Ψ_k Newsletter

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

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Editor: Z. (Dzidka) Szotek
E-mail: psik-coord@dl.ac.uk

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Contents

1 Editorial

In this Psi-k newsletter we have three workshop reports, however without abstracts of presented papers. The complete reports are to be found on the Psi-k Portal in the 'Psi-k Repository'. How to upload reports and other information to the Psi-k Portal is described in the following section.

This time we also have one report on a collaborative visit of a young researcher from Barcelona to ETH Zurich, a few job and event announcements and a number of abstracts of the newly submitted or recently published papers.

The scientific highlight of this issue is by Y. Pouillon (Louvain-la-Neuve and San Sebastian) and X. Gonze (Louvain-la-Neuve) on "Harnessing the power of modern package management tools for a large Fortran-90-based project: the mutation of ABINIT".

Since this is the last newsletter of this calendar year, we would like to take this opportunity and thank everybody who contributed to the Psi-k newsletters of this year. We also wish everybody all the best in the personal and professional activities in the New Year. We hope for an increased number of contributions to the future newsletters. The *Networks* have a home page on World

Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:

http://www.psi-k.org.uk/

Please submit all material for the next newsletters to the email address below.

The following email addresses, which remain in operation, are repeated for your convenience, and are the easiest way to contact us.

	function
psik-coord@dl.ac.uk	**messages to the coordinators, editor & newsletter**

Dzidka Szotek, Martin Lüders and Walter Temmerman
e-mail: psik-coord@dl.ac.uk

2 General News

2.1 Uploading Information to Psi-k Portal

As already mentioned in the past newsletters, the Psi-k Portal is the only means for distributing and receiving Psi-k related information. We do not advise using 'Mailtool' facility on the Portal, as it does not allow to store the distributed information on the Psi-k Portal in the Psi-k Announcements' pool. Thus it cannot be seen by anybody who chooses to check for the new announcements on the Portal.

Since uploading information to the Psi-k Portal seems to give problems to some users, below we enumerate the steps one needs to follow to successfuly upload e. g. an announcement to the Psi-k Portal and having it distributed by e-mail to all the Portal members.

1. **'Login to Psi-k Portal'**, accessed from http://www.psi-k.org, by clicking on the former while on the Psi-k web page
2. While already on the Psi-k Portal click on **'Psi-k Announcements'**
3. Click on **'Add'** to get a window for uploading an announcement and then fill in all the required fields
4. Hyperlinks have to be added to any URLs of the web pages ocurring in the body of the announcement by clicking on the option above the main body window which looks like **'binnacles on a blue ball'** and typing the URL into the subsequently opened field
5. **Add Attachements**, if any, by pressing this option
6. When all is typed and filled, then press **'Preview'** to see if all looks right
7. If yes, then for **'Email Notification'** choose **'High - All Participants'**
8. **Don't do** anything about 'Access' or 'Availability', and leave them as they are by default
9. Press **'Add Announcement'**, and all is done.

Our 'java experts' are presently looking into the possibility of combining the Mailtool option and the uploading option in such a way that both create a similar interface and in addition store the announcement on the Portal. Of course, using Mailtool one can choose an option that will allow to store the announcement in the 'Mailtool Archive', but until now no-one using

Mailtool has chosen to do so. In any case storing announcements in two different places would be inconvenient. Thus, until we have a better way of dealing with the Mailtool, please do follow the steps above for the announcements. Thank you.

2.2 Uploading Reports on Workshops and Other Events to Psi-k Portal

It has been our long-term practice to publish in the Psi-k Newsletters reports on all workshops/meetings supported by the Psi-k Network. They have consisted of a short summary, a programme, list of participants and abstracts of presented papers. Unfortunately, as the number of yearly events has increased with time, the reports have become longer, leading to newsletters often approaching 200 A4 pages.

