AB INITIO BASED MODELING OF ADVANCED MATERIALS AMM-2016

Satellite Conference of XX Mendeleev Congress on general and applied chemistry

Ekaterinburg
22 – 24 September, 2016

Organizers

Institute of Quantum Materials Science CJSC

Institute of Metal Physics Ural Branch RAS

Ural Hi-Tech Park

Ural Federal University

Chairmans

Yuri Gornostyrev (Ekaterinburg, Russia)
Mikhail Katsnelson (Nijmegen, Netherlands)

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. Particularly the conference will focus on the development of theoretical approaches and physical principles of accelerated materials design, discussion of novel trends in materials science and promote direct interaction between theory and experiment. The aim is to provide a distinguished atmosphere and framework for exchanging the newest 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.

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AMM-2016 conference program

22 September

9:30 –10:30	Registration. Coffee is served
10:30 –10:45	Opening. Welcome talk
SESSION 1: DMFT AND ALL THAT	
10:45–12:40	**Chair Mikhail Katsnelson**
10:45 –11:25	**Alexander Lichtenstein**, University Hamburg, Hamburg, Germany *Strong Electronic Correlations in magnetic materials*
11:25 –11:50	**Andrey Katanin**, IMP Ural Branch RAS, Ural Federal University, Ekaterinburg, Russia *Non-local effects in strongly-correlated systems*
11:50 –12:15	**Ivan Leonov**, University of Augsburg, Augsburg, Germany *Electronic structure and phase stability of correlated electron materials under extreme conditions*
12:15 –12:40	**Sergey Streltsov**, Igor Mazin, IMP Ural Branch RAS, Russia, NRL, USA *Molecular orbitals in hexagonal ruthenates*
13:00 –14:00	**Lunch**
14:00-16:10	**Chair Tamio Oguchi**
14:00 –14:40	**Vladimir Anisimov**, IMP Ural Branch RAS, Ekaterinburg, Russia *Magnetic and structural properties of iron and its alloys in LDA+DMFT*
14:40 –15:20	**Olle Eriksson**, Uppsala university, Uppsala, Sweden *Theory of x-ray and photoelectron spectroscopy with DMFT*
15:20 –15:45	**Leonid Pourovskii**, CPHT-Ecole Polytechnique, CNRS, Université Paris-Saclay, France *Impact of electronic correlations on point-defect thermodynamics and transport in iron metal*

15:45 –16:10	**Igor Nekrasov**, Institute of Electrophysics Ural Branch RAS, Ekaterinburg *Magnetocaloric effect in strongly correlated systems*
16:10 –16:40	**Coffee break**
16:40-17:55	**Chair Vladimir Anisimov**
16:40 –17:05	**Alessandro Toschi**, Institute of Solid State Physics, TU Wien, Austria, *Quantum many-body theory at the two-particle level*
17:05 –17:30	**Georg Rohringer**, Vienna University of Technology, Wien, Austria *Impact of non-local correlations over different energy scales: a dynamical vertex approximation study*
17:30 –17:55	**Alexey Rubtsov**, Russia Quantum Center, Moscow, Russia *Modeling of the impurity dynamics in ultracold atomic media*
18:00 –20:00	**Poster session and reception (beer and food)**

23 September

SESSION 2: MAGNETISM AND ALL THAT	
10:00-12:20	**Chair Alexander Lichtenstein**
10:00 –10:40	**Tamio Oguchi**, ISIR, Osaka university, Japan *Electronic properties associated with spin-orbit coupling and broken symmetry*
10:40 –11:05	**Igor Solovyev**, National Institute for Materials Science, Tsukuba, Japan *Origin and microscopic mechanisms of magnetoelectric coupling in multiferroic manganites*
11:05 –11:30	**Vladimir Mazurenko**, Ural Federal University, Ekaterinburg, Russia *Methods for calculation and analysis of the Dzyaloshinskii-Moriya interaction*

11:30 –11:55	**Mikhail Korotin**, Institute of Metal Physics, Ekaterinburg, Russia *Coherent potential approximation for strongly correlated systems with spin-orbit coupling*
11:55 –12:35	**Sergey Savrasov**, University of California, Davis, CA, USA *Weyl semi-metal: a new topological state in condensed matter*.
13:00 –14:00	**Lunch**
14:00-16:05	**Chair Olle Eriksson**
14:00 –14:25	**Alexander Tsirlin**, University of Augsburg, Augsburg, Germany *Ab initio evaluation and experimental verification of magnetic exchange parameters in insulators*
14:25 – 14:50	**Sergey Skornyakov**, Institute of Metal Physics, Ekaterinburg, Russia *Electronic correlations and topological Fermi surface transition in the iron-based chalcogenides*
14:50 – 15:15	**Sergey Khmelevskyi**, Vienna University of Technology, Wien, Austria *Functional antiferromagnetic materials for spintronics applications: challenge for ab initio computations.*
15:15 – 15:40	**Tilmann Hickel**, X. Zhang, J. Rogal, Jörg Neugebauer, MPIE, Dusseldorf, Germany *The role of interfaces for structural transformations among austenite, ferrite and cementite in Fe-C alloys*
15:40 –16:10	**Coffee break**
16:10 –18:40	**Master class** **Alexander Poteryaev**, IMP Ural Branch RAS, Ekaterinburg, Russia *Application of the AMULET code for DFT+DMFT calculations of realistic compounds*

24 September

SESSION 3: ALLOYS, STRUCTURE AND ALL THAT	
10:00-12:25	**Chair Pavel Korzhaviy**
10:00 –10:40	**Jörg Neugebauer**, A. Glensk, F. Koermann, B. Grabowski, T. Hickel, MPIE, Dusseldorf, Germany *Ab initio thermodynamic description of advanced structural materials: Status and challenges*
10:40 –11:20	**Igor Abrikosov**, Linköping University, Linköping, Sweden *Finite temperature effects in ab initio simulations of alloy thermodynamics*
11:20 –11:45	**Alexander Rudenko**, Radboud University, Nijmegen, Netherlands *Intrinsic transport properties of monolayer black phosphorus*
11:45 –12:10	**Danil Boukhvalov**, Department of Chemistry, Hanyang University, Korea *Locally destroyed crystal order in Ti-Fe alloys.*
12:10 –12:35	**Alexander Mirzoev**, A. Verkhovykh, South Ural State University, Chelyabinsk, Russia *The interaction of hydrogen interstitials with grain boundaries in bcc iron*
13:00 –14:00	**Lunch**
14:00-16:05	**Chair Igor Abrikosov**
14:00 –14:25	**Sergey Simak**, Linköping University, Linköping, Sweden *Temperature-driven martensitic phase transitions from first principles*
14:25 –14:50	**Vsevolod Razumovskiy**, D. Scheiber, L. Romaner, Materials Center Leoben Forschung GmbH (MCL), Leoben, Austria *Impurity segregation and its effect on the grain boundary embrittlement in Ti: effects of chemical and structural contributions*
14:50 –15:15	**Nadezhda Medvedeva**, Institute of Solid State Chemistry, Ekaterinburg, Russia *Ab initio simulation of phosphorus in bulks, at surfaces and interface of fcc Fe and K-carbide*
15:15 –15:40	**Oleg Gorbatov**, Institute of Quantum Materials Science, Ekaterinburg, Russia *Effect of composition on antiphase boundary energy in NI3AL based alloys*
15:40 –16:05	**Mikhail Petrik**, Institute of Metal Physics Ural Branch RAS; Institute of quantum materials science, Ekaterinburg, Russia

	Ab initio investigation of grain boundary segregation in Al=X (X=Mg,Zn,Si,Cu) alloys
16:05 –16:30	**Coffee break**
16:30-18:40	**Chair Yuri Gornostyrev**
16:30 –17:10	**James Morris**, Oak Ridge National Lab, Oak Ridge, TN, USA *Ab initio modeling for understanding and predicting novel alloy behavior*
17:10 –17:50	**Pavel Korzhavyi**, Royal Institute of Technology, Stockholm, Sweden *Ab initio based models of disordered materials*
17:50 –18:15	**Mikheil Sekania**, University of Augsburg, Augsburg, Germany *Scaling behavior of the Compton profile of alkali metal elements*

Poster Session and Reception
22 September, 18:00 – 20:00

1	V. Greshnyakov, E. Belenkov, Chelyabinsk State University, Chelyabinsk, Russia *Ab initio modelling of diamond-like materials*
2	M. Shundalov, A. Matsukovich, S. Gaponenko, Belarusian State University; B.I. Stepanov Institute of Physics, Minsk, Belarus *DFT and multi-reference perturbation theory calculations of the structures and uv-vis spectra of adamantane-containing molecules, potential antibacterial agents*
3	A. Gerasimov, V. Mazurenko, S. Skornyakov, Ural Federal University; Institute of Metal Physics Ural Branch RAS, Ekaterinburg, Russia *Modelling of the magnetic interaction of strongly correlated systems*
4	I. Kashin, I. Solovyev, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia; National Institute for Materials Science, Tsukuba, Japan

	Effect of dynamical electron correlations on collective magnetic excitations in CrO_2
5	S. Andreev, I. Solovyev, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia; National Institute for Materials Science, Tsukuba, Japan *Pressure dependence of the electronic structures of $Sr_3Ir_2O_7$*
6	O. Sotnikov, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia *A method for calculating paramagnetic exchange interactions*
7	I. Nekrasov, N. Pavlov, M. Sadovskii, A. Slobodchikov, Institute of Electrophysics of the Ural Branch RAS; Institute of Metal Physics Ural Branch RAS, Ekaterinburg, Russia *The electronic structure of a monolayer FeSe on the $SrTiO_3$ substrate*
8	V.V. Bannikov, V.S. Kudyakova, A.A. Elagin, M.V. Baranov, A.R. Beketov , Ural Federal University, Ekaterinburg, Russia; University of Michigan, USA; Hamburg University, Germany *Electronic structure and magnetic properties of hexagonal and cubic modifications of aluminium nitride doped with sp-impurities (B, C, O)*
9	D. Medvedeva, V. Mazurenko, S. Iskakov, A. Lichtenstein, Ural Federal University, Ekaterinburg, Russia; University of Michigan, USA; Hamburg University, Germany *Calculation scheme based on the extended equations of DMFT for square and triangular lattices*
10	J. Komleva, S. Nikolaev, A. Tsirlin, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia; University of Augsburg, Germany *Lattice dynamics in copper chloride $CuCl_2$*
11	D. Badrtdinov, S. Nikolaev, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia *Spin-orbit coupling effects in adatom systems Si(111):{C,Si,Sn,Pb}*
12	D. Zakir'yanov, V. Chernyshev, Ural Federal University, Russia *Lead oxyhalides $Pb_3X_2O_2$ (X=Cl, Br, I): ab initio calculations of phonon spectra and optical properties*
13	A. Stepanenko, D. Vesnina, P. Igoshev, A. Katanin, Ural Federal University, Institute of Metal Physics Ural Branch RAS, Ekaterinburg, Russia *The Kohn anomalies in three-dimensional systems*
14	V. Protsenko, A. Katanin, Institute of Metal Physics Ural Branch RAS; Ural Federal University, Ekaterinburg, Russia *Electron transport through double quantum dots: the functional renormalization group approach*

15	D. Prishchenko, A. Rudenko, V. Mazurenko, M. Katsnelson, Ural Federal University, Ekaterinburg, Russia; Radboud University, Nijmegen, Netherlands *Plasmons and screening in phosphorus: beyond wavelength limit*
16	S. Sozykin, V. Beskachko, South Ural State University, Chelyabinsk, Russia *Contacts of carbon and gold nanotubes: first principles calculations*
17	I. Tikina, N. Barbin, Ural Institute of state fire service of EMERCOM of Russia; Ural state agrarian University, Ekaterinburg, Russia *Thermodynamic modeling of thermal dissociation of the intermetallic compounds $PbBi_2Sn_2$*
18	M. Petrik, D. Badrtdinov, Institute of Metal Physics Ural Branch RAS; Institute of quantum materials science; Ural Federal University, Ekaterinburg, Russia *Magnetic anisotropy effects in Fe-Ga alloys*
19	D. Nazipov, A. Nikiforov, L. Gonchar, Ural Federal University; Ural State University of Railway Transport, Ekaterinburg, Russia *Structure and lattice dynamics of $BiMnO_3$: Ab initio calculations*
20	V. Chernyshev, A. Nikiforov, V. Petrov, Ural Federal University, Ekaterinburg, Russia *Structure and lattice dynamics of PrFe3(BO3)4: Ab initio calculation*
21	I. Leonidov, V. Petrov, V. Chernyshev, A. Ishchenko, E. Konstantinova, A. Nikiforov, Institute of Solid State Chemistry UB RAS; Ural Federal University, Ekaterinburg, Russia *Lanthanide-Doped Germanates: DFT Study of Lattice Dynamics and Electronic Structure of Optical Hosts*
22	Z. Pchelkina, O. Volkova, V. Mazurenko, A. Vasiliev, Institute of Metal Physics Ural Branch RAS, Ural Federal University, Ekaterinburg, Lomonosov Moscow State University, National University of Science and Technology "MISiS," Moscow, Russia *Electronic structure and magnetic properties of the strong-rung spin-1 ladder $Rb_3Ni_2(NO_3)_7$*
23	I. Piterskikh, D. Boukhvalov, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia; Hanyang University, Seoul, Republic of Korea *Full potential study of electronic and magnetic properties of functionalized graphene*
24	D. Suetin, Institute of Solid State Chemistry, Ural Branch RAS, Ekaterinburg, Russia *Structural, electronic properties, stability and fermi surfaces of ternary borides CaM_2B_2, CaM_3B_2, $Ca_2M_5B_4$, $Ca_3M_8B_6$ (M = Rh, Ir)*
25	M. Ivonina, P. Snegurov, V. Sizov, Saint Petersburg State University, Saint Petersburg, Russia *Oxygen ion diffusivity in scandia-stabilized zirconia: molecular dynamics simulations*

	and ab initio calculation
26	L. Kar'kina, I. Kar'kin, A. Kuznetsov, Institute of Metal Physics Ural Branch RAS; Institute of quantum materials science, Ekaterinburg, Russia *Atomistic simulation of stacking faults in cementite*
27	A. Stroev, Yu. Gornostyrev, Institute of Metal Physics Ural Branch RAS; Institute of quantum materials science, Ekaterinburg, Russia *Precipitation kinetics and GPZ formation in Al-based alloys. Master equation approach with ab-initio parameterization*
28	I. Shmakov, I. Razumov, Yu. Gornostyrev, Institute of Metal Physics Ural Branch RAS; Institute of quantum materials science, Ekaterinburg, Russia *Decomposition kinetics in Fe–Cu dilute alloys. Monte Carlo simulations*
29	K. Nekrasov, N. Kichigina, Ural Federal University, Ekaterinburg, Russia *Molecular dynamics simulation of bulk xenon diffusion in UO_2: a comparison of ab initio interaction potentials*
30	I. Lomaev, D. Novikov, S. Okatov, Yu. Gornostyrev, S Burlatsky, Institute of Quantum Materials Science, Institute of Metal Physics UB RAS, Ekaterinburg, Russia, United Technologies Research Center (UTRC), USA *Size misfit versus electronic effects in diffusion of substitutional impurities in ni matrix*
31	A. Kardashin, V. Mazurenko, Ural Federal University, Ekaterinburg, Russia *Electronic and magnetic properties of iron impurities on W(110)*
32	A. Pravednicov, A. Tsirlin, D. Prishchenko, V.G. Mazurenko, Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany; Ural Federal University, Ekaterinburg, Russia *Modeling the electronic structure and dynamics of the crystal lattice $TiPO_4$*

ABSTRACTS
INVITED AND CONTRIBUTED TALKS