



PROGRAM

Day 1 (Tuesday, Aug 13th)

Time *Activity*

- Morning
- 8:30: Registration
 - 8:50: Welcome address
 - 9:00-10:00: **K.Schwarz**: Density functional theory (DFT) and the concepts of the augmented-plane-wave plus local orbitals (APW+lo) method
 - 10:30-12:00: **P.Blaha**: An overview of the WIEN2k package for beginners
- Afternoon
- 13:30-14:30: **P.Blaha**: Input files, Volume optimization, AIM,
 - Exercises

Day 2 (Wednesday, Aug 14th)

- Morning
- 9:00-9:30: **P.Blaha**: Forces, structure optimization, supercells, surfaces, phonons
 - 9:30-10:00: **K.Schwarz**: Magnetism (FM, FSM, AFM)
 - 10:30-11:30: **F. Tran**: Advanced DFT: Hybrid-DFT, vdW-DFT, LDA+U, mBJ
 - 11:30-12:00: **J. Tomczak**: DMFT
- Afternoon
- 13:30-14:30: **R.Laskowski**: Relativistic effects, non-collinear magnetism (NCM)
 - Exercises

Day 3 (Thursday, Aug 15th)

- Morning
- 9:00-10:00: **O.Rubel**: Wannier functions + Berry phases + fold2Bloch
 - 10:30-12:00: **P. Blaha, R.Laskowski**: Optical properties, XPS, XAS, EELS, BSE
- Afternoon
- Exercises



Day 4 (Friday, Aug 16th)

- Morning
- 9:00-10:00: P.**Blaha**: Hyperfine interactions
 - 10:30-11:30: R. **Laskowski**: NMR shifts
 - 11:30-12:00: Poster

Afternoon

- 13:30-14:30: G.**Madsen**: Boltztrap2 (Transport)
- Exercises
- 18:30: Conference Dinner

Day 5 (Saturday, Aug 17th)

- Morning
- 9:00-10:00: M. **Arrigoni**: Point defects in solids
 - 10:30-11:00: M. **Arrigoni**: "Spinney"
 - 11:00-12:00: P.**Blaha**: Installation of Wien2k, parallelization
 - 12:00-12:30: Round table & closing

Afternoon

- Free Exercises

Abstracts of Poster session

A DFT study: Electronic and magnetic structure of spintronic Sr₂CoO₄

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In past few years, Sr₂CoO₄ (SCO) based two-dimensional (2D) layered cobalt oxides have been the subject of hot interest among spintronics materials [1]. SCO exhibits ferromagnetism (T_C=255K) and metallic behavior, which is unique in such materials. Besides this, few theoretical predictions of half metallicity make this compound a potential candidate for the spintronics industry. The compound possesses a complex electronic structure, consisting of two kinds of O atoms, namely planar (O1) and apical oxygen (O2), while the Co atoms occupy eight corners and body-centered positions of tetragonal SCO lattice. In these materials, the 2D nature of the CoO₂ network reduces the bandwidth of e_g electrons as compared to the 3D network, and hence gives rise to various fascinating electronic, electrical and magnetic properties [2, 3]. Co⁴⁺ in SCO can possess in three electronic configurations of t_{2g}⁴e_g¹, t_{2g}⁵ and t_{2g}³e_g² revealing three possible spin states.

Ab-initio calculations have been performed with different approaches to study the electronic and magnetic properties of SCO. In the present work, spin dependent electronic and magnetic properties are evaluated using mBJ exchange potential. BJ approach was introduced by Becke and Johnson [4] for orbital dependent expression for exchange energy. It takes into account the shape of atomic optimized effective potential. The approach was then modified by Tran and Blaha in 2009 [5], termed as mBJ. Fermi surface topology for spin states of SCO have also been discussed.

Wien2k with various possible exchange correlations gives us freedom to evaluate the electronic, optical, electrical and magnetic structure of any compound. We further aim to effectively use the WIEN2k DFT tool for the new novel materials modelling, such as pyro-electric IR sensors for clinical thermometry and humidity-moisture sensors for metrological applications. Presenting author will discuss with the peers to explore these possibilities and collaborations.

References:

- [1] K. Takada, et al. Nature **422**, 53 (2003).
- [2] X. L. Wang and E. Takayama-Muromachi, Phys. Rev. B **72**, 064401 (2005).
- [3] K.-W. Lee and W. E. Pickett, Phys. Rev. B **73**, 174428 (2006).
- [4] A. D. Becke and E. R. Johnson, J. Chem. Phys. **124**, 221101 (2006).
- [5] F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009).

Electronic, dynamical, and thermoelectric properties of noncentrosymmetric B20-RhGe

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We present ab initio study of noncentrosymmetric B20-type phase of RhGe, which is not found in nature and can be synthesized only at high pressures and temperatures. We trace the pressure evolution of electronic, dynamical, transport, and thermoelectric properties using the DFT calculations and Boltzmann transport equations. We demonstrate an appreciable transformation of the phonon spectrum under high pressure, including a vanishing anisotropy of the transverse acoustic phonon modes. B20-RhGe is shown to be a poor metal with a moderate carrier density. The symmetry-conditioned Dirac-like features in the electronic spectrum are essential for the Fermi surface topology. Pressure-induced successive Lifshitz transitions are considered, which can manifest themselves in quantum oscillations and anomalies of thermopower and conductivity. The application of high pressure tunes the conductivity and thermopower of B20-RhGe in the same way as a low-level hole-doping does. The temperature dependence of the charge and heat transport properties is evaluated within the semi-classical Boltzmann approach. Using the quasi-harmonic approximation, we determine the range of pressures and temperatures, in which the phase B20-RhGe is stable, and make recommendations for optimizing the synthesis conditions to reduce the number of defects that occur in a sample during solidification under pressure.

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Quantum-mechanical description of Fe₃Al: a review of different GGA parametrizations

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The materials based on Fe and Al represent one of the most promising classes of alloys intended for high-temperature structural applications. One of the most important intermetallic compounds from this family is Fe₃Al which crystallizes under ambient conditions in the D0₃ structure. Interestingly, many parametrizations of the generalized gradient approximation (GGA) predict the ground-state structure of Fe₃Al incorrectly - the L1₂ structure is energetically preferred instead. For example, Lechermann *et al.* [1] showed that the Perdew-Burke-Ernzerhof (PBE) [2] parametrization of the GGA cannot correctly predict the D0₃ structure as the ground state of Fe₃Al (in contrast to the local density approximation (LDA) which predicts the correct hierarchy of structures). Similarly, Connetable and Maugis [3] calculated structural, magnetic, elastic and vibrational properties of Fe₃Al employing the PBE parametrization [2] and found out that Fe₃Al has lower energy in the L1₂ structure.

The above mentioned findings led us to systematically searching for a reliable computational set up when using the GGA and the projector-augmented waves (PAW) potentials. Surprisingly, the Perdew-Wang parametrization [4] has turned out to be an optimum in the case of Fe₃Al.

- [1] F. Lechermann, F. Welsch, C. Elsässer, C. Ederer, M. Fähnle, J. Sanchez, B. Meyer, *Phys. Rev. B* **65**, 132104 (2002).
- [2] J.P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [3] D. Connetable, P. Maugis, *Intermetallics* **16**, 345 (2008).
- [4] J.P. Perdew, Y. Wang, *Phys. Rev. B* **45**, 13244 (1992).

The ground state and Fermi-surface nesting phenomenon in antiferromagnetic CeAuSb₂.

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Abstract

Recently, it was reported that, under an external magnetic field (≤ 3 T) along the c -axis, the in-plane wave vector of the spin-density wave (SDW) is $(\eta, \eta, \frac{1}{2})$ with $\eta \approx 0.136$ for CeAuSb₂ compound. To elucidate this SDW and the ground state we investigate the electronic structure of antiferromagnetic (AFM) CeAuSb₂ using the full-potential linearized-augmented-plane-wave method. The results of volume optimize calculations and total energy show that $1 \times 1 \times 2$ unit cell construction with $\uparrow \uparrow \downarrow \downarrow$ AFM configuration is the ground state, which are well matched with experiments. Fermi surface (FS) on the ab -plane exhibit FS nesting along the (110) direction. The nesting vector $\mathbf{q} = (\zeta, \zeta, \frac{1}{2}) (2\pi/a)$ with $\zeta \sim 1/7$, is very similar to the results of experiment. To confirm the relation between this FS nesting and SDW we will calculate the generalized susceptibility $\chi(\mathbf{q})$.

Electric field gradients in noncentrosymmetric B20-RhGe: DFT simulation and experiment

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Single-phase polycrystalline samples of RhGe with a cubic B20-type non-centrosymmetric crystal structure (space group P2₁3) have been synthesized under high pressure of 8 GPa [1]. Here, we present new experimental data on RhGe obtained by the time-differential perturbed angular $\gamma\gamma$ -correlation (TDPAC) method on the ¹¹¹In/¹¹¹Cd and ¹⁸¹Hf/¹⁸¹Ta probes. We also report on DFT-calculations performed using the Wien2k package, with the PBE-96 approximation for the exchange–correlation potential. The lattice parameter a and the internal atomic coordinates u_{Rh} and u_{Ge} were optimized. For ¹¹¹Cd- TDPAC, at $T = 300, 160,$ and 90 K, the experimental electric field gradients (EFG), V_{zz} , corresponding to the measured quadrupole frequencies, ν_Q , are 6.68, 6.71, and 6.75 [$\times 10^{17}$ V/cm²], respectively.

The calculated V_{zz}^{Rh} and V_{zz}^{Ge} are opposite in sign and weakly increase with pressure. At $p = 0$, $V_{zz}^{\text{Rh}} = 1.7 \times 10^{17}$ V/cm², while V_{zz}^{Ge} is several times larger and equal to -7.4×10^{17} V/cm². The experimental value of $V_{zz}^{\text{Cd}} = 6.75 \times 10^{17}$ V/cm² significantly exceeds V_{zz}^{Rh} and differs by only 10% from V_{zz}^{Ge} . This suggests that ¹¹¹Cd probes apparently occupy the Ge sites in the metalloid sublattice and therefore, provide information on the germanium environment in B20-RhGe. Although the experimental V_{zz}^{Cd} weakly increases with decreasing temperature, even its hypothetical zero-temperature value would hardly reach the calculated V_{zz}^{Ge} , as the non-sphericity of electron density on Ge atom with its directed p-orbitals is more pronounced than for Cd atom with filled d-shells.

Our ¹⁸¹Hf/¹⁸¹Ta-TDPAC measurements were performed on RhGe samples doped with 2% and 1% of Hf. At room temperature, two EFG values were observed, with practically coinciding populations of corresponding sites. We also made such TDPAC measurements for the phases HfRh, Hf₃Rh₅, and Hf₂Rh to verify that they do not form in the sample.

The initial concentration of In atoms in ¹¹¹Cd-TDPAC measurements was about 0.01%, so the B20 lattice can be considered as undistorted. To the contrary, in ¹⁸¹Ta measurements with initial Hf concentration of 2% and 1%, the lattice was noticeably distorted. Thus, in DFT simulations of RhGe doped with small amount of Hf/Ta atoms, we had to use triclinic supercells. As a result, the EFG values at all sites turned out different. Average values at Rh and Ge sites are $\langle V_{zz}^{\text{Rh}} \rangle = 2.1 \times 10^{17}$ V/cm² (most V_{zz}^{Rh} are positive) and $\langle V_{zz}^{\text{Ge}} \rangle = 10.0 \times 10^{17}$ V/cm² (all V_{zz}^{Ge} are negative). We also determined the EFG at impurity Hf/Ta atoms substituted for Rh and Ge. Our preliminary results show that the problem of two frequencies needs further study.

This work was supported by Russian Science Foundation (Grant RSF # 18-12-00438).

[1] A.V. Tsvyashchenko, V.A. Sidorov, A.E. Petrova et al. *J. Alloys Compd.* **686**, 431 (2016).

PERTURBED ANGULAR CORRELATION STUDY OF $\text{SrMnGe}_2\text{O}_6$, $\text{SrCoGe}_2\text{O}_6$ AND $\text{CaMnGe}_2\text{O}_6$

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ABSTRACT

Multiferroic materials have been under the spotlight due to their fundamental scientific interest and for potential applications in technology. Among these interesting materials are the group of compounds belonging to the Pyroxene family with general chemical formula $\text{AM}(\text{Si},\text{Ge})_2\text{O}_6$. More specifically, $\text{SrMnGe}_2\text{O}_6$, $\text{SrCoGe}_2\text{O}_6$ and $\text{CaMnGe}_2\text{O}_6$ are isostructural, crystallizing with monoclinic C2/c symmetry and are characterized by zigzag chains of MnO_6 octahedra linked by edge-sharing, separated by GeO_4 tetrahedra chains along the same axis, linked by corner-sharing. Due to this arrangement these systems present a rich diversity of low-dimensional magnetic properties. The existence and possible interplay of low dimensionality and magnetic frustration results in multiferroic and/or magnetoelectric properties.

Since these properties might arise from local structural features that are not well described by methods based on long-range average structural models, the use of local probe studies is essential. In this context, hyperfine methods, such as perturbed angular correlation (PAC) spectroscopy where the study of the electric field gradient (EFG) in the vicinity of a probe atom, allows reconstructing of the atomic and electronic environment of the probe in the material, helps to clarify the origin of the properties exhibited in these systems. In this work a temperature dependent EFG study will be presented and discussed, guided by EFG simulation results using ab-initio WIEN2k, attempting to clarify the experimental observation of two different local environment for in $\text{SrMnGe}_2\text{O}_6$ and $\text{SrCoGe}_2\text{O}_6$, as opposed to three in $\text{CaMnGe}_2\text{O}_6$.

References:

[1] Lei Ding et al, *J. Mater. Chem C*, 2016, **4**, 4236

[2] Lei Ding et al, *Physical Review B* 2016, **93** 064423

[3] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran and L. D. Marks, *WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2018. ISBN 3-9501031-1-2*

Electronic, structural, vibrational and magnetic properties of interstitially doped L1₀-FeNi:N Alloy

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Abstract. In modern technological society, permanent magnets (PMs) are crucial for electrical and mechanical energies, such as a motor in an electric vehicle and a generator in a wind turbine [1]. For these applications, the PMs composed of critical rare-earth (RE) (Nd, Sm, and Dy) and transition-metal (TM) elements, e.g. Nd-Fe-B and Sm-Co are exclusively used due to their superior properties. However, due to so called “rare-earth crisis” [2], there is a need to look for development of new high performance novel RE free PMs. Among possible materials for replacing RE elements in PMs, the ordered L1₀-FeNi [3-6] is the one, with extraordinary magnetic response; large saturation magnetization of ~ 1.5 T and Curie temperature of at least 830 K which is sufficiently larger than that of Nd₂Fe₁₄B ~ 590 K. However, its magnetocrystalline anisotropy oscillates around 1.0 MJ/m³ which is insufficient for PMs. There is still a possibility to tune its magnetocrystalline anisotropy by certain modifications like introducing tetragonal strain, with interstitial doping or by substitutional alloying.

First principles studied of electronic, structural, vibrational and magnetic properties of L1₀-FeNi via inducing tetragonal distortion with interstitial N-doping have performed using full potential linearized augmented plane wave (FPLAPW) method within generalized gradient approximation (GGA). We have investigated two types of interstitial N-doping in Fe/Ni-layer of the parent alloy. The structure stability was revealed by calculated formation energy as well as phonon spectra. As per our calculations, N-doping results in structural distortion that promotes the magnetocrystalline anisotropy at a small cost of magnetization. This increment in magnetocrystalline anisotropy is more for N-doping in Fe-layer. Hence, interstitial N-doping has raise potential of L1₀-FeNi to act as a novel material for permanent magnets.

Keywords: Permanent magnets; DFT; Magnetization; MCA; FPLAPW; SOC

References

1. L. H. Lewis et al., Metallurgical and Materials Transactions A **44** (2013).
2. K. S. Stegen et al. Ener. Polc. **79**, 1–8 (2015).
3. L. H. Lewis et al., J. Phys.: Cond. Matr. **26**, 064213 (2014).
4. M. Mizuguchi et al., J. Magn. Soc. Japan **35**, 370-373 (2011).
5. E. Poirier et al., J. Appl. Phys. **117**, 17E318 (2015).
6. J. Paulevé et al., J. Appl. Phys. **39**, 989-990 (1968).