With the introduction of the Psi-k Portal, we have opted for shorter reports (without abstracts) published in the newsletters, while asking the events' organizers to upload the complete reports (including abstracts), in the pdf-format, to the Psi-k Portal.

Hereby, we would like to remind all the organizers of the events supported by the Psi-k Network to submit short reports (consisting of short summary, programme and list of participants), in the latex format, by e-mail to

psik-coord@dl.ac.uk,

to be published in the Psi-k newsletter, subsequent to the event, and to upload complete reports (with abstracts of presented papers), in the pdf-format, to the 'Psi-k Repository' on the Psi-k Portal.

All the reports are stored in the Repository for an easy access if anybody is interested to read also the abstracts of papers presented at a given event.

The Psi-k Portal is accessed from the Psi-k Network webpage

http://www.psi-k.org

by choosing the option **'Login to Psi-k Portal'**.

3 Psi-k Core Activities

"Towards Atomistic Materials Design"

3.1 Reports on Psi-k Workshops

3.1.1 Report on IAC-V

Fifth International Alloy Conference (IAC-V)

11-14.09.2008, Cliff-Hotel Ruegen, Germany

Sponsored by Psi-k Programme

The triennial International Alloy Conferences (IACs) aim at the identification and promotion of the common elements developed in the study, either experimental, phenomenological, or theoretical and computational, of materials properties across materials types, from metals to minerals. To accomplish this goal, the IAC-V brought together scientists from a wide spectrum of materials science including experiment, theory, modelling, and computation, engaged in the study of a broad range of materials properties. This conference provided a forum for presentations of state-of-the-art experimental, theoretical, and computational developments in studying, understanding, and predicting the properties of materials. It also encouraged interdisciplinary contributions, such as between the fields of condensed matter physics and earth sciences and geophysics

Main emphasis in the talks was given to the fields of basic science, e.g., electronic structure and related properties, experimental science, e.g., assessing alloy phase diagrams, semiconductor physics, mineral science, and phenomenology. The emphasis on cross-fertilization of subject matter and the interdisciplinary character of the presentations made this meeting unique.

A number of specialized sessions covered the following topics:

Electronic structure calculations for alloys (wave functions and density functional theory for excited states, the EMTO method and applications to disordered alloys, as well as an implementation of the Non-local CPA alloy theory have been addressed);
Thermodynamics of alloys (with an emphasis on configurational thermodynamics of alloys and studies of thermodynamic properties and phase diagrams from first principles, as well as on the double defect method);
Metals and alloys at high pressure and temperature: theory and experiment (new trends in high-pressure alloys synthesis, in particular, high-pressure alloying of immiscible metals, and alloys characterisation using synchrotron radiation have been shown; new experimental and theoretical results of investigations of phase transformations and structural stability in beta-brass CuZn, FeCr and Mo under pressure have been reported);
Strongly correlated materials have been presented on example of density-functional studies

of Pu-U-Zr alloys as well as investigation of the influence of two-particle correlations on electron-emission spectra thermal signatures of the volume collapse in cerium;
Alloys with special properties session gave a broad overview on metastable pseudobinary alloys of transition metal nitride thin films with resultant age hardening, on binary and multi-component phase diagrams for titanium carbonitride, as well as on para- to ferroelastic transformations in NiTi shape memory alloys and elastic constants of Pt-Sc alloys
High-pressure and thermal properties of Fe and Fe- alloys demonstrated a strong relation between earth's and materials sciences on example of mineral physics quest to the Earth's core and theoretical investigations of structural and magnetic properties of Fe and Fe based alloys under pressure
TM oxides and compounds under high pressure session broadened the scope of presented materials due to reports on HP studies of FeMgO, FeMgSiO3, FeMg, and (Mg,Fe)O systems
Atom kinetics and electron transport in alloys was demonstrated on example of Fe-Cr, Cu-Fe, and other intermetallics ((Cu,Ni)MnSb), including nano-sized precipitates in alloys, modelling

For statistics, 43 scientists from 11 countries (Sweden, USA, Germany, Russia, United Kingdom, Czech Republic, the Netherlands, Japan, France, Austria, and Israel) took part in this scientific forum. Among them there were 13 women and 10 young scientists.

Programme

September 11, Thursday
12.00-18.00 Registration
12:30- 14:00 Lunch
17:00- 17:30 Coffee
18.00 - 18.30 Conference opening
18.30-19.30 **Opening session**

1. I. Abrikosov "Theoretical physics, steel and alloys" - 30 min
2. Yu. Vekilov "Electronic and Thermal properties of Quasicrystalline Alloys at Low and High Temperatures" - 30 min

19:30-21:00 Dinner

September 12, Friday

7:30- 8:30 Breakfast

8.30-10.00 **Electronic structure calculations for alloys**

3. T. Gonis "Wave functions and density functional theory for excited states in electronic structure calculations" -30 min
4. L. Vitos "The EMTO method and applications to disordered alloys" - 30 min
5. H. Ebert "An efficient implementation of the Non-local CPA alloy theory and its application

to study magnetic and transport properties" - 30 min

10.00-10.30 - Coffee

10.30 - 12.30 **Thermodynamics of alloys**

6. A. V. Ruban "Configurational thermodynamics of alloys from first principles" - 30 min
7. V. Vinograd "The Double Defect Method" - 30 min
8. K. Masuda-Jindo "First Principles Study of Thermodynamic Properties and Phase Diagrams of High Temperature Bcc Mo-Ta-W Alloy Systems: Inclusion of liquid phase" - 30 min
9. P. Korzhavyi "First-principles thermodynamic modeling of multicomponent alloys" - 30 min

12.30-14.00 Lunch

14-00-15.00 - **discussions and posters**

15.00 -16.30 **Metals and alloys at high pressure and temperature: theory and experiment**

10. N. Dubrovinskaia "High-pressure alloying" - 30 min
11. S. Pascarelli "Effects of Pressure on Magneto-Elastic Properties of Alloys" - 30 min
12. T. Mohri "First principles calculation of phase equilibria and lattice expansion of Fe-Ni system" - 30 min

16.30-17.00 - Coffee

17.00-19.00

13. O. Degtyareva "Structural transformation in beta-brass CuZn compressed to 90 GPa" - 30 min
14. V. Degtyareva "Structural stability of the sigma phase FeCr under pressure to 77 GPa" - 30 min
15. A. Mikhaylushkin "Electron Concentration and Pressure-Induced Structural Changes in Alloys InA (A = Cd, Sn)" - 30 min
16. C. Asker "First-principles solution to the problem of lattice stability in Molybdenum" - 30 min

19:30-21:00 Dinner

21.30 - **after dinner panel discussion**

September 13, Saturday

7:30- 8:30 Breakfast

8.30-10.00 **Strongly correlated materials**

17. A. Landa "Density-functional studies of Pu-U-Zr alloys" - 30 min
18. J. Berakdar "Influence of two-particle correlations on electron-emission spectra" - 30 min
19. M. Lipp "Thermal signatures of the volume collapse (VC) in cerium" - 30 min

10.00-10.30 - Coffee

10.30-12.30 **Alloys with special properties** 20. L. Hultman "Secondary phase transformations in metastable pseudobinary alloys of transition metal nitride thin films with resultant age hardening" - 30 min
21. D. A. Andersson "First-principles based calculation of binary and multicomponent phase diagrams for titanium carbonitride" - 30 min
22. W. Schmahl "Para- to ferroelectric transformations in NiTi shape memory alloys" - 30 min
23. E. I. Isaev "Elastic constants of Pt-Sc alloys" - 30 min

12.30-14.00 Lunch

14-00-15.00 - **discussions and posters**

15.00-17.00 **High-pressure and thermal properties of Fe and Fe alloys**

24. L. Dubrovinsky "Mineral physics quest to the Earth's core" - 30 min
25. S. I. Simak "Iron and its alloys under high pressure" - 30 min
26. L. Vocadlo "Elasticity of iron phases in the Earth's core" - 30 min
27. S. Mankovsky "Structural and magnetic properties of Fe and Fe based alloys under pressure" - 30 min

17.00-17.30 - Coffee

17.30-19.30 **TM oxides and compounds under high pressure**

28. R. Ahuja "High pressure study on FeMgO, FeMgSiO3 and FeMg systems" - 30 min
29. R. Pentcheva "Cation, charge and magnetic ordering in the Fe2O3/FeTiO3 system: Insights from correlated band theory" - 30 min
30. G. Kh. Rozenberg "Metallization of TM compounds under pressure and accompanying magnetic/electronic phenomena" - 30 min
31. Natalia Skorodumova "Theoretical study of high- to low-spin transition in (Mg,Fe)O under pressure" - 30 min

20.00- Conference dinner

September 14, Sunday

7:30-8:30 Breakfast

8.30-10.30 **Atom kinetic and electron transport in alloys**

32. P. Olsson "Fe-Cr modeling" - 30 min
33. W. Puschl "Monte-Carlo simulation of atom kinetics in intermetallics: Correcting the jump

rates" - 30 min
34. V. Vaks "Stochastic statistical theory of nucleation and growth of nano-sized precipitates in alloys with application to precipitation of copper in iron" - 30 min
35. V. Drchal "Electronic, magnetic, and transport properties of halfmetallic semi-Heusler (Cu,Ni)MnSb alloys" - 30 min

10.30-11.00 - Coffee

11.00-11.10 Conference closing

12.30 Lunch and departure

Poster presentations

1. G. M. Bhuiyan "Entropy of Mixing for AgSn liquid binary alloys"
2. L. Isaeva "Dinamical stability of the defect phase of palladium hydride: ab initio studies"
3. E. Kabliman "Ab initio calculations of formation energies of the Fe-Cr sigma-phase in magnetic state"
4. A. I. Kartsev "Stability of the face-centered-cubic phases of CoN under pressure"
5. A. Lodder "Electromigration force on a proton with a bound state"
6. S. Mankovsky "Structural and magnetic properties of Cr telluride-selenide alloys"
7. O. Narygina "Fe-Ni-C system at high pressure"
8. A. Ponomareva "Tuning of magnetic state in high-pressure synthesis of cubic phase in Fe-Si system"
9. E. Sterer "Irreversible pressure-induced amorphization of the cation deficient perovskite La1/3NbO3"
10. K. Tarafder "Phase stability in disordered alloys: An approach via augmented space recursion based orbital peeling technique"
11. O. Vekilova "First-principles investigation of multiple hydrogen occupancy of vacancies in Pd"
12. N. Bondarenko "Lattice stability of simple metals and phase transitions at ultrahigh pressure"
13. E. Zarechnaya "New HPHT boron phase"
14. L. Pourovskii "Electronic properties of rare earth monoarsenides and rare earth iron oxyarsenides"
15. W. Wunderlich "Ab-initio calculations and experiments on CoSbTi-based Half-Heusler phases for thermoelectric applications"

List of participants

1. Igor Abrikosov
Email: igor.abrikosov@ifm.liu.se

Department of Physics
Chemistry and Biology (IFM)
Linkoping University
581 83 Linkoping
Sweden

2. R. Ahuja
Email: rajeev.ahuja@fysik.uu.se
Physics Department
Uppsala University
Sweden

3. D. A. Andersson
Email: andersson@lanl.gov
Los Alamos National Lab
USA

4. C. Asker
Email: chrgo@ifm.liu.se
Department of Physics
Chemistry and Biology (IFM)
Linkoping University
581 83 Linkoping
Sweden

5. Jamal Berakdar
Email: jamal.berakdar@physik.uni-halle.de
University of Halle
Heinrich-Damerow-Strasse 4
06120 Halle
Germany

6. Nina Bondarenko
Email: bondnina@gmail.com
Moscow Steel and Alloys Institute
Theoretical Physics Department
Leninskii pr. 4
119049 Moscow
Russia

7. Olga Degtyareva
Email: o.degtyareva@ed.ac.uk
CSEC and School of Physics
University of Edinburgh
King's Buildings, Mayfield Road
Edinburgh EH9 3JZ
United Kingdom

8. Valentina Degtyareva
Email: degtyar@issp.ac.ru
Institute of Solid State Physics
142432 Chernogolovka
Russia

9. Vaclav Drchal
Email: drchal@fzu.cz
Institute of Physics
Academy of Sciences of the Czech Republic
Na Slovance 2
182 21 Praha 8
Czech Republic

10. Natalia Dubrovinskaia
Email: Natalia.Dubrovinskaia@min.uni-heidelberg.de
Institute of Earth Sciences
University of Heidelberg
Im Neuenheimer Feld 234-236
D-69120 Heidelberg
Germany

11. Leonid Dubrovinsky
Email: Leonid.Dubrovinsky@uni-bayreuth.de
Bayerisches Geoinstitut
University of Bayreuth
95440 Bayreuth
Germany

12. Hubert Ebert
Email: Hubert.Ebert@cup.uni-muenchen.de
Universitat Munchen
Department Chemie und Biochemie
Physikalische Chemie
Butenandtstr. 5-13
D-81377 Munchen
Germany

13. Antonios Gonis
Email: gonis@comcast.net
Lawrence Livermore National Laboratory
P.O. Box 808, L-353
Livermore, CA 94550
USA

14. Lars Hultman
Email: larhu@ifm.liu.se
Linkoping University

Thin Film Physics Division
IFM, S-58183 Linkoping
Sweden

15. Eyvaz Isaev
Email: isaev@ifm.liu.se
Department of Physics,
Chemistry and Biology (IFM)
Linkoping University
581 83 Linkoping
Sweden

16. Leyla Isaeva
Email: leyla@isaeva@yahoo.com
Department of Physics
M.V. Lomonosov Moscow State University
1-2 Lenin Hills
119992 Moscow
Russia

17. Pavel Korzhavyi
Email: pavel@mse.kth.se
KTH Stockholm
Sweden

18. Alexander I. Landa,
Email: landa1@llnl.gov
Lawrence Livermore National Laboratory
Physical Sciences Directorate
7000 East Ave L-045
Livermore, CA 94550-0808
USA

19. Magnus Lipp
Email: lipp1@llnl.gov
Lawrence Livermore National Laboratory
H-Division, Physical Sciences, 7000 East Ave
Livermore, CA 94550
USA

20. A. Lodder
Email: adrilodder@msn.com
Amstelveenseweg 749
!081 JE Amsterdam
The Netherlands

21. Sergiy Mankovskyy
Email: Sergiy.Mankovskyy@cup.uni-muenchen.de

Ludwig-Maximilians-Universitat Munchen
Department Chemie/ Physikalische Chemie
Butenandtstra?e 11
81377 Munchen
Germany

22. Kinichi Masuda-Jindo
Email: kmjindo@issp.u-tokyo.ac.jp
University of Tokyo
Japan

23. Tetsuo Mohri
Email: tmohri@eng.hokudai.ac.jp
Graduate School of Engineering
Hokkaido University
Kita-13 Nishi-8, Sapporo 060-8628
Japan

24. Olga Narygina
Email: Olga.Narygina@uni-bayreuth.de
Bayerisches Geoinstitut
University of Bayreuth
95440 Bayreuth
Germany

25. Par Olsson
Email: olsson.par@gmail.com
EDF R&D
France

26. S. Pascarelli
Email: sakura@esrf.fr
ESRF
6 rue Jules Horowitz
BP220
38043 Grenoble cedex
France

27. R. Pentcheva
Email: Rossitza.Pentcheva@lrz.uni-muenchen.de
Department of Earth and Environmental Sciences
Section Crystallography
Ludwig-Maximilians-University Munich
Theresienstr. 41
80333 Munich
Germany

28. Alena Ponomareva
Email: alenaponomareva@yahoo.com
Moscow Steel and Alloys Institute
Theoretical Physics Department
Leninskii pr. 4
119049 Moscow
Russia

29. Wolfgang Puschl
Email: wolfgang.pueschl@univie.ac.at
Fakultat fur Physik der Universitat Wien
Department
Dynamics of Condensed Systems
Boltzmanngasse 5
A-1090 Wien
Austria

30. G. Kh. Rozenberg
Email: emtsm@post.tau.ac.il
School of Physics & Astronomy
Tel-Aviv University,
Ramat-Aviv, Tel-Aviv 69978
Israel

31. A. V. Ruban
Email: a.v.ruban@gmail.com
KTH Stockholm
Sweden

32. Prof. Wolfgang Schmahl
Email: wolfgang.schmahl@lrz.uni-muenchen.de
Department of Earth and Environmental Sciences
Section Crystallography
Ludwig-Maximilians-University Munich
Theresienstr. 41
80333 Munich
Germany

33. Sergei I. Simak
Email: sergeis@ifm.liu.se
Department of Physics
Chemistry and Biology (IFM)
Linkopings universitet
581 83 Linkoping
Sweden

34. N. Skorodumova
Email: Natalia.Skorodumova@fysik.uu.se

Physics Department
Uppsala University
Sweden

35. Valentin Vaks
Email: vaks@mbslab.kiae.ru
Russian Research Centre "Kurchatov Instituite"
Kurchatov square 1
Moscow 123182
Russia

36. Olga Vekilova
Email: olgav@ifm.liu.se
Department of Physics
Chemistry and Biology (IFM)
Linkoping University
581 83 Linkoping,
Sweden

37. Yuri Vekilov
Email: yuri_ vekilov@yahoo.com
Moscow Steel and Alloys Institute,
Theoretical Physics Department
Leninskii pr. 4
119049 Moscow
Russia

38. V. Vinograd
Email: V.Vinograd@kristall.uni-frankfurt.de
Inst. f. Geowissenschaften
FE Mineralogie / Abt. Kristallographie
Universitaet Frankfurt
Altenhoeferallee 1
D-60438 Frankfurt am Main
Germany

39. Levente Vitos
Email: Levente.Vitos@fysik.uu.se
MSE-KTH Stockholm
Sweden

40. Lidunka Vocadlo
Email: l.vocadlo@ucl.ac.uk
Department of Earth Sciences
UCL
Gower Street
London
WC1E 6BT

UK

41. Wilfried Wunderlich
Email: wi-wunder@rocketmail.com
Tokai University
Materials Science Department
259-1292 Hiratsuka-shi, Kanagawa
Japan

42. M. Winklhofer
Email: michael@geophysik.uni-muenchen.de
Department of Earth and Environmental Sciences
Geophysics
Ludwig-Maximilians-University Munich
Theresienstr. 41
80333 Munich
Germany

43. Evgeniya Zarechnaya
Email: ezarechnaya@yahoo.com
Bayerisches Geoinstitut
University of Bayreuth
95440 Bayreuth
Germany

3.1.2 Report on 2008 Tutorial Hands-on-FPLO

IFW Dresden, Germany

24-28 August, 2008

Sponsored by

Psi-k Network
IFW Dresden e. V.
Alexander von Humboldt-Stiftung

The 2008 Tutorial Hands-on-FPLO was the seventh tutorial of its kind, in annual succession. After the 2007 La Plata (Argentina) tutorial, it was again placed at IFW Dresden (2002, 2003, 2004, and 2006 - IFW Dresden, 2005 - UC Davis, California). This time, we combined the tutorial with a workshop called "DFT meets experiment". This way the interaction of computation and experiment on actual topics was demonstrated to young participants. A particular focus was on invited talks given by experimentalists who reported successful collaborations with DFT groups and gave an overview over some of the available techniques that can be combined with electronic structure calculations. In particular, experimental reports were given on quantum oscillations (J. Wosnitza), spectroscopy of organic complexes (M. Knupfer) and rare earth compounds (C. Laubschat), and high-pressure experiments (U. Schwarz).

The theoretical part combined recent research on new functionals for highly correlated magnetic systems (W. Pickett, P. Novák), with further development of electronic structure codes (B. Delley - DMol3, P. Gianozzi - Quantum Espresso, V. Blum - FHI-aims) and specific applications (I. Opahle - magnetic shape memory alloys, A. Mykhaylushkin - Fe-alloys under earth's core conditions, A. Tsirlin - low dimensional spin systems, F. Tasnádi - piezoelectricity, M. Gruner - magnetic clusters, H. Eschrig - superconducting Fe-pnictides, D. Kasinathan and H. Rosner - orbital order, B. Hamad - magnetic multi-layers). Eleven contributed talks and several posters completed the program. Most of the lectures can be downloaded from http://www.fplo.de/workshop/ws2008/index.html.

The total number of participants, 59, was higher than in the previous meetings. The tutorial was attended by 27 of the participants, which is at the limit of our local possibilities. The setup of the input and specific features of the FPLO code were presented in introductory lessons. Then, the participants were invited to try FPLO-8 (a pre-release) and to perform a number of calculations like convergence tests for numerical settings, modification and re-compilation of the source code, fixed-spin moment calculations, LSDA+U and LSDA+OPC calculations on cuprate oxides and on the magnetic anisotropy of hcp Co, respectively, determination of Heisenberg model parameters, and the magnetic ground state of transition metal dimers. The related tasks and solutions can be downloaded (http://www.fplo.de/workshop/ws2008/index.html). Partly, they repeat recently published FPLO results.

Finally, I would like to thank, on behalf of all organizers, all participants for their contributions

and the funding institutions (Psi-k network and IFW Dresden) for financial support.

Manuel Richter.

Sunday, August 24

19:00 Registration and get-together reception

Monday, August 25

Morning session: Workshop DFT meets Experiment, invited talks

9:00 Helmut Eschrig (Dresden): Opening

9:05 Warren Pickett (Davis): LDA, DMFT, FPLO: The Story of U

9:50 Jochen Wosnitza (Rossendorf): Magnetic quantum oscillations in strongly correlated metals - experimental data meets theoretical predictions

10:35 Coffee

10:50 Pavel Novák (Prague): Spin and orbital polarization in DFT methods

11:35 Ingo Opahle (Frankfurt): Origin of the tetragonal distortion in FePd shape memory alloys

12:20 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Getting started and installation)

14:00 Getting started with FPLO-8 (Manuel Richter)

15:00 Task I: Convergence of k summation

15:30 Coffee

16:00 Installation and modification of the code (Ulrike Nitzsche)

16:30 Task II: Code modification and installation

17:00 Ressources and performance (N.N.)

17:15 Break

Evening session: Workshop DFT meets Experiment, contributed talks

17:30 Martin Diviš (Prague): Crystal Field calculated for alloys

17:50 Iryna Kondakova (Kiev): Structure optimization with FPLO7: Perovskites and doped II-VI semiconductors

18:10 Erik Ylvisaker (Davis): Charge self-consistency in LDA+DMFT: Application to Yb valence transition

18:30 Sanjubala Sahoo (Duisburg-Essen): Magnetic anisotropy in transition metal clusters

18:50 End of session

Tuesday, August 26

Morning session: Workshop DFT meets Experiment, invited talks

- 9:00 Bernard Delley (Villigen): DMol3 applications from molecules to surfaces and solids
- 9:45 Martin Knupfer (Dresden): