Science Meeting – Scientific Report

Scientific report (one single document in WORD or PDF file) should be submitted online within two months of the event. It should not exceed seven A4 pages.

***Proposal Title**: Workshop "Computational exploration of atomistic structures and their interrelation with physical properties" and Tutorial "Hands-on-FPLO"*

Application Reference N°: Science Meeting 4609

1)Summary (up to one page)

The Workshop "Computational exploration of atomistic structures and their interrelation with physical properties" and the Tutorial "Hands-on-FPLO" took place at IFW Dresden, Germany, from November 4 till 8, 2013. The program contained 14 invited lectures (40 min.) with speakers from China, Germany, USA, Denmark, Estonia, and Sweden; 8 contributed lectures (30 min., local speakers); 16 poster presentations with authors from Switzerland, Japan, Poland, Morocco, Germany, Korea, USA, Estonia, India, Sweden, and Russia. The total number of participants, including the organizers, amounted to 59.

The meeting was opened with a welcome reception in the evening of November 4. While the lectures were presented in the morning sessions on November 5 to 8 and in the afternoon of November 8, three afternoons were reserved for the tutorial.

During the tutorial, the participants were trained in the handling of the full-potential local-orbital (FPLO) code, the interpretation of its output, and in the solution of simple handling problems. Seven tutors first gave an introduction into a certain class of problems which can be treated by density-functional methods and then assisted the participants in solving a number of related tasks. These tasks were chosen from real scientific questions, but partly transferred to smaller systems to allow for calculations within the available time. The tasks were solved in 12 groups of two participants each. Since the number of applications for the tutorial was almost two times larger than the capacity (24 places were available due to the given number of laptops and the size of the lecture room), we decided to offer a second tutorial for local participants. This second tutorial (with 20 participants) took place at the Max-Planck-Institute for Chemical Physics of Solids Dresden on December 9 and 10, 2013.

The event was financially supported by ESF-psik, by the German Science Foundation (DFG), by the IFW Dresden, and by the MPI-CPfS Dresden.

2)Description of the scientific content of and discussions at the event (up to four pages)

The workshop was focussed on the computational exploration of atomistic structures, i.e., on the investigation of energy landscapes of chemcial systems with the aim to find stable and low-lying metastable structures of these systems with a pre-defined chemical composition. Further, it was intended to pay attention to the interrelation between structure and physical properties. This interrelation is mutual: systems with the same chemical composition, but with different structure, can show distictly different properties; on the other hand, the specific physical (e.g., magnetic) state may affect the structure.

The first two speakers, Yanming Ma from Jilin University (China) and Christian Schön from Stuttgart University (Germany), presented specific methods for the prediction of structures with density functional methods and discussed their advantages and shortcomings. Yanming Ma described several optimization strategies implemented in the "CALYPSO" code, developed by his group, and showed a number of successful applications, in particular the prediction of high pressure structures of several important systems, including elemental lithium, polymeric nitrogen, and calcium hydride. Up to now, the largest structural unit considered with this code contained 160 atoms. Christian Schön payed particular attention to unsolved problems which are inherent to the subject. The speakers agreed in the observation, that empirical pair potentials can be used to find the relevant low-energy basins which can be refined by DFT approaches.

Gerd Steinle-Neumann from Bayreuth University (Germany) reported his results on structure prediction for materials under the pressure of the earth (and other planet's) core. Such investigations considerably extend the possibilities of experimental high-pressure results and yield important input data for geophysical and astrophysical research.

Helge Rosner and Deepa Kasinathan from the MPI-CPfS Dresden (Germany) considered two aspects of structural transitions: the impact of local magnetism, which may considerably affect the bond length and the atomic volume, and the general question of the accuracy of density-functional calculations for the description of structural transitions.

Antia S. Botana from UC Davis, California (USA), discussed the effect of the surface on the physical properties of CrN. This compound is a magnetic semiconductor but has a metallic surface due to structural relaxation. A similar class of materials (PbS, PbSe, PbTe, and SnTe) was investigated by Niels E. Christensen from Aarhus University (Denmark). Here, the exceptional thermoelectric properties of these compounds motivated the interest. It was shown that the electronic structure at the gap was incorrectly described in the local density approximation. A self-consistent GW calculation cured the problem and provided correct band gap deformation potentials.

Markus Gruner from the University Duisburg/Essen (Germany) presented results on magnetic shape-memory alloys which are of recent interest for applications as

miniaturized actuators. He proved that the experimental observation of complicated modulated structures can be viewed as nano-twinned stackings of much simpler structural units.

Manuel Richter from IFW Dresden (Germany) showed possibilities to tune the dispersion and the location of topology-protected surface states in strong topological insulators. While the very existence of these states is determined by the bulk electronic structure, their properties can severely be influenced by surface decoration or by the choice of the surface facet. This insight is important for possible spintronic applications.

Klaus Koepernik from IFW Dresden (Germany) reported on the electronic structure of stacking faults in graphite. The energy of such faults is much smaller than the chemical bond energy within the carbon planes; nonetheless, the low-energy properties are essentially influenced by the imperfect stacking of the planes. As a result, the electric conduction parallel to the planes is mainly governed by the faults. Another effect of defects was described by Alexander Tsirlin from the National Institute of Chemical Physics and Biophysics Tallinn (Estonia), who considered their influence on structure and magnetism of Han purple, an ancient mineralic color.

Gotthard Seifert from Dresden University (Germany) presented details of the density-functional tight-binding (DFTB) method. This approximate method allows to treat large structural units (up to about 10.000 atoms) and may be used as a bridge between the less accurate empirical potential methods and the very accurate density functional methods for structure prediction.

Oleg Janson from the National Institute of Chemical Physics and Biophysics Tallin (Estonia) explained the possibility to evaluate microscopic model parameters for magnetic insulators by density-functional total energy calculations. In this way, density-functional theory can be used as input for quantum magnetic calculations.

Arnulf Möbius from IFW Dresden (Germany) resumed the discussion about structure prediction and introduced a new concept for the exploration of the huge space of possible atomic structures. He suggested to combine partial distortions with quench cycles and showed the success of this concept for benchmark systems using empirical pair potentials.

Hongbin Zhang from Rutgers University (USA) considered the J_{eff} = 1/2 insulating state of iridates by means of a dynamical mean-field approach. He showed, that higher-J states essentially contribute to the properties of such systems. Another aspect of spin-orbit coupling was investigated by Ulrich Rößler from IFW Dresden (Germany) who presented results for mesoscopic magnetic structures, so-called skyrmions.

Stephan Schönecker from KTH Stockholm (Sweden) reported his finding, that epitaxial films may show isostructural first-order phase transitions, if the substrate lattice parameter is varied, for instance by means of a piezoelectric crystal. At such a transition, all intrinsic physical properties show a discontinuity which can be expoited, e.g., in sensor or electronic applications. The further development of conventional electronic circuits calls for insulators with very low dielectric constant. Such low-k bulk insultors were simulated by Helmut Hermann from IFW Dresden (Germany).

Stefan Lebernegg from MPI-CPfS Dresden (Germany) described the effect of hydrogen positions on the exchange coupling of Cu-minerals. The experimental determination of these positions is complicated, since X-ray methods fail to resolve them.

Ivan Leonov from Augsburg University (Germany) computed the equilibrium crystal structure and phase stability of several correlated electron materials using the dynamical mean-field approach. In particular, he calculated the electronic and structural properties of paramagnetic iron at the bcc - fcc phase transition as a function of temperature.

Wenxu Zhang from Chengdu University (China) reported about his progress in the search for new carbides and dichalcogenides with global crystal structure searching codes. Previously reported carbides with rocksalt or wurtzite structures were found to be unstable in these structures.

Finally, Ingo Opahle from Bochum University (Germany) presented his results in the field of materials for energy applications, in particular materials with promising thermoelectric and magnetocaloric properties. These materials were identified by density-functional screening of a number of structure classes and their properties were evaluated.

Posters comprised results on unknown structures discovered by density-functional approaches (Amsler, reconstruction of the Boron (111) surface); suggestion of a novel material for spintronic application (Ghimire, half-metallic Sr4Rh3O10); the relation between chemical charges and physical properties (Goraus, BaFe2As2 and SrFe2As2 superconductors); the effect of doping (El Hachimi, Nd-doped ZnO); pressure-dependent intermolecular coupling (Höppner, picene); the interplay of structure and correlation (Jung, perovskite NaOsO3); results of spin-fluctuation pairing calculations for superconductors (Kreisel, Wang); the effect of distance variation on graphene bilayers (Naji); the effect of crystal fields and exchange interactions in magnetite and nickel ferrite (Ouaissa); a microscopic model of Cu(OH)Cl (Pungas); the relation between electronic and magnetic properties of Ni-Fe-Ga Heusler alloys (Sahariah); the effect of correlation and spin-orbit coupling in metal-aluminum-X phases (Sun); a comprehensive investigation of Fe-Co-Ga solid solutions (Verchenko); and the effects of size, substitution and electric field on the properties of carbon and boron-nitride quantum dots (Yamijala).

3)Assessment of the results and impact of the event on the future directions of the field (up to two pages)

The whole meeting was characterized by a critical discussion of the open problems in the field. While advanced search algorithms offer the principle possiblity to exhaust the search space in a much more efficient way than a straightforward scanning would do, the problem is, from a mathematical point of view, non-polynomial hard and, thus, the effort for large systems grows exponential with the system size. It has to be concluded that a so-called educated guess of the possible structure for a given chemcial composition may essentially reduce the search space and has to be applied in order to make the search tractable for systems sizes of interest.

An important observation is, that in many cases empirical potentials allow to find basins of low-energy solutions which are the same as those found with density-functional codes. This means, that empirical potentials which are computationally cheap can be used to explore the user-defined search space. The obtained low-energy solutions can be further refined (or, evaluated) by more accurate, but also more expensive, density-functional methods. This procedure could possibly be extended into a three-step algorithm with an intermediate refinement by an approximate density-functional method like DFTB. Such an approach has not yet been tested, to the best of our knowledge.

We are confident, that the workshop will contribute to the further development of electronic-structure based methods for materials research. In particular, the development and distribution of software for the search of yet unknown structures will gain from the combination of several presented techniques. This will finally foster the application of computational screening methods in the search for new materials with specific properties. Though the computational effort of such a screening is high, in it will many cases be still cheaper than related experimental screening.

The tutorial was over-booked and was for this reason extended in a second session. It attracted in total 44 participants who learned the ins and outs in the handling of the full-potential local-orbital (FPLO) code. Under the supervision of experienced tutors, the participants solved realistic tasks and were successfully educated in avoiding problems in the handling of electronic structure codes. This event will certainly contribute to the further distribution of electronic structure methods in general and to the use of the FPLO code in particular.

Manuel Richter and Helge Rosner

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Monday, November 4

18:00 – 20:00 Welcome reception at IFW / Registration
D2E.27 (2nd floor)

Lecture Hall Attachment of posters

Tuesday, November 5

08:30 – 09:00 Registration

09:00 – 12:50 / Lecture Hall Session 1 Chair:
Manuel Richter

09:00 Yanming Ma Atomistic structure prediction via CALYPSO methodology: principles and applications

09:40 Christian Schön Investigation of energy landscapes of chemical systems on ab initio level

10:20 Coffee and Posters Lecture Hall

11:10 Gerd Steinle-Neumann Magnetism in iron under high pressure

11:50 Helge Rosner Structural transitions under pressure: How relevant is local magnetism?

12:20 Deepa Kasinathan Structural transitions under pressure: How accurate are DFT calculations?

13:00 Lunch IFW Restaurant

14:00 – 18:00 / Room B3E.26 Tutorial Hands-on-FPLO

16:00 Coffee break D2E.27 (2nd floor)

18:00 Sandwiches IFW Restaurant

Dinner for the invited speakers

Wednesday, November 6

09:00 – 12:50 / Lecture Hall **Session 2** **Chair:** Deepa Kasinathan

09:00 Antia S. Botana Electronic structure of CrN: from macro to nano

09:40 Niels E. Christensen Electronic quasiparticle states of PbX (X=S,Se,Te) and SnTe

10:20 Coffee and Posters *Lecture Hall*

11:10 Markus Gruner Magnetoelastic coupling and the formation of adaptive microstructures in magnetic shape memory alloys

11:50 Manuel Richter Yet the surface matters: Anisotropy and position of topological states

12:20 Klaus Koepernik Electronic structure of stacking faults in graphite

13:00 Lunch *IFW Restaurant*

14:00 – 18:00 / Room B3E.26 **Tutorial Hands-on-FPLO**

16:00 Coffee break *D2E.27 (2nd floor)*

18:00 – 20:00 / Lecture Hall **Beer, Sandwiches, and Posters**

Thursday, November 7

09:00 – 12:50 / Lecture Hall **Session 3** **Chair:** Stefan Lebernegg

09:00 Gotthard Seifert Density-Functional Tight Binding (DFTB) – an approximate DFT Method

09:40 Alexander Tsirlin Structure and magnetism of Han Purple ($BaCuSi_2O_6$) revealed by DFT: how the defects matter

10:20 Coffee and Posters *Lecture Hall*

11:40 Oleg Janson Evaluation of microscopic model parameters for magnetic insulators: a computational approach

12:20 Arnulf Möbius Structure optimization via "partial distortion"- quench cycles

13:00 Lunch *IFW Restaurant*

14:00 – 18:00 / Room B3E.26 **Tutorial Hands-on-FPLO**

16:00 Coffee break *D2E.27 (2nd floor)*

18:00 Sandwiches *IFW Restaurant*

Removal of posters

Friday, November 8

09:00 – 12:50 / Lecture Hall **Session 4** **Chair:** Klaus Koepernik

09:00 Hongbin Zhang J_{eff} = 1/2 insulating state in Ruddlesden-Popper iridates: An LDA+DMFT study

09:40 Stephan Schönecker Bain paths of metals: From isostructural instabilities in epitaxial films to the ideal strength of random alloys

10:20 Coffee break *Lecture Hall*

10:40 Ulrich Rößler Itinerant magnetism modified by spin-orbit coupling: Intermetallic compounds with B20 structure and related systems

11:10 Helmut Hermann Simulation of low-k bulk insulators for application in semiconducting devices

11:40 Stefan Lebernegg Hydrogen positions and their effect on exchange couplings of Cu-minerals

12:10 Ivan Leonov Total energy and force calculations for correlated materials

13:00 Lunch *IFW Restaurant*

14:00 – 15:20 / Lecture Hall S**ession 5** **Chair:** Helge Rosner

14:00 Wenxu Zhang Searching for New Carbides and Dichalcogenides

14:40 Ingo Opahle Density functional screening of materials for energy applications

15:20 Coffee break *Lecture Hall*

18:00 Farewell Dinner

Posters

Gulzar Ahmed Electronic structure of lead halides using Compton scattering technique

Maximilian Amsler Conducting boron sheets formed by the reconstruction of the ??-Boron (111) surface

Madhav Ghimire	Novel material for spintronics applications: Sr4Rh3O10
Jerzy Goraus	Mulliken charges calculated for iron based superconductors-BaFe2As2 and SrFe2As2 either doped with cobalt or under external pressure
Abdel Ghafour El Hachimi	Structural and magnetic properties of Nd-doped ZnO
Marc Höppner	From molecules to crystals: pressure-dependent intermolecular coupling in picene
Myung-Chul Jung	Structural and Correlation Effects in the Itinerant Insulating Antiferromagnetic Perovskite NaOsO3
Andreas Kreisel	Symmetry of gap functions and pairing instabilities in multiband superconductors: 3D effects
Mohamed El-Amine Moussa	DFT+U Study of Strongly correlated materials: ABO4 compounds
Sufyan Saleh Ahmed Naji	On Distance Variation Effects on Graphene Bilayers
Mohamed Ouaissa	Magnetic properties dependence on crystal fields and exchange interactions in magnetite
Mohamed Ouaissa	Effects of Crystal Fields and Exchange Interactions on Magnetic Properties of Nickel Ferrite

Taavi Pungas	Microscopic magnetic model of Cu(OH)Cl: Shastry-Sutherland lattice with spatial anisotropy
Munima Bora Sahariah	Electronic and magnetic properties of Ni-Fe-Ga Heusler alloy
Weiwei Sun	Correlation and relativistic effects in MAX phases
Valeriy Verchenko	Intermetallic Solid Solution Fe1-xCoxGa3: Synthesis, Physical Properties, NQR Study and Electronic Band Structure Calculations
Yan Wang	Superconducting gap in LiFeAs from three dimensional spin fluctuation pairing calculations
Sharma Yamijala	Structural Stability, Electronic, Magnetic and Optical Properties of Rectangular Graphene and Boron-Nitride Quantum Dots: Effects of Size, Substitution and Electric Field

Annex 4b: Full list of speakers and participants

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