



PROGRAM

Day 1 (Monday, Sept 18th)

<i>Time</i>	<i>Activity</i>
Morning	<ul style="list-style-type: none">• 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	<ul style="list-style-type: none">• 13:30-14:00: P.Blaha: Volume optimization, QTL, AIM• Exercise I: Getting started, struct file, init, scf, charge density, DOS, bands, FS• Exercise II: Volume optimization

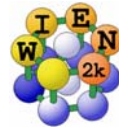
Day 2 (Tuesday, Sept 19th)

Morning	<ul style="list-style-type: none">• 9:00-9:30: P.Blaha: Forces, structure optimization, supercells, surfaces, phonons• 9:30-10:00: K.Schwarz: Magnetism (FM, FSM, AFM)• 10:30-11:15: F. Tran: advanced DFT: Hybrid-DFT, vdW-DFT, LDA+U• 11:15-12:00: R.Laskowski: Optical properties, Core-level spectra (XAS, EELS)
Afternoon	<ul style="list-style-type: none">• 13:30-14:30: X. Rocquefelte: Relativistic effects, non-collinear magnetism (NCM)• Exercise III: Structure optimization, supercells and surfaces• Exercise IV: magnetism

Day 3 (Wednesday, Sept 20th)

Morning	<ul style="list-style-type: none">• 9:00-10:00: O.Rubel: Wannier functions + Berry phases + Bloch2fold• Exercises
Afternoon	<ul style="list-style-type: none">• 13:30-14:15: G.Madsen: Boltztrap2 (Transport)• Poster session• Exercises
Evening	<ul style="list-style-type: none">• 18:30: Conference Dinner

24th Wien2k Workshop, 18. - 22.Sept. 2017, Vienna



Day 4 (Thursday, Sept 21th)

Morning

- 9:00-9:30: P.Blaha: Hyperfine interactions
- 9:30-10:15: K. Khoo: NMR shifts
- Exercises

Afternoon

- 13:30-14:15: P.Blaha: Installation of Wien2k, parallelization
- Exercises

Day 5 (Friday, Sept 22th)

Morning

- 9:00-9:30: R. Laskowski: GW + BSE
- 9:30-10:00: J. Tomczak: DMFT
- Exercises
- 11:30-12:30: Round table & closing

Afternoon

- Free Exercises



POSTER:

(We, Sept. 20th, 14:15-15:00)

- J. Fernandez Afonso and J. Kunes:
Excitonic magnetism in d^6 perovskites
- Hana Cencarikova and Dominik Legut:
First-principles study of electronic and mechanical properties in correlated electron system with the atomic number $Z=112$
- Arup Chakraborty, Boris Markovsky, Doron Aurbach, Dan T. Major:
Effect of high-valent metal-ion doping on the properties of NCM-523 Li-ion battery materials
- R. M. Costa, J. H. Belo, M. Barbosa, J. P. Araújo and A. M. Pereira:
Nature of the structural transition in Er_5Si_4
- Sourav Kumar Dey, Chandi Charan Dey, and Satyajit Saha:
Electric field gradients at ^{181}Ta probe in $\text{Zr}_7\text{Ni}_{10}$ and $\text{Hf}_7\text{Ni}_{10}$ intermetallic binary alloys; investigations by time-differential perturbed angular correlation spectroscopy
- Douglas H. Fabini, Geneva Laurita, Emily C. Schueller, Constantinos C. Stoumpos, Ting-Ann Siaw, Songi Han, Mercuri G. Kanatzidis, and Ram Seshadri:
Structure and Dynamics of Main-Group Halide Perovskite Photovoltaics
- A. Ghosh and R. Thangavel:
Electronic band structure of $\text{Cu}_2\text{ZnAS}_{4-x}$ and CuZn_2AS_4 ($A = \text{Al, Ga, In}$) nanocrystals for solar energy conversion applications
- H. Kara, K. Özdoğan:
Searching magnetic phase, electronic structure and thermoelectric properties of Ti_2MnAl Heusler material
- H. Kara, K. Özdoğan:
A DFT based thermoelectric energy research: Co_2MnSn Heusler alloy as a direct thermal energy conversion material
- Sandeep Kumar, Prabhakar P. Singh and Dan Thomas Major:
First-principles Study of Electronic Properties of Si-doped $\text{FeSe}_{0.9}$ Alloys
- William Lafargue-Dit-Hauret, Vinko Šurija, Tonči Cvitanić, Mihael Grbić, Mirta Herak, Xavier Rocquefelte:
Magnetic anisotropy and spectroscopic properties of SeCuO_3
- Alicia Lecomte, Xavier Rocquefelte, Camille Latouche, Laurent Calvez, XiangHua Zhang:
Experimental and Theoretical Investigation of a Photovoltaic glass-ceramic material based on the heterojunction $\text{Sb}_2\text{Se}_3\text{-GeSe}_2\text{-CuI}$
- Masoud Mansouri, Tahereh Mahmoodi, Raheleh Kimia:
Electronic and magnetism properties of vacancy-defected and adsorption on MoO_3 (010) Surface: a first-principles study
- I.I. Nazarenko, S.N. Sofronova, E.M. Moshkina:



The Magnetic Properties Investigation of Nickel and Cobalt Oxyborate Compounds with a Kotoite Structure

- M.Nedyalkova, H. Alexandrov, B. Donkova I. Koleva:
Mn-oxalates - experimental and theoretical approach
- Dominik Nöger, David Holec:
Optimised structural models of solid solutions for tensorial properties
- Hardev Singh, Manish K. Kashyap:
A first principle calculation of half metallic ferromagnetism in transition metal doped BeS
- Mukhtiyar Singh, Manoj K. Sharma, Hardev S. Saini, Manish K. Kashyap:
Spin gapless character of Ti_2MnAl inverse Heusler alloy under uniform and tetragonal strain
- S. Stavric, M. Belic, Z.Sljivancanin:
Planar versus three-dimensional growth of metal nanostructures at 2D heterostructures
- Bouchra Taychour, Lalla Btissam Drissi:
Theoretical study of structural, electronic and magnetic properties in Mn_2RuSn and Mn_2RuGe Heusler alloys: Cu_2MnAl type and Hg_2CuTi type
- R. Teixeira, G.N.P. Oliveira, M. B. Barbosa, J. N. Gonçalves, J. Schell, T. M. Mendonça, J.G. Correia, A.M.L. Lopes and J. P. Araujo:
EFG study of orbital melting and Jahn-Teller distortions in $LaMnO_3$ Manganite
- Alexander Udovsky, Dmitry Vasilyev:
Verification of ab-initio mixing enthalpy using thermodynamic simulation of phase equilibrium and the temperature dependences of the heat capacity of the bcc ferro- and paramagnetic Fe-Cr alloys
- A.V. Ushakov, A. O. Shorikov, V. I. Anisimov, N. V. Baranov, and S. V. Streltsov:
Suppression of magnetism under pressure in FeS: A DFT+DMFT study