electron-phonon interactions in these materials, whereas the electron-electron interaction has mostly been ignored. In this talk, we show that in NbS_2 the local Coulomb interaction is by itself strong enough to turn the material insulating. Screening by the electron-phonon and the non-local Coulomb interaction restores the metallic phase, leads to a broadening of the electronic spectral function, and to a coexistence of strong charge and spin fluctuations. These results are obtained by combining an ab-initio determination of the band structure and Coulomb interaction with the Dual Boson approach for the extended Hubbard model.

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MODELING RESONANT X-RAY EMISSION AND RESONANT INELASTIX X-RAY SCATTERING IN THE LDA+DMFT FRAMEWORK

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I will discuss a theoretical description of photon-in/photon-out resonant x-ray spectroscopies, which is based on the Anderson impurity model. The parameters of the model are determined with the aid of the material-specific LDA+DMFT method, and the spectra themselves are calculated using a combination of the Krylov subspace techniques.

I will briefly demonstrate that the proposed method accurately reproduces the resonant x-ray emission spectra (RXES) measured at the L-edge in lanthanides under pressure [1], and then I will show how one can use it to deduce and quantify the increase of fluctuations of the 4f-states occupation with increasing compression [2].

As a second application, I will discuss the valence-to-core resonant inelastic x-ray scattering (RIXS) at the europium L_3 edge in the ferromagnetic semiconductor EuS. In this setup, the main signal comes from the direct RIXS: an Eu 2p core electron is excited to an empty Eu 5d band above the Fermi level, and then another electron from an Eu 5d state hybridized with the S 3p bands (located below the Fermi level and hence occupied) fills back the Eu 2p core hole. I will analyze if one can expect to detect also indirect RIXS processes where additional excitations are induced by the Coulomb potential of the 2p core hole.

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INTERPLAY OF ELECTRONIC STRUCTURE, MAGNETIC STATE AND LATTICE STABILITY IN IRON OXIDES UNDER EXTREME CONDITIONS

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Iron oxides are important minerals in our planetary system and are among the major constituents of the deep Earth's interior. The theoretical understanding of their electronic structure, magnetic properties, and structural phase stability is of fundamental importance for modeling the properties and evolution of the Earth's lower mantle and outer core. Here, we employ a combination of the *ab initio* band structure methods and dynamical mean-field theory (DFT+DMFT) to determine the electronic structure, magnetic state, and crystal structure phase stability of the paramagnetic phases of wüstite FeO, hematite Fe_2O_3, and pyrite-type FeO_2 at high pressures. Our results reveal a complex interplay between electronic correlations and the lattice in the above-mentioned compounds under extreme conditions. In particular, in the vicinity of a pressure-induced Mott transition FeO and Fe_2O_3 are found to exhibit a series of complex electronic, magnetic, and structural transformations, which are accompanied by a collapse of local magnetic moments and delocalization of the Fe *3d* electrons under pressure. Our results for structural optimization of FeO_2 within DFT+DMFT show that FeO_2 is a metal and that the oxidation state of Fe is equal to nearly 3+. In contrast to the previous claims, we found no noticeable oxygen-oxygen bonding in FeO_2 to at least 180 GPa (no evidence for the O_2 dimerization), implying that the oxidation state of oxygen in pyrite-type FeO_2 is 1.5- due to the oxygen-to-metal negative charge transfer. This suggests that similar to iron, oxygen may have multiple valence states in the deep Earth's interior. Moreover, our calculations of the relative stability of FeO, FeO_2 and Fe_2O_3 reveal that FeO_2 is unstable below ~40 GPa. In agreement with experiment, it is found to decompose into Fe_2O_3 with release of oxygen, suggesting the importance of iron oxides in oxygen cycling between Earth's reservoirs. Under ultra-high pressures above ~220 GPa, Fe_2O_3 decomposes into FeO and FeO_2. Our results demonstrate that electronic correlations are critically important to explain the electronic state and the lattice stability of iron oxides under pressure.

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LOW-VALENCE LAYERED NICKELATES: A CLOSE ANALOGUE TO THE ELECTRONIC STRUCTURE OF CUPRATE HIGH-TEMPERATURE SUPERCONDUCTORS

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For decades, physicists have struggled to understand the underlying physical mechanisms behind the high-temperature superconductivity in layered copper oxides. One possible route towards finding new clues about the puzzle is the search for electronic structure analogue systems. The closest one, in principle, would be nickel oxides, since Ni^{+} is isoelectronic to Cu^{2+}. However, finding a parent insulating antiferromagnetic Ni^{+}-based oxide looks difficult, $LaNiO_2$ being metallic [1]. Other examples, based on Ni^{3+} systems, such as $LaNiO_3$ superlattices, seem not to give the Jahn-Teller distortion that splits the e_g electronic bands so strongly in the parent cuprates and hence have limited applicability in connection to the cuprates [2].

In this talk, we will discuss some recent findings [3-7] about the electronic structure and magnetic properties of low-valence layered nickelates. We have carried out a series of calculations in various members of the series $R_{n+1}Ni_nO_{3n+2}$ formed by n NiO_2 planes separated by a wide RO spacing layer leading to a quasi-two-dimensional structure where antiferromagnetism together with insulating behaviour appears in a region of the phase diagram close to the d-band filling where cuprates become superconducting.

We will show how recent experimental and theoretical efforts are happening to drive this type of system closer to the nominal Ni^{+}:d^9 filling where comparisons with the cuprates can be carried out systematically. We will discuss the various different phases that have been obtained, both theoretically and experimentally and provide an outlook towards future directions within this kind of systems.

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ELECTRONIC STRUCTURE AND PHASE STABILITY OF THE SUPERCONDUCTING CHALCOGENIDES: THE CASE OF THE PARENT COMPOUNDS FeSe AND FeS

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We report results of a detailed theoretical study of the structural, electronic and magnetic properties of the tetragonal paramagnetic phase of Fe(Se,S) employing a fully charge self-consistent method combining density functional theory and dynamical mean-field theory (DFT+DMFT). In particular, we perform a structural optimization and compute the evolution of the electronic structure and the symmetry of magnetic correlations of the tetragonal (space group P4/nmm) paramagnetic phase of FeSe and FeS upon lattice compression and expansion. We show that in both compounds the equilibrium lattice parameters determined within nonmagnetic DFT are underestimated compared to experiment, implying a crucial importance of electronic correlations. By contrast, the lattice parameters obtained within DFT+DMFT are in good quantitative agreement with experimental data. Most importantly, our results reveal a topological change of the Fermi surface (Lifshitz transition) upon expansion (in FeS) and both compression and expansion (in FeSe) of the lattice volume. Namely, in FeSe upon compression the Lifshitz transition is accompanied by a two- to three-dimensional crossover and a small reduction of the quasiparticle mass renormalization as compared to ambient pressure. The behavior of the momentum-resolved magnetic susceptibility is consistent with the observed reduction of the degree of the in-plane π,π stripe-type nesting. Upon a moderate expansion of the lattice both FeSe and FeS show a remarkable change of the electronic structure accompanied by a complete reconstruction of the Fermi surface. The phase transition now results in a strong enhancement of orbital-selective electronic correlations and a change of the symmetry of dominant magnetic correlations from π,π to $\pi,0$ in FeSe and an overall enhancement of spin fluctuations in FeS. This transition is associated with a crossover from itinerant to orbital-selective localized magnetic moments.

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DYNAMICAL VERTEX APPROXIMATION FOR THE KAGOME-LATTICE HUBBARD MODEL

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[2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany
[3] UC Davis, USA

In recent years the geometrically frustrated Kagome lattice has been in the focus of many model studies. However, most of them were done in the context of the Heisenberg model, whose ground state is believed to be a spin-liquid. Much less is known about the parent Hubbard model, which includes both electron hopping and local Coulomb repulsion on equal footing. Therefore it is very difficult obtain even approximate solutions.

A very successful approximation is made in the dynamical mean-field theory, where one obtains an auxiliary impurity model. To overcome its inherent restriction to local correlations, we employ the dynamical vertex approximation [1]. Here, the momentum dependence is generated through Feynman diagrams, with a local (but dynamical) irreducible two-particle vertex as a basic building block [2]. It has been successfully applied to lattices without frustration, but the current project is the first application of dynamical vertex approximation to a frustrated system.

As a result, we obtain sizable non-local components in the self-energy. The effect of geometrical frustration becomes manifest in the magnetic structure factor, which is essentially independent of temperature at low temperatures.

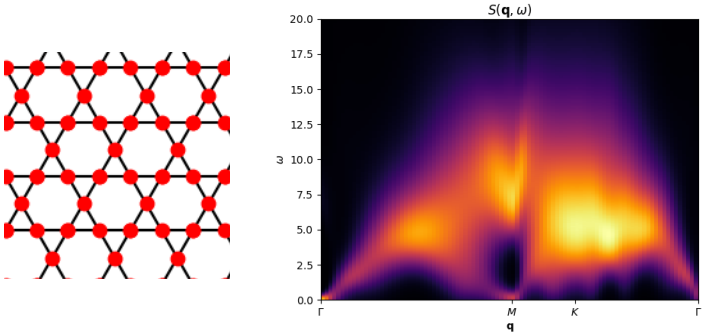

Fig. 1: Kagome lattice (left), dynamical structure factor (right)

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NEW NANOSCALE VTe_2/GRAPHENE AND VTe_2/GRAPHENE/VTe_2 HETEROSTRUCTURES FOR SPINTRONIC APPLICATIONS

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The structural, magnetic and electronic properties of bilayer and threelayer vertical heterostructures based on graphene and ferromagnetic VTe_2 monolayers were studied using a DFT approach. The results show that the interaction between monolayers changes the electronic structure of 2D *T*-VTe_2 from metallic to half-metallic (see at Fig. 1). The electronic subsystem of graphene fragment is slightly hole doped with exchange-mediated spin splitting at the Dirac point. In contrast to the freestanding monolayer the *T*-VTe_2 fragment has magnetic easy axis along *x* direction. The TMR ratio estimated within the Julliere model for favorable triple heterostructure is 220%. Proposed triple heterostructure can be used as magnetic tunnel junction for novel spintronic devices.

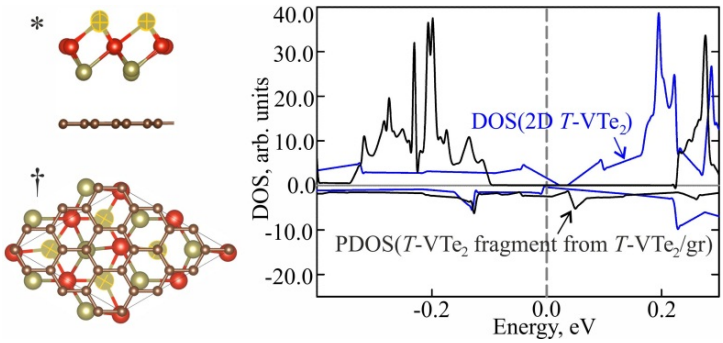

Fig. 1 Side (*) and top (†)views of bilayer *T*-VTe_2/graphene and the electronic structure of *T*-VTe_2 fragment (black lines) versus the electronic structure of freestanding 2D *T*-VTe_2 (blur line)

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METASTABLE STATES OF MATTER: A PATH TOWARDS NEW ADVANCED MATERIALS

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Theory of Gibbs [1] is the foundation for understanding of materials stability. It is broadly used by scientists and engineers, and its predictive power is well established for materials in the equilibrium state, the state with the lowest energy called the ground state. However, deep insights into mechanisms leading to the formation of metastable phases with energies above the ground state energy are missing, despite their wide appearance in nature and the broad use in technology. The luck of a consistent theory in this field limits our ability to discover and design novel materials.

The interest in developing quantitative accurate theoretical tools to predict metastable phases is great. However, the complexity of the problem, that address thermodynamics and kinetics of phase transformations makes its solution truly challenging. Ceder's group has made perhaps the first attempt to address the challenge systematically within the first-principles approach [2], making an attempt to quantify the thermodynamic scale of metastability in terms of the energy differences between stable and metastable structures. It turned out that the scale was broad. Moreover, it depended on chemistry and composition, varying from ~10 meV/atom for iodides to ~190 meV/atom for nitrides. The study made it clear that fundamental understanding of metastable states of matter is in its infancy, at best.

Indeed, our studies of the behavior of matter at high pressure challenge the accepted energy scale accessible to metastable materials. In particular, two new high-pressure silica phases, coesite-IV and coesite-V have just been discovered in experiments [3]. Their crystal structures are built of four-, five-, and six-coordinated silicon, coesite-IV and coesite-V contain SiO_6 octahedra, which, at odds with 3rd Pauling's rule, are connected through common faces. This has never been observed or even expected in silica, silicates or glasses. Our theoretical calculations have confirmed that within the experimentally studied pressure range (30-50 GPa) coesite-IV and coesite-V are ~400 meV/ion above the ground state, which is well beyond all know metastability limits [2]. However, calculated structural parameters are in perfect agreement with experiment and phonon dispersion relations indicate the dynamic stability of the phases. We further illustrate intriguing features of recently discovered polynitrides [4], as well as transition metal nitrides relevant for industrial applications [5,6].

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AB INITIO BASED FINITE TEMPERATURE PHASE STABILITIES OF HARD-MAGNETIC MATERIALS

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Recent developments in electrical transportation and renewable energies have significantly increased the demand of hard magnetic materials with a reduced critical rare-earth content, but with properties comparable to (Nd,Dy)-Fe-B permanent magnets. Though promising alternative compositions have been identified in high-throughput screenings [1], the thermodynamic stability of these phases in a realistic microstructure against decomposition into structures with much less favorable magnetic properties is often unclear. In the case of Ce-Fe-Ti alloys we have used finite temperature ab initio methods to provide this missing information [2]. We have first evaluated the performance of density functional theory (DFT) for the calculation of thermodynamic properties of the rare-earth element Ce and its alloys. Afterwards the Helmholtz free energy, F(T; V), is calculated for the desired hard magnetic $CeFe_{11}Ti$ phase and all relevant competing phases. Though the electronic and vibrational contributions are significant, the magnetic contribution turned out to be decisive for this competition. Our ab initio based free energy calculations reveal that the presence of the $CeFe_2$ Laves phase suppresses the formation of $CeFe_{11}Ti$ up to 700 K. The result is in agreement with experiments based on reactive crucible melting (RCM) and energy-dispersive X-ray spectroscopy (EDS). The insights obtained are used to screen a large set of transition metals in a quaternary extension of the Ce-Fe-Ti system to improve the stability of the $CeFe_{11}Ti$ phase. This approach is discussed in the broader context of simulation platforms [3] for extending high throughput materials discovery to finite temperatures.

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STRUCTURE, STABILITY, AND MOBILITY OF ATOMIC DEFECTS IN STRONGLY BONDED COMPOUNDS

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Transition-metal (TM) oxides, nitrides, and carbides combine ceramic-like properties with metal-like properties, which is a desirable combination of for many existing and emerging applications of these compounds [1]. Ab inito calculations can give us the energies of atomic defects and defect arrangements, as well as the possibility to simulate the processes of defect migration through the lattice. This information is essential for modeling the structure and property evolution in these materials during manufacturing and service.

Systematic *ab initio* studies show that the formation energy of di-vacancies (Schottky defects) in cubic TM–*X* compounds decreases along the series *X* = C, N, O. Thus, for example, vacancies are stable defects in TiO [2], while in TiC the formation energy of a dissociated Schottky pair in TiC appears to be too high for Ti mono-vacancies to be mediators of Ti self-diffusion [3]. Other mediators of TM diffusion have thus been considered, including clusters of vacancies [4] and interstitial atoms [5,6].

We revisit the diffusion mechanisms in TiC, based on the recent finding of a new (symmetry-broken) configuration of a Ti mono-vacancy that is almost twice as low in energy as its usually considered (symmetric) configuration. This configuration does not form by itself as a result of structural relaxation, because the symmetric configuration is a local energy minimum. We explore the configurational space of Ti mono-vacancy to locate other energy minima. Among them, a planar symmetry-broken configuration with the optimal number, length, and angles of C—C bonds is found to be the global energy minimum. Formation of these symmetry-broken configurations is essential for describing Ti self-diffusion in TiC by the Ti mono-vacancy mechanism.

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NEURAL NETWORK APPROACHES FOR MATERIAL SCIENCE AND QUANTUM COMPUTING

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Amazing progress in development of machine learning techniques changing our everyday life can also facilitate the solution of challenging problems in material science and related fields in physics [1,2].

In my talk, I will discuss neural network approaches we developed for recognition and classification of the complex non-collinear magnetic structures formed in two- and three-dimensional materials at finite temperatures and magnetic fields [3,4]. In contrast to standard methods of machine learning such approaches allow one to analyse transitional areas between different phases. A special focus will be on recurrent neural network classifier of ultrafast magnetization processes in systems with Dzyaloshinskii-Moriya interaction. The last part of my talk will be devoted to a new neural network eigensolver for quantum computers [5].

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ELECTRON CORRELATIONS IN MAGNETIC AND SUPERCONDUCTING MATERIALS

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Effects of electron correlations in real materials, including magnetic transition metals and superconducting compounds will be discussed. Modern density functional theory (DFT) describe in principle only ground state properties but not magnetic excitations and superconducting d-wave pairing in strongly correlated materials [1]. We used realistic dynamical mean field theory (DFT+DMFT) which allowed to study the correlations effects in different d- and f-systems. In order to investigate charge and spin non-local excitations we formulate a general framework which start from the DMFT solution for strongly correlated materials within a numerically exact continuous-time Quantum Monte Carlo impurity solver [2]. Then we use a path integral transformation to find an optimal diagrammatic series for many-body Green functions as extension of GW scheme [3]. Prospects of self-consistent theoretical description for correlated systems based on GW++ theory with strong non-local magnetic fluctuations will be addressed.

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MICROSCOPIC ORIGINS OF PLASTIC ANISOTROPY IN MAGNESIUM

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It has been known for many years that the total energy in a free electron like metal may be cast into real space, where it becomes a long-ranged oscillating pair potential. This result is exact to first order in the pseudopotential. However, the pair potential is dominated by a term depending only on the average atomic volume, and moreover the pair potential is itself a function of the volume. These difficulties have meant that the generalized pseudopotential theory of John Moriarty is seldom used in atomistic simulations. We have overcome these difficulties, and I will present million atom simulations with electronic structure accuracy which serve to determine core structures of <a> dislocations in pure magnesium. The very strong plastic anisotropy can be partially understood from these simulations. From a metallurgical point of view, it will be valuable to extend the method into an alloy theory. Our ultimate goal is to find substitutions for the politically strategic rare-earths which can confer the same beneficial properties in terms of formability and the reduction of basal texture.

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INTERPLAY BETWEEN STRUCTURE AND MAGNETISM IN $(Fe, Cr)_7C_3$ TERNARY SYSTEM

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The ternary iron-chromium-carbon alloy system is the foundation stone of the large class of industrially important materials – stainless steels and white cast irons. It is known that iron-chromium-carbon melt forms upon crystallization a series of carbidic and mixed carbidic phases, moreover, their relative stability experiences significant changes near the concentration point of 13 at.% of chromium. This fact is very important for practical metallurgy, but the cause of the phenomenon is poorly understood. Recently, with ab initio simulations, it was found that magnetic frustration caused by competing ferromagnetic Fe-Fe and antiferromagnetic Cr-Cr interactions tends to either strongly reduce local magnetic moments on atoms of transition elements while maintaining collinearity or leads to non-collinear magnetic structures. This effect is responsible for the short-range inversion in Fe-Cr alloys at a Cr concentration of 11 at. %. This suggests that one of the factors determining the stability of various carbide phases may be the change in magnetic moments on iron atoms introduced by chromium impurities.

We present the results of the ab initio simulations of binary and intermediate $(Fe, Cr)_7C_3$ carbides in orthorhombic and hexagonal phases. It was found, that the relative stability of the phases changes as the concentration of iron increases. The reasons for the possible phase transition are outlined and the influence of the resultant short-range magnetic order is emphasized. The results are supported by the investigation of the structure of the system in the liquid state close to the melting point.

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KITAEV MAGNETISM AND DIMERIZATION INSTABILITY IN HONEYCOMB IRIDATES

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Iridium oxides with the honeycomb and related geometries are one of the best platforms to study Kitaev magnetism – bond-anisotropic magnetic interactions that may stabilize a peculiar quantum spin liquid state. Tuning real materials toward this interesting limit requires an application of pressure that not only changes magnetic interactions but also brings a dimerization instability as a competing effect.

In this talk, I will present computational and experimental results on the behavior of α-Li_2IrO_3 and β-Li_2IrO_3 under hydrostatic pressure. Our single-crystal x-ray diffraction study shows that both compounds undergo a first-order structural phase transition around 3.8 GPa accompanied by an abrupt shortening of the Ir-Ir distances into dimers [1]. This binds valence electrons of iridium and renders both iridates non-magnetic. Density-functional calculations reveal a strong dependence of this dimerization instability on the strength of electronic correlations. In the absence of correlations, the honeycomb iridates would be dimerized already at ambient pressure, whereas a realistic U_{eff} = 1.5-2.0 eV leads to dimerization pressures in good agreement with the experiment.

Below 3.8 GPa, both α-Li_2IrO_3 and β-Li_2IrO_3 remain magnetic, and their magnetism can be tuned. From magnetization and muon spin relaxation measurements under pressure, we infer that long-range magnetic order in β-Li_2IrO_3 is suppressed above 1.4 GPa as a result of pressure-induced changes in the competing exchange interactions. We quantify these changes from density-functional and quantum-chemistry calculations, and discuss the nature of the pressure-induced spin-liquid state [2].

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PHASE DIAGRAM OF HIGH-TC CUPRATES CALCULATED WITHIN A MULTSCALE SCHEME WITH CONTROLLABLE APPROXIMATIONS

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The desirable theory for the high-Tc cuprates should account within the same framework a number of phenomena occurring at wide range of energy and length scale. Collective modes are characterized by a low energy scale of about 10-2 eV. It is important that different strongly developed collective phenomena, in particular spin fluctuations and superconductivity, coexist and can essentially compete/interact with each other. This means that they should be threaten unperturbatevely on equal footing, without a prejustice to some particular mode. `High-energy' single-electron phenomena, such as Hubbard band formation, occur at the typical energy of several eV. An account of these effects for the regime of intermediate correlations U ~ W implies an accurate analysis of the local on-site psychics. At the same time possible effect of the van Hove physics on the spin fluctuations means that large length scale of at least several dozens of lattice sites should be accounted to resolve van Hove singularities in the k-space. One extra requirement is that the theory should be controllable in a sense that the validity of all assumptions can be verified, at least in principle. These means that if the analysis is performed for a cluster of certain size, a calculation for the doubled-size case should also be doable without an unacceptable slowing down of the program.

We believe that our theory fulfills the above conditions. It includes the following three steps. First, we account the local on-site phenomena by the exact transformation to dual fermions. This transformation leads to the action characterized by local in space dispersive interaction, which rapidly decays at high frequency arguments. This allowed us to integrate over high Matsubara frequencies as a second step. This yields an effective low-energy action. Our third step is a solution of the full parquet equations for this action yielding the instability channels of the system. Since the low energy action is defined on just a few Matsubara frequencies, the solution of parquet equations is possible for large enough lattices, up to 32x32 sites. Our calculations show a very reasonable agreement with the experimentally known domains of the antiferromagnetism and d-wave superconductivity in the phase diagram.

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ELECTRIC POLARIZATION INDUCED BY SKYRMIONIC ORDER IN GaV_4S_8: FROM FIRST-PRINCIPLES CALCULATIONS TO MICROSCOPIC MODELS

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The lacunar spinel GaV_4S_8 was recently suggested to be a prototype multiferroic material hosting skyrmion lattice states with a sizable polarization $\boldsymbol{P}$ coupled to magnetic order. We explain this phenomenon on the microscopic level. On the basis of density functional theory, we construct an effective model describing the behavior of magnetically active electrons in a weakly coupled lattice formed by *molecular* orbitals of the $(V_4S_4)^{5+}$ clusters. By applying superexchange theory combined with the Berry-phase theory for $\boldsymbol{P}$, we derive a compass model relating the energy *and polarization* change with the directions of spins $\boldsymbol{e}_i$ in magnetic bonds. We argue that, although each skyrmion layer is mainly formed by superexchange interactions in the same plane, the spin dependence of $\boldsymbol{P}$ arises from the stacking misalignment of such planes in the perpendicular direction, which is inherent to the lacunar spinel structure. We predict a strong competition of isotropic, $\sim \boldsymbol{e}_i\boldsymbol{e}_j$, and antisymmetric, $\sim \boldsymbol{e}_i \times \boldsymbol{e}_j$, contributions to $\boldsymbol{P}$ that explains the experimentally observed effect. Finally, we consider how all these properties will change in the series of lacunar spinels GaV_4S_8, GaV_4Se_8, and $GaMo_4S_8$, which differ by the ferroelectric distortion and the number of magnetically active electrons.

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SPIN-ORBIT COUPLING AND JAHN-TELLER EFFECT: FRIENDS OR FOES?

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Spin-orbit (SO) Mott insulators are regarded as a new paradigm of magnetic materials, whose properties are largely influenced by the SO coupling and featured by highly anisotropic bond-dependent exchange interactions between the spin-orbital entangled Kramers doublets, as manifested in 5d iridates and 4d ruthenates. We will show that a very similar situation can be realized in cuprates, when the Cu^{2+} ions reside in a tetrahedral environment, like in spinel compounds. A special attention will be paid to $CuAl_2O_4$, which was experimentally found to retain cubic structure and does not show any long-range magnetic ordering down to very temperatures (0.5 K). We argue that these are the strong Coulomb correlations and the spin-orbit coupling, which conspire to suppress the Jahn-Teller distortions in $CuAl_2O_4$. The spin-orbit-entangled $j_{eff}=1/2$ state is then naturally realizing in the situation of t_{2g}^5 configuration and degenerate t_{2g} subshell. This in turn explains unusual magnetic properties of $CuAl_2O_4$. Using first-principles electronic structure calculations, we construct a realistic model for the diamond lattice of the Cu^{2+} ions in $CuAl_2O_4$ and show that the magnetic properties of this compound are largely controlled by anisotropic compass-type exchange interactions that dramatically modify the magnetic ground state by lifting the spiral spin-liquid degeneracy and stabilizing a commensurate single-q spiral.

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ANTIFERROMAGNETIC PHASE TRANSITION IN Cr_2As VIA ANISOTROPY OF EXCHANGE INTERACTIONS

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Intermetallic compounds of 3d metals with As or Sb possessing a tetragonal crystal structure of the Cu_2Sb-type have garnered significant interest from the research community for their diverse magnetic structures. For example, Mn_2Sb is a ferrimagnet, and Mn_2As, Fe_2As and Cr_2As are antiferromagnets. The antiferromagnet Cr_2As is distinguished by two aspects: the small magnetic moments of the atoms ($M(Cr_I) = 0.4\mu_B$, $M(Cr_{II}) = 1.34\mu_B$) and its magnetic structure. This should lead to uncorrelated ordering of both subsystems, i.e. to the existence of two transition temperatures.

Calculations of the electronic structure and exchange integrals in *Cr_2As* are performed by fully relativistic Korringa-Kohn-Rostoker method [1]. The magnetic moments of chromium in the ferrimagnetic ($M(Cr_I) = -0.72\mu_B$, $M(Cr_{II}) = 1.45\mu_B$) and antiferromagnetic ($M(Cr_I) = 0.87\mu_B$, $M(Cr_{II}) = 1.65\mu_B$) phases agree with the experimental data [2] ($M(CrI) = 0.4\mu_B$, $M(CrII) = 1.34\mu_B$) and the results of other calculations. The interatomic exchange integrals were calculated by the method [3]. Their dependence on the interatomic distance is shown in Fig.1 for the basic FIM(left figure) and AF states(right figure).

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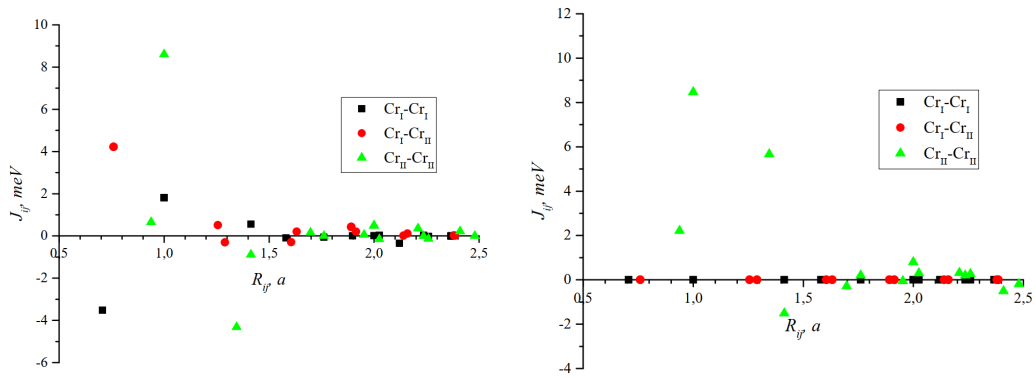

Fig. 1. Interatomic exchange interactions in *Cr_2As*

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NEW INSIGHTS INTO THE MAGNETIC EXCHANGE INTERACTIONS OF MULTIFERROIC $SRMNO_3$

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Perovskite structure$SrMnO_3$ has received attention due to the possibility of strain engineering its Multiferroic properties [1,2], possibly leading to fascinating new magnetoelectric coupling phenomena [3]. Total energy DFT calculations revealed that the Mn-Mn magnetic exchange interactions in the material change sign from antiferro- to ferromagnetic, in an unexpected manner, with increasing atomic distance [2]. The magnetic behaviour of the compound is thus not fully understood and, furthermore, exhibits a notable non-Heisenberg behaviour. For enhanced understanding of the magnetism of $SrMnO_3$, we use a recent method, complementing total energy DFT calculations, to evaluate magnetic exchange interactions in $SrMnO_3$. This is done via a mapping of DFT plane-wave pseudopotential calculations on Wannier functions, and by evaluating second order energy variations due to spin rotations [4]. This leads to significant new insights into the exchange interactions, via energy and orbital decomposition. We show that partial occupancy of the e_g states gives rise to the sign change in the nearest neighbour exchange interaction with increased atomic distance and, furthermore, the e_g-contributions are particularly non-Heisenberg.

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CONSISTENT DESCRIPTION OF COLLECTIVE ELECTRONIC FLUCTUATIONS BEYOND DYNAMICAL MEAN-FIELD THEORY

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Collective electronic fluctuations in correlated materials give rise to various important phenomena, such as charge ordering, superconductivity, Mott insulating and magnetic phases, and plasmon and magnon modes. Description of these correlation effects requires a significant effort, since they almost entirely rely on strong local and nonlocal electron-electron interactions. Some collective phenomena, such as magnetism, can be sufficiently described by simple Heisenberg-like models that are formulated in terms of bosonic variables. This fact suggests that other many-body excitations can also be described by simple bosonic models in the spirit of Heisenberg theory. Here, I will show how an effective bosonic problem can be derived for charge and spin degrees of freedom for the extended Hubbard model. It can be shown that in the regime of strong collective excitations the obtained model reduces to a classical Hamiltonian of effective Ising and Heisenberg models, respectively. The derived expressions for the exchange interaction and susceptibility are then expressed in terms of single-particle quantities, which can be efficiently used in realistic calculations of multiband systems. This, in particular, allows an accurate prediction of phase boundaries between the normal and ordered states (see e.g. Fig. 1).

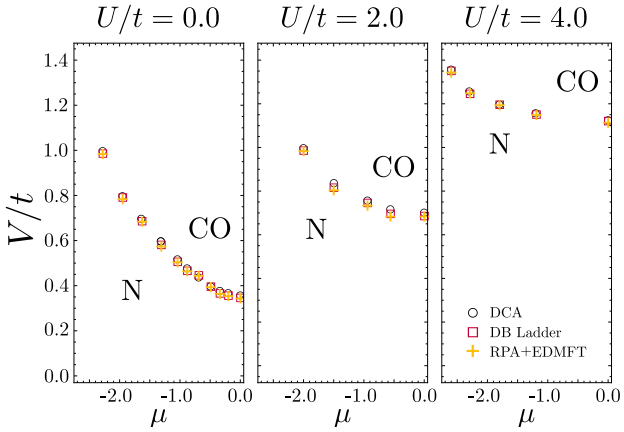

Fig. 1 Phase boundary between the normal (N) and charge-ordered (CO) states of the extended Hubbard model. t, μ, U, and V are hopping amplitude, chemical potential, local and nonlocal Coulomb interaction, respectively.

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VACANCY MEDIATED GUINIER-PRESTON ZONES TO Θ′-PHASE TRANSFORMATION IN AL-CU BASED ALLOYS

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Interest to solute clustering and precipitation phenomena in Al alloys has been recently revived in connection with the development of new precipitation-strengthened Al alloys, as well as thanks to the advances in the instrumentation and methodology of experimental and computational studies. The progress in computational modeling techniques allows the researchers to reveal the microscopic mechanisms of early precipitation stages and to make the important step in modeling studies from binary to ternary and multicomponent alloy systems. In this work, the energetics of point defect interactions with a Guinier-Preston zone (GPZ) in Al alloys is systematically studied using ab initio calculations and a supercell approach. We find that vacancies can be trapped by GPZs and that the presence of a vacancy in a Cu layer qualitatively changes the solute–GPZ interactions [1].

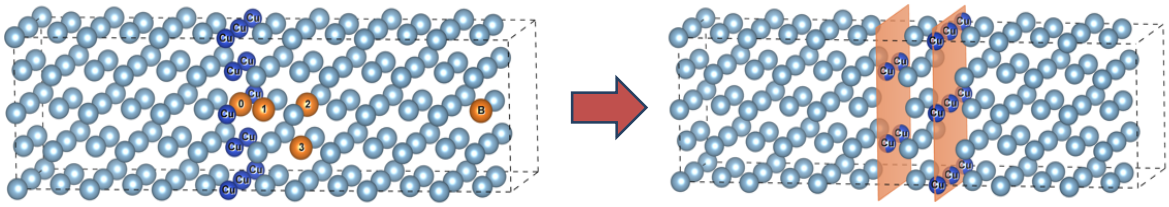

Fig.1 Schematic representation of Guinier-Preston zone vacancy mediated transformation into θ′-phase. Light blue spheres are aluminum atoms, dark blue are copper atoms and orange spheres are the sites of point defects disposition.

A vacancy mediated mechanism of GPZ to θ′-phase transformation is suggested and shown to be thermodynamically feasible, which involves the formation of structural vacancies and splitting of a GPZ layer into two half-vacant Cu layers. In presented results we considered different types of solute- θ′-phase interactions to shed the light on the complicated processes of precipitates formation in complex Al-Cu based alloys.

This work was supported by the RSCF (Grant No. 18-12-00366).

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LATTICE DYNAMICS AND PRESSURE INFLUENCE ON MEF2 (ME=CA, SR, BA): AB INITIO CALCULATION

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Interest to the study of fluorites due to their varied application. Fluorites are used as solid electrolyte in electric batteries [1] as well as optical materials [2, 3]. Some fluorites exist in two phases (cubic β-phase and orthorhombic α-phase), which can be transformed into each other by means of external pressure and temperature. The study of this phase transition is of practical interest, since such a phase transition can occur in epitaxial films of alkaline-earth metal fluorides with a difference in the thermal expansion coefficients of the film and substrate [4]. Crystal structure and phonon spectrum of MeF_2 crystals (Me = Ca, Sr, Ba) in both cubic and orthorhombic phases have been investigated in this work. The investigation was done within the framework of the MO LCAO approach. The hybrid DFT functionals was used. The functionals take into account the contribution of nonlocal exchange in the Hartree-Fock formalism. The frequencies and types of IR, Raman and silent modes are determined. The effect of hydrostatic pressure on MeF_2 crystals was also investigated. Calculations were carried out in the program CRYSTAL14 [5], designed to simulate periodic structures within the MO LCAO approach.

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AB INITIO CALCULATIONS OF ELECTRONIC PROPERTIES OF THERMOELECTRIC Mg_2X-Mg_2Y (X,Y=Si,Ge,Sn) ALLOYS

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There has been a wide interest in the Mg2X-Mg2Y substitutional alloys, between the isoelectronic X,Y=Si,Ge,Sn, for technological applications and fundamental research. We use the Bloch spectral density function, defined within the coherent potential approximation in the KKR method, to map an electronic band structure, to explore the electronic nature, and to extract parameters relevant for transport such as energy gaps and effective masses. We discuss the physical consequences of the formalism, compared to available experimental data, as well as the trends of the measurements for intermediate compositions. In general, we have found non-linear dependencies of the lattice constant, and energy gaps, as the composition changes. The effective masses also show non-linearity with composition, anisotropies, and a singular behavior at intermediate compositions of $Mg_2X_{(1-x)}Sn_x$, where the lowest conduction bands converge [1-3].

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OPTICAL PROPERTIES OF DEFECTIVE CARBON NANOTUBE (11,0)

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Properties of carbon nanotubes depend not only on their chirality, but also on the presence of atomic structure defects. During the previous research, we investigated the effect of the most common defects on electronic and optical properties of CNT (7.7) with metallic conductivity [1]. The difference in the nature of the spectra (peaks in the low-energy part of the spectrum, as well as blurring of M_{11}, M_{22} and M_{33} peaks) indicates the possibility of identifying the type of defect by empirical means. The present paper is devoted to a similar study of the properties of CNT (11.0) with a semiconductor type of conductivity.

In order to verify the modeling technique, we determined the band structure, the density of states, and the optical absorption spectrum of a defectless CNT (11.0) (Fig. 1). These properties are in good agreement with the results of other authors [2-5]. This ensures the reliability of new results for defective nanotubes obtained using this technique.

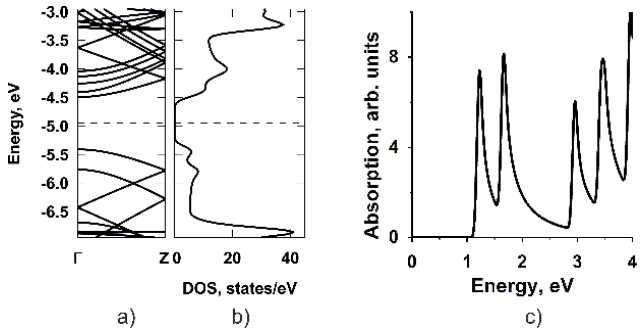

Fig. 1 Properties of SWNT (11,0): a) band structure, b) DOS, c) absorption spectra

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AB INITIO MODELING OF P, S AND C INTERACTION WITH THE GRAIN BOUNDARIES IN A -IRON

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The brittle intergranular fracture was experimentally observed in many different materials: iron and steel; nickel, copper, and high-melting alloys. Impurities with low solubility in the volume accumulate at the grain boundaries (GB) and locally reduce the cohesive strength of a metal. Though researchers have been studied the influence of various impurities on the interatomic bonds on GB for several decades, some problems remain unsolved The intergranular embrittlement, which caused weakening of bonds at the grain boundary, is associated either with a chemical mechanism [1] related to the features of impurity capture or with a mechanical impact related to the atomic size of the impurity [2]. The predominant mechanism depends on a type of impurity and a material boundary.

We investigated the interaction of non-metallic interstitial (C) and substitutional (P, S) impurities with the grain boundaries in α-iron via first-principles calculations. Modeling was performed using density functional theory with generalized gradient approximation (GGA'96), implemented in the WIEN2k package. We studied three fully relaxed tilt grain boundaries: Σ5(310), Σ5(210), and Σ3(111); and constructed the supercells of tilt grain boundaries by the coincidence site lattice model. We showed that for the symmetric grain boundaries Σ3(111) and Σ5(310) phosphorus and sulfur induce the material's embrittlement, while carbon increases the interatomic the bonds between Fe-atoms on the grain boundary. These results are in good agreement with the available literature data. In case of asymmetrical grain boundary Σ5(210) phosphorus also weaken the interatomic bonds between Fe-atoms on the grain boundary, though sulfur enhances them. We assume that this effect stems from the geometry of the surrounding matrix. Magnetic moments of impurity atoms are very small and, in most cases, are antiparallel to magnetic moments of nearby Fe atoms.

We also investigated not only the individual effect of carbon and phosphorus impurities on the grain boundaries properties, but also it co-segregation.

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UNUSUAL COLLINEAR MAGNETIC ORDER AT SPINEL-TYPE Cu_2GeO_4 SYSTEM

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In the classical approximation, the J_1 - J_2 model with S = 1/2 adopts spiral order in the range of $|J_1|/J_2 < 4$. Previous theoretical results predicted such an order in Cu_2GeO_4 [1], which contradicts recent neutron diffraction data that reveal the collinear up-up-down-down (UUDD) order instead [2]. Using revised density functional theory (DFT) calculations, as well as superexchange theory supplied with the direct exchange interaction estimated on the level of random phase approximation (RPA), we show that the nearest-neighbor coupling J_1 should be significantly suppressed in comparison to the next-nearest J_2 and interchain J exchange integrals. The new parameter regime supports the collinear magnetic order, as demonstrated by Luttinger-Tisza (LT) analysis, that yields a commensurate propagation vector. The eventual UUDD magnetic order is stabilized by symmetric anisotropic terms, arising due to spin-orbit coupling effects in the system.

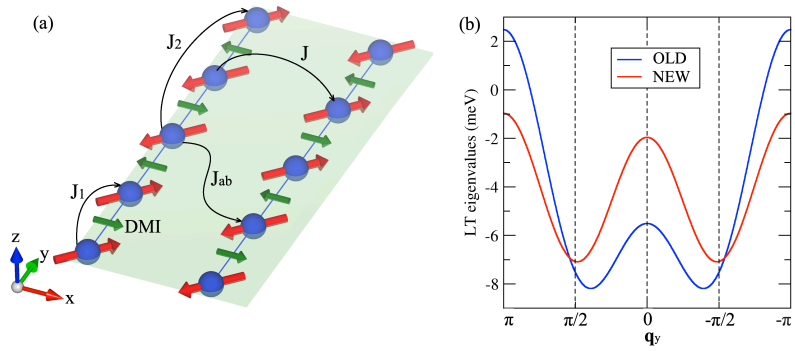

Fig. (a) Magnetic model of Cu_2GeO_4 with main exchange integrals. Red arrows represent the UUDD magnetic ordering revealed by neutron diffraction. (b) LT method eigenvalues for two sets of magnetic parameters.

The reported study was funded by RFBR according to the research project No. 18-32-00018.

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WANNIER FUNCTIONS IN ELK CODE FOR DFT+DMFT SOLVER

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Density functional theory combined with dynamical mean field theory (DFT+DMFT) [1,2] is a powerful approach for simulating physical properties of strongly correlated materials. There are different numerical implementations of the DFT+DMFT approach. In this work we propose a distinct one based on the combination of the full-potential Elk [3] package for electronic structure calculations and Wannier90 [4,5] package for constructing the maximally localized Wannier functions [6]. In turn, the DMFT problem in our approach is solved within the AMULET [7] toolbox.

Using the developed numerical scheme, we have studied the magnetic state in the B2 FeCo alloy at different temperatures. One of the important results is the temperature dependence of magnetic moments in the range from 1000K to 2200K (see at Fig. 1). We observe a critical temperature of 2023K that can be associated with the Curie temperature. The overestimation of the experimental value of T_c by 30% can be explained by the fact that the density-density form of the Coulomb interaction U in DMFT approach breaking the rotational invariance of the system was used.

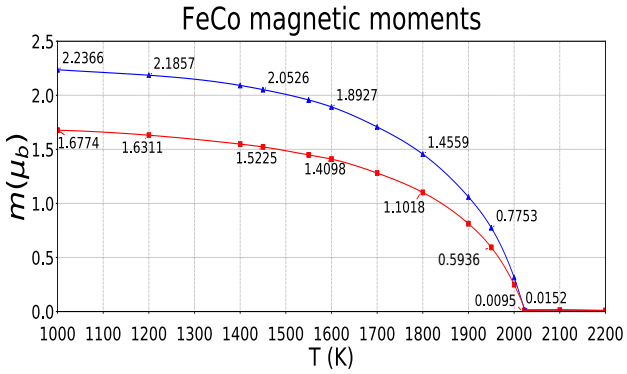

Fig. 1 Magnetic moments on Fe (blue) and Co (red) atoms in B2 FeCo alloy with respect to the temperature.

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EFFECT OF HUBBARD CORRELATIONS ON THE SODIUM DIFFUSION AND REDOX PROPERTIES OF MOLYBDATES WITH ALLUAUDITE STRUCTURE

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Alluaudite-type compounds have been recently proposed as new promising cathode materials for sodium batteries due to their high operating voltage, high capacity and good cyclability [1-3]. In this work, we present the GGA and GGA+U studies of sodium diffusion and (de)intercalation mechanism in alluaudite $Na_{2+2x}M_{2-x}(MoO_4)_3$ (M = Mn, Fe, Co, Ni), as well as their electronic structure and magnetic properties. The calculations were performed using the Vienna *Ab Initio* Simulation Package (VASP) [4,5] and the projector-augmented wave approach (PAW). The Na diffusion was studied with the nudged elastic band method.

We predict that, unlike the known alluaudite sulfates, the Na-ion migration in alluaudite molybdate should occur not only through 1D channels along the *c* axis, but also due to their cross-linking, which is responsible for 2D diffusion. These cross-channel sodium hops with the low-energy barriers may reduce the negative influence of defects and improve rate. They can also provide additional mobile ions to the main channels and play an important role in (de)intercalation. The mechanism of the charging process involves the Na^+ extraction in a specific sequence from different Na sites, which is accompanied by a redox reaction and has an average redox potential of ~3–5 V as dependent on transition metal. Large volume shrinkage during the last desodiation stages narrows the Na migration channels that impedes the diffusion and removal of all Na from molybdates. We found that the GGA+U functional predicts more accurately the band gap and redox potentials in $Na_{2+2x}M_{2-x}(MoO_4)_3$ than the GGA scheme.

This work was supported by the RSCF (Grant No. 18-12-00395).

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GATE-TUNABLE INFRARED PLASMONS IN ELECTRON-DOPED SINGLE-LAYER ANTIMONY

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We report on a theoretical study of collective electronic excitations in single-layer antimony crystals (antimonene), a novel two-dimensional semiconductor with strong spin-orbit coupling. Based on a tight-binding model, we consider electron-doped antimonene and demonstrate that the combination of spin-orbit effects with external bias gives rise to peculiar plasmon excitations in the mid-infrared spectral range. These excitations are characterized by low losses and negative dispersion at frequencies effectively tunable by doping and bias voltage. The observed behavior is attributed to the spin-splitting of the conduction band, which induces interband resonances, affecting the collective excitations. Our findings open up the possibility to develop plasmonic and optoelectronic devices with high tunability, operating in a technologically relevant spectral range.

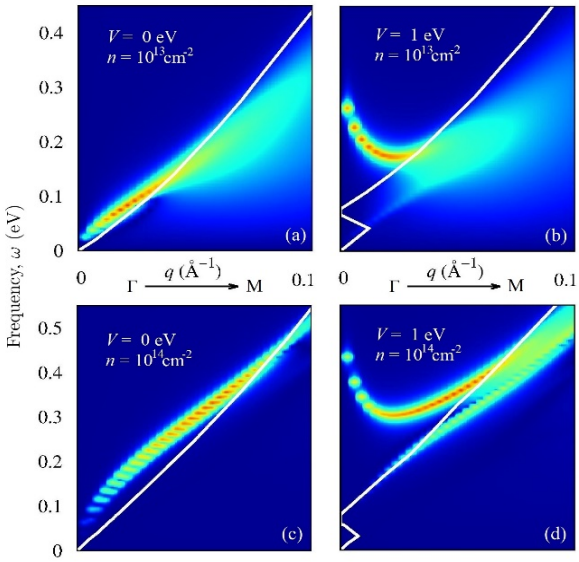

Fig. 1 Plasmon loss function in single-layer antimony

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RAMAN SPECTRUM AND ELASTIC PROPERTIES OF RARE-EARTH OXYORTHOSILICATES R2SIO5: AB INITIO CALCULATION

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Oxyorthosilicate single crystals R_2SiO_5, where R – rare earth ion, are actively studied at the present time as a good optical matrixes and advanced laser materials. Doped with rare-earth ions the crystals are used as gamma rays detectors [1] and in positron emission tomography [2].

In this work ab initio calculation of crystal structure, Raman spectra and elastic properties for range of rare-earth oxyorthosilicates R_2SiO_5 (R – La, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb) has been performed within the framework of density functional theory (DFT) using hybrid DFT/HF functionals. Calculations made in program package CRYSTAL14 using molecular orbitals approximation (MO LCAO) with gauss-type basis sets and pseudopotentials. The results for lutetium oxyorthosilicate are compared with recent experimental data [3]. For the first time the complete set of fundamental vibrations, their frequencies, types and intensities in the Raman spectrum for various polarizations are calculated.

Based on crystal structure calculations, elastic moduli for all range of R_2SiO_5 also predicted. Spatial dependences of Bulk modulus, Young modulus and Poisson's ratio have been described. Lu_2SiO_5 is being studied as a material with good characteristics for use as a thermal barrier coating. Calculated it this work values of lattice thermal conductivities for range R_2SiO_5 (R – La, Pr, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, Lu) presented in Figure 1.

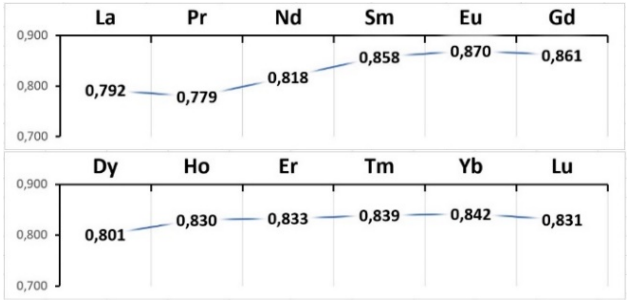

Fig. 1 Theoretically predicted lattice thermal conductivities of R_2SiO_5 with A-type structure (upper) and B-type structure (lower) .

This study was supported by the Government of the Russian Federation (contract no. 02.A03.21.0006, resolution no. 211)

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FIRST-PRINCIPLES INVESTIGATION OF FERROMAGNETISM IN CHROMIUM TRIIODIDE MONOLAYER

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Under our investigation is chromium triiodide (CrI_3) monolayer, being remarkable representative of 2D materials class, possessed by ferromagnetism, which could be identified as induced by van der Waals mechanism [1]. Also important to mention the role of magnetic anisotropy, lifting restrictions of Mermin-Wagner theorem [2].

In order to theoretically interpret the magnetic properties of the given compound we employ first-principles calculations by means of DFT-GGA approach. Then the low-energy tight-binding model was configured in basis of maximally localized Wannier functions. The model contains Cr(*3d*) and I(*5s5p*) states. The resulting Green's functions were used to extract pairwise isotropic exchange interactions in frame of infinitesimal spin rotations approximation.

For the first and the second coordination spheres we found non-negligible $J_1 = -0.13$ meV, $J_2 = 0.9$ meV, establishing two Cr ferromagnetic sublattices, connected by weak antiferromagnetic interaction. The nature of J_1 was enlightened by orbital decomposition, which revealed the competing character of individual specific contributions. Namely, in accordance with Kugel-Khomskii formalism [3], highly occupied Cr(*3d*) orbitals interact antiferromagnetically with intensity of -3.1 meV, whereas highly and lowly occupied ones are found connected by ferromagnetic interplay of +3.1 meV. It allows one to ascribe the former interaction to be of super-exchange type, and the latter to have the nature of interatomic exchange interaction, followed by Hund's rule. It also confirms the magnetic anisotropy to have the decisive rule in forming of the CrI_3 monolayer ferromagnetism.

Thus, accomplished explanation favors further theoretical and experimental investigations of CrI_3 monolayer, compound with intriguing magnetic properties and large perspectives of application in modern spintronic devices.

This work was supported by the RSCF Grant No. 17-72-20041.

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PRESSURE-INDUCED INSULATOR-TO-METAL TRANSITION IN BINIO3 CONTROLLED BY LATTICE EFFECTS

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The physical properties of rare-earth nickelate perovskites RNiO$_3$ (R = Lu, Y, Nd, etc.) with high Ni^{3+} oxidation state have attracted much recent attention due to their complex site- and orbital-selective correlations. Under ambient conditions, RNiO$_3$ exhibit a site-selective Mott insulating phase with a strong site-selective alternation of the local magnetic moments and complex charge ordering on the Ni ions. Here, we discuss an application of the DFT+DMFT computational scheme to explore the electronic structure, local magnetic moments, and lattice properties of BiNiO$_3$, an isoelectronic system of RNiO$_3$. In particular, we will present our results for the pressure-induced Mott insulator-metal transition (MIT), which is found to be accompanied by a structural transformation and melting of charge disproportionation in BiNiO3. In contrast to RNiO$_3$, where the MIT arises from a site-selective Mott MIT accompanied by a charge transfer between the Ni 3d and O 2p states, our results suggest the important role of the Bi 4s charge ordering (with a charge difference of ~0.52 electrons) in BiNiO$_3$. The MIT in BiNiO$_3$ is driven by a charge transfer between the Bi 4s and O 2p states, whereas the Ni sites preserve a Ni^{2+} configuration. Interestingly, the energy gap in the insulating phase of BiNiO$_3$ is found to increase under pressure that results in a sufficient enhancement of charge disproportionation between the Bi 4s states. Our DFT+DMFT results suggest that the MIT in BiNiO$_3$ is driven by the structural effects. We conclude that electronic correlations are important to explain the electronic structure, magnetic state, and lattice stability of BiNiO$_3$.

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MOTT INSULATOR-METAL TRANSITION AND MELTING OF CHARGE ORDERING IN $YNiO_3$ UNDER PRESSURE

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The electronic, magnetic, and crystal structure properties of the rare-earth-element nickelate perovskites RNiO$_3$ (R = rare earth: Lu, Y, Nd, Sm, etc.) with a formally high Ni^{3+} oxidation state have attracted much recent attention because of their intriguing physical properties. Upon compression and/or heating RNiO$_3$ compounds exhibit a sharp metal-insulator transition (MIT) [1,2]. The MIT is accompanied by a structural phase transformation, complicated by the appearance of unusual charge order and non-collinear magnetic phases in the Mott insulating state. Here, we will discuss an application of the DFT+DMFT computational scheme to explore the electronic structure, local magnetic moments, and lattice properties of paramagnetic $YNiO_3$. In particular, we will present our results for the pressure-induced Mott MIT, which is found to be accompanied by a structural transformation and melting of charge disproportionation. In agreement with previous studies, we found that the MIT arises from a site-selective Mott transition, controlled by a charge transfer between the Ni *3d* and O *2p* states. Thus, the Ni sites exhibit a strong site-selective variation of the local magnetic moments. Based on our constrained DFT+DMFT calculations in which an oxygen-breathing distortion has been treated as an external potential acting on the Ni *3d* states, we propose that the MIT in $YNiO_3$ is triggered by the structural effects. We point out the importance of electronic correlations to explain the electronic structure, magnetic state, and lattice stability of $YNiO_3$.

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FIRST-PRINCIPLES CALCULATION FOR ALLOYED CEMENTITE (Fe-Ni-Cr)$_3$C

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Cementite, which exists as a disperse phase in carbon steels, strongly affects their mechanical and magnetic properties. Doping elements of steel can also enter the cementite lattice, thus changing the size, shape, and properties of the cementite particles and of the steel also. In particular, nickel, which in itself is not a carbide-forming element, when using in a steel to improve its mechanical properties, enters the cementite lattice as an iron-substituting element and changes its magnetic properties as was shown in [1].

Mechanical alloying allows one to produce nonequilibrium meta stable compounds, in particular to obtain samples with a high content of cementite (up to 95–100 \% [2]). In [3-5], cementite with nickel or/and chromium was obtained by mechanical alloying and subsequent thorough annealing. The samples with 0 - 20 \% of Ni/Cr replacing the iron atoms were then studied by X-ray diffraction, magnetic measurements, and Mössbauer spectroscopy.

In this work, we perform first-principles calculations of electron structure of cementite with Ni and Cr replacing iron atoms with concentration close to that in [3-5] (one or two of 12 Fe atoms in the $Fe_{12}C_4$ unit cell), to acquire additional information on the local atomic structure of samples and the hyperfine parameters. The unit cells are fully relaxed through finding the minimum of total energy over the lattice parameters and atomic positions. The details of calculation are given in [6]. The obtained data for total magnetization, atomic magnetic moments, and parameters of hyperfine interaction of Fe nuclei are compared with those for pure cementite and used to interpret experimental magnetic and Mössbauer data. Special attention is drawn to the calculated values of electric field gradient and its appearance in Mossbauer spectra through the corresponding quadrupole splitting.

This study was performed as the State Task (no. AAAA-A17-117022250038-7).

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FIRST-PRINCIPLES CALCULATIONS FOR TERNARY ALLOYS BASED ON FE–AL

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Neutron diffraction in ordered Fe-Al system revealed incommensurate spin density waves in alloys known to be spin glasses. We investigate the spin arrangement for Fe-Al system using variation of topological and electronic properties by doping of the M atoms (Ga, B V, Mn) to $Fe_{65}Al_{35}$. The results of magnetic and Mössbauer measurements [1] on Fe-Al-M ternary systems required studying by first-principle calculations. First-principles calculations for the hyperfine magnetic fields, magnetic moments and lattice parameters of various periodic Fe-Al systems with the subsequent replacement of one Al or Fe atom by the elements Ga, Mn, V and B are carried out for comparison. The Fe-Al-M alloys are simulated with supercells of different Al content, on the basis of a bcc lattice. Calculations were performed using the full-potential linearized augmented plane wave (FP LAPW) technique contained in the WIEN2k software package [1]

The majority of results are coordinated with experiments [2]. A small experimentally observed increase in the hyperfine magnetic field when Ga is added to the Fe-Al alloy, is confirmed by calculations in the concentration range 25 – 35 at.% and is explained by an increase in the lattice constant. An increment in the Fe hyperfine magnetic field with addition of B to Fe-Al can result from the increase in the contribution to the polarization of core electrons associated with an increase in the local magnetic moment. This occurs due to a decrease in the overlap of the wave functions of *d*- electrons located at different sites and concomitant narrowing of the *d*-band. The decrease in the Fe hyperfine magnetic field with a small addition (3 at.%) of Mn in the experiment is confirmed by calculations with all concentrations under the assumption that Mn atoms replace Fe atoms. Replacement of iron atoms by V leads to reduction of hyperfine magnetic field according to experiments.

This work was funded by the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities (3.7352.2017/8.9).

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STRUCTURAL AND OPTICAL PROPERTIES OF $HoGa_3(BO_3)_4$

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The present work devoted to ab-initio theoretical study of the structural and optical properties of $HoGa_3(BO_3)_4$ crystal. The crystals of the huntite family with the general formula $RX_3(BO_3)_4$ (R = lanthanide ions, X = Al, Ga, Fe, Cr) attract the interest of the investigators. The stability of the huntite crystal structure due to rigidity of the BO_3 polyhedron. The optical nonliner and multiferroic properties lead to different practical applications of these materials [1-6]. The structure of two magnetic ions of different types (3d and 4f) gives rise to magnetic order at low temperatures [5]. Coexistence of structural and magnetic order parameters can open new opportunities to control their physical characteristics. The $HoGa_3(BO_3)_4$ crystal exhibits a strong magnetoelectric effect [6]. The calculation is based on the Density Functional Theory (DFT) approach with a plane-wave (PW) basis set using the generalized gradient approximation parameterized (GGA-PBE) [7].

This work is financially supported by the Russian Foundation for Basic Research № 18-02-00754.

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ELECTRONIC STRUCTURE AND ZERO SPIN FLUCTUATION IN QUANTUM FERROMAGNETS

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The electronic structure of the helicoidal ferromagnet MnSi with a broken symmetry of the crystal lattice (the absence of an inversion center in the cubic structure) has not yet been definitively established. In current work it is shown that the cause of the difficulties arising in the LDA and GGA calculations of the electronic structure is that MnSi belongs to the group of quantum ferromagnets with Dzyaloshinsky-Moriya interaction. Moreover, significant zero spin fluctuations occur in the ground state of these compounds. The initiative electron spectrum was calculated in the LDA+U+SO method. To estimate the fluctuation effects we calculated the electron Green function of a system of strongly correlated electrons interacting with fluctuating exchange fields. The amplitudes of zero fluctuations are determined in the approximation of the saddle point for the energy functional. The inclusion of zero fluctuations leads to the parameter of the intermode interaction, which corresponds to a stable ferromagnetic ground state. The values of the parameters of the Hubbard and Hund interactions for which the calculated local magnetization is in good agreement with experimental data are established.

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SHORT-RANGE ORDER IN ADVANCED SOFT MAGNETIC ALLOYS

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[2]*Institute of Quantum Materials Science, Ekaterinburg, Russia*
[3]*Institute of Physics and Technology, Ural Federal University, Ekaterinburg, Russia*

Substitutional alloys Fe-X (X = Al, Si, Ga, Ge) based on bcc Fe are of considerable interest due to their unusual magnetic properties such as induced magnetic anisotropy (Fe-Al, Si), giant magnetostriction (Fe-Ga) and a significant decrease in the elastic moduli (Fe-Ga, Ge). According to the existing concepts, features of physical properties of these alloys are due to formation of a certain short-range order (SRO), however, the nature and reasons for its currently remain the subject of debate.

To clarify the mechanisms of SRO formation, we carried out Monte Carlo simulation of the structure of the alloys under consideration, depending on temperature and magnetic state, using the effective interactions energies between solute atoms from first principles (VASP-PAW) calculations. It also took into account the presence of a high concentration of non-equilibrium vacancies generated during intensive treatment of the material (irradiation, large plastic deformation) and/or due to the formation of stable vacancy-impurity complexes (Vac-X) with alloying elements.

It was shown that the energy of the effective X–X interaction in bcc Fe strongly depends on the magnetic state of the matrix. As a result, the B2-type SRO, which is responsible for the enhancement of magnetic anisotropy, is formed at $T > T_C$ and is fixed during quenching, while in the ferromagnetic state ($T < T_C$) the $D0_3$-type SRO is equilibrium. We found that the binding energy of a vacancy with an impurity is high in the case of Ga, Ge (~ 0.45 eV) and half as much (~ 0.24 eV) in the case of Al, Si; a similar relationship between the binding energies is retained also during the formation of X-Vac-X complexes. As a result, the formation of B2-type SRO in Fe-X alloys (X = Ga, Ge) is preferable even in the presence of equilibrium vacancies, while in Fe-X alloys (X = Al, Si), additional external treatment is needed.

The results obtained reveal the important role of magnetism in the formation of short-range order in these alloys, as well as the possibility of its significant enhancement due to the presence of vacancies and allow us to explain the experimentally observed structural features depending on the composition and temperature.

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ELECTRONIC STRUCTURE OF SNAS: DFT AND ARPES STUDY

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Currently active research is under way on binary compounds such as SnAs. This is a superconductor material and it is promising in particular in terms of topological superconductivity search.

Recently new experimental data from angle-resolved photoemission spectroscopy has been obtained [1]. To explain this new ARPES data we carried out DFT calculation of electronic properties of SnAs using Wien2k [2] package. We obtained band dispersions in high-symmetry directions КГК and МГМ' both for bulk material and for the slab with the {111}.

For more realistic comparison of DFT bands with ARPES spectral function maps we take into account several particular experimental details: the photoemission cross-section, the experimental energy and angular resolutions and the core-hole lifetime effects.

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CRYSTAL STRUCTURE AND LATTICE DYNAMICS OF $Gd_2Ge_2O_7$ CRYSTAL: AB INITIO CALCULATION

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Rare-earth pyrochlores germanates $R_2Ge_2O_7$ (R-rare earth ion) have recently been synthesized [1]. These crystals are of cubic symmetry (S.G. 227). $Gd_2Ge_2O_7$ crystal is representative of this series. In this work the ab initio investigation of the crystal structure, phonon spectrum, and elastic properties of $Gd_2Ge_2O_7$ was carried out for the first time.

Crystal structure and phonon spectrum at Gamma point were studied within the framework of density functional theory (DFT) and MO LKAO approach. The calculations were performed by using hybrid functionals that takes into account both local and nonlocal (in the Hartree–Fock formalism) exchange. The calculations were performed in the CRYSTAL17 program [2] intended for simulating periodic structures in the MO LCAO approximation. For the description of gadolinium the pseudopotential replacing internal orbitals including 4*f* orbitals was used. External 5*s* and 5*p* orbitals defining chemical bond were described by valence basis sets.

The fundamental vibration frequencies of $Gd_2Ge_2O_7$ were calculated. The relative intensities of the Raman lines and the oscillator strengths of the IR-active modes have been calculated. An analysis of the displacement vectors obtained from the ab initio calculation, made it possible to estimate the degree of the ion participation in the vibrational mode.

The elastic constants of the crystal have been calculated too. The elastic anisotropy of $Gd_2Ge_2O_7$ lattice have been investigated.

This study was supported by the Ministry of Education and Science of the Russian Federation (project no. 3.9534.2017/8.9).

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RECURRENT NETWORK CLASSIFIER FOR ULTRAFAST SKYRMION DYNAMICS

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Understanding of relaxation processes in magnetic materials due to the ultrafast pulses realized with different experimental techniques plays a crucial role for creating next-generation magnetic storage and spintronic technologies. In the static case the magnetic state recognition and classification problems can be effectively solved neither with standard methods of machine learning such as support vector machine, k-means and others or with neural network approach[1]. In our study we follow the idea "classify a movie rather than snapshot"[2] and propose a recurrent neural network classifier for ultrafast skirmion processes of picosecond scale in two-dimensional materials (see at Fig. 1). The magnetic configurations calculated with LLG [3] approach at different times of the relaxation process are used as input for the recurrent neural network. Having trained the recurrent neural network, we have constructed a phase diagram of processes realized in the ferromagnetic material depending on external parameters (damping constant and magnetic pulse width).

This work was supported by the Russian Science Foundation Grant 18-12-00185.

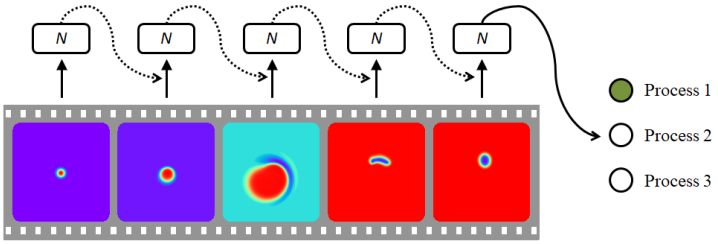

Fig. 1 Illustration of idea of the ultrafast skyrmionic process recognition. Magnetization dynamics is used frame by frame as an input for recurrent neural network providing the process classification.

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QUANTUM NANOSKYRMION

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Skyrmions in condensed matter physics appear as classical topological spin structures. This nontrivial state can be obtained solving the corresponding micromagnetic model. Here, we introduce a new concept of quantum skyrmions of a nanoscale size. This distinct magnetic state can be formed in spin-1/2 low dimensional magnets characterized by a strong Dzyaloshinskii-Moriya interaction and the quantum Hamiltonian [1]:

$$H = \sum_{i<j} \vec{D}_{ij} \cdot [\vec{S}_i \times \vec{S}_j] - \vec{B} \sum_i \vec{S}_i. \qquad (1)$$

The usual way to distinguish the skyrmion state is calculation of topological charge [2], however, it is not possible to calculate this value in quantum case. On the other hand, one can treat skyrmion as superposition of spiral states, which can be determined with magnetic structure factor.

This concept can also be applied to usual spin systems characterized by a nonzero exchange interaction if the quantum solution of the problem is accessible. We observe that the quantum skyrmionic state is stabilized even when the corresponding classical skyrmionic solution has already undergone a phase transition towards the polarized ferromagnetic state.

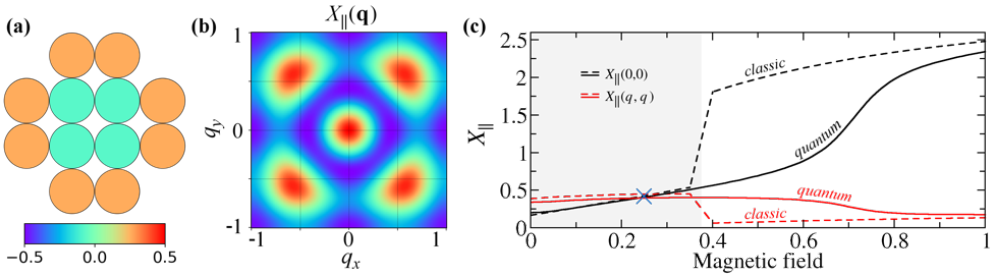

Fig. 1 (a) z-components of local magnetization of considered cluster calculated at field B = 0.25D. (b) Corresponding magnetic structure factor. (c) Dependence of susceptibility on magnetic field. Here, q = 0.56π.

The work of M.V.V., S.O.M., and S.E.A. was supported by the Russian Science Foundation Grant 18-12-00185. The work of K.M.I. was supported by NWO via Spinoza Prize. The work of C.J. and M.F. is supported by the Swiss National Science Foundation. Details of this research were published and available at Ref. [3].

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NEURAL NETWORK SOLUTION OF THE KAGOME PROBLEM

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Investigations of the frustrated low-dimensional spin systems belong to the most challenging problems of the modern condensed matter theory [1]. Negative sign problem [2] prevents one from using most advanced numerical techniques such as Quantum Monte Carlo family approaches for studying such systems. In this situation the exact diagonalization can be used to simulate small clusters with number of spins up to 50 [3]. The main problem to consider quantum systems of larger sizes is the exponential growth of the Hilbert space. Such a problem can be partially solved with the recently proposed neural network approach by Carleo and Troyer [4] in which the quantum state of a system is effectively compressed by using the restricted Boltzmann machine.

Here we focus on the spin-1/2 Heisenberg model on the kagome lattice. Analyzing the ground state energies we found, that the difference between obtained solutions and ED results is about 1% and decreases when we increase α parameter, which shows how many times the number of hidden neurons is bigger than the number of atoms. Similar behavior can be traced out from the evolution of spins structural factors with respect to the number of hidden neurons (see at Fig. 1).

This work was supported by the Russian Science Foundation Grant 18-12-00185.

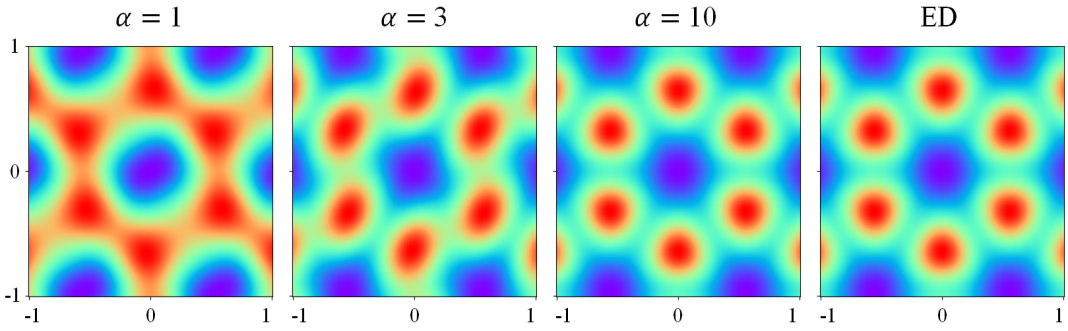

Fig. 1 Correlation functions obtained for supercell with 12 spins by using neural network with various values of α and exact diagonalization.

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STRUCTURAL PHASES TRANSITION IN VSE2: ENERGETICS, ELECTRONIC STRUCTURE AND MAGNETISM.

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Monolayer VSe2 is the one of the most intriguing members of the family of two-dimensional (2D) transition-metal dichalcogenides. This material attracts a special interest of the scientific community due to several recent discoveries, including in-plane piezoelectricity [1], a pseudogap with Fermi arc [2] at temperatures above the charge-density-waves transition (~220 K for the monolayer [3])

Results of first-principles calculations (see at Fig. 1) demonstrate that the energy barrier for transition between two structural states of VSe2 monolayer by a step-by-step rotation of the whole selenium layer is rather low (about 0.6 eV in monolayer). The energies of the rotation of the selenium layer up to 10 degree is very low, therefore, the realistic theoretical description of VSe2 (from monolayer to bulk) should take into account these small deviations from ideal crystal structure.

This work was supported by the Russian Science Foundation Grant 18-12-00185.

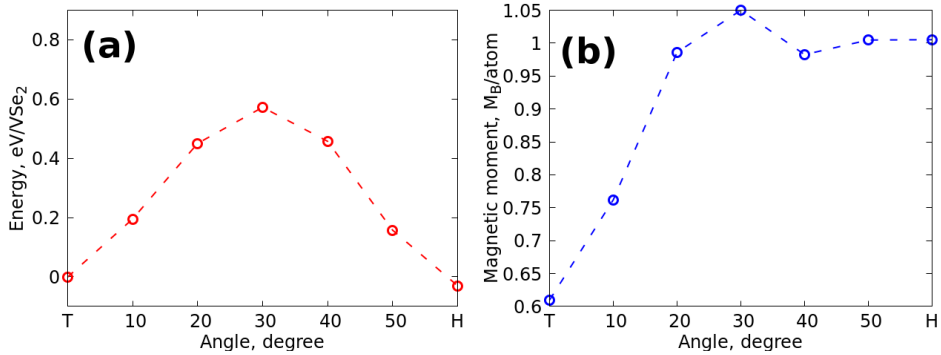

Fig. 1 Evolution of the total energy (a) and magnetic moment (b) during rotation of whole Se upper layer of VSe2 monolayer.

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MAGNETIC INTERACTIONS IN $SR_3IR_2O_7$

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5d transition - metal oxides have attracted a considerable attention, since their properties are mainly determined by the strong spin orbit (SO) coupling. In this work we study the magnetic properties of $Sr_3Ir_2O_7$. For that we construct the following spin Hamiltonian

$$\widehat{H} = \sum_{i<j} D_{ij}\left[\widehat{S}_\iota \times \widehat{S}_J\right] + \sum_{i<j} \widehat{S}_i \overleftrightarrow{\Gamma}_{ij} \widehat{S}_j + \sum_{i<j} J_{ij} \widehat{S}_i \widehat{S}_j ,$$

where $\hat{S}_i$ is the spin operator, J_{ij}, D_{ij} and $\overleftrightarrow{\Gamma}_{ij}$ are the isotropic exchange coupling, antisymmetric anisotropic (Dzyaloshinskii-Moriya), and symmetric anisotropic interactions, respectively. These parameters can be defined within the superexchange theory [1, 2]. The first step of our investigation is to define the hopping integrals with spin-orbit coupling. For that we performed first-principles calculations by using the plane wave pseudopotential method, as implemented in the Quantum - ESPRESSO simulation package. To construct the minimal low-energy model in the Wannier functions basis, we used the procedure of maximal localization [3,4] implemented in the Wannier90 package [5].

The obtained magnetic interaction between nearest neighbors in the plane are J=32meV and D^Z=29meV. The calculated $\overleftrightarrow{\Gamma}_{ij}$ tensors are characterized by nonzero negative zz components. It means that for antiferromagnetic configuration between nearest neighbors the spins will have in-plane orientation, which contradicts to the experiment. Thus, one-band model with spin-orbit coupling doesn't give correct description of magnetic properties in the case of $Sr_3Ir_2O_7$. One needs to use a multi-orbital Hubbard model taking into account all t_{2g} states of Ir and spin-orbit coupling.

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AB INITIO BASED MODELLING OF THE LATTICE PROPERTIES OF SUPERCONDUCTING 115 COMPOUNDS

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Department of Physics, Ural Federal University, Russia

The 115 compounds family share the chemical formula AMX_5, where A is actinide metal (Np, U, Pu), M is transition metal (Co, Rh, Fe) and X is Ga or In. These compounds began to attract attention of condensed matter and material science community since the discovery of superconducting $PuCoGa_5$ compound with T_c~18,5 K, which is anomalously high for the actinide-based intermetallics. Subsequent studies have shown unconventional nature of superconductivity in $PuCoGa_5$ meaning that electronic correlations are responsible for the superconductivity. $PuCoIn_5$ has the unit cell volume ~30% higher than that of $PuCoGa_5$, which is similar for the volume difference between alpha and delta phases of plutonium and which can considerably affect the electron correlation effects. In the present contribution we present *ab initio* calculations of the ground state energy of $PuCoGa_5$ and $PuCoIn_5$ as a function of unit cell volume. By supplementing it with the vibrational energy calculated in terms of the generalized Debye-Einstein model we have simulated temperature dependencies of thermal and elastic properties of the considered systems. We show that $PuCoIn_5$ exhibit considerably stronger phonon anharmonicity as compared to $PuCoGa_5$.

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EASTMAG Program

Sunday, 08.09.2019. "Ural" Center

16:00 Opening Ceremony

16:30 (Plenary talk) Sang-Wook CHEONG. Chirality, Helicity, Spirality and Moire Patterns in Intercalated Transition Metal Dichalcogenides

17:10 (Plenary talk) Gen TATARA. Spintronics theory without spin current

Monday, 09.09.2019

9:30 (Plenary talk) Oleg TRETIAKOV. Spintronics with (Anti)Skyrmions and Bimerons (Plenary talk)

10:10 (Plenary talk) Alexey KIMEL. Anomalies of spin dynamics in ferrimagnets (Plenary talk)

10:50 Coffee break

11:20 Invited/Oral talks

Spintronics and magnetic nanostructures	Magnetic soft matter	Soft and hard magnetic materials	Magnetism of strongly correlated electron systems

12:50 Lunch time

15:00 Invited/Oral talks

Spintronics and magnetic nanostructures	Magnetic soft matter	Soft and hard magnetic materials	Magnetism of strongly correlated electron systems

17.15 Coffee break

17:30 Poster session: Spintronics and magnetic nanostructures. Magnetic soft matter. Soft and hard magnetic materials. Magnetism of strongly correlated electron systems

Tuesday, 10.09.2019

9:30 Invited/Oral talks

Spintronics and magnetic nanostructures	Magnetism in biology and medicine	Spin dynamics and magnetic resonances	Magnetism of strongly correlated electron systems

11:00 Coffee break

11:30 Invited/Oral talks

Magnetoelastic, magnetocaloric and shape memory effect	Magnetism in biology and medicine	Spin dynamics and magnetic resonances	Magnetism of strongly correlated electron systems	Magnetic soft matter

13:00 Lunch time

15:00 Invited/Oral talks

Magnetoelastic, magnetocaloric and shape memory effects	Round table "Modern equipments and methods"	Spin dynamics and magnetic resonances	Magnetism of strongly correlated electron systems	Magnetic soft matter

17:15 Coffee break

17:30 Poster sessions: Spin dynamics and magnetic resonances. Magnetoelastic, magnetocaloric and shape memory effects. Magnetism in biology and medicine. Magnetic semiconductors, multiferroics, topological insulators. Magnetic non-destructive testing

Wednesday, 11.09.2019

9:30 (Plenary talk) Andrei ROGALEV. X-ray magnetic circular dichroism: recent advances
10:10 (Plenary talk) Theo RASING. All Optical Magnetic Switching and Brain-inspired Concepts for low energy Information Processing
10:50 Coffee break
11:20 Invited/Oral talks

Low dimensional magnetism	Frustrated and disordered magnetism	Magnetism and superconductivity

Thursday, 12.09.2019
9:30 (Plenary talk) Ramamoorthy RAMESH. Electric field control of magnetism for ultralow power electronics
10:10 Break
10:15 Invited/Oral talks

Low dimensional magnetism	Magnetotransport, magnetooptics and magnetophotonics	Magnetism and superconductivity	Domain walls, vortices and skyrmions

11.15 Coffee break
11:45nvited/Oral talks

Low dimensional magnetism	Magnetotransport, magnetooptics and magnetophotonics	Magnetism and superconductivity	Domain walls, vortices and skyrmions	Magnetic semiconductors, multiferroics, topological insulators

13:15 Lunch time
15:00 Invited/Oral talks

Low dimensional magnetism	Magnetotransport, magnetooptics and magnetophotonics	Magnetism and superconductivity	Domain walls, vortices and skyrmions	Magnetic semiconductors, multiferroics, topological insulators

17:15 Coffee break
17:30 Poster sessions: Low dimensional magnetism. Domain walls, vortices and skyrmions. Magnetotransport, magnetooptics and magnetophotonics. Frustrated and disordered magnetism. Magnetism and superconductivity

Friday, 13.09.2019
9:30 Invited/Oral talks

Low dimensional magnetism	Frustrated and disordered magnetism	Magnetic semiconductors, multiferroics, topological insulators	Soft and hard magnetic materials	Magnetic non-destructive testing

11:45 Coffee break
12:30 Closing Ceremony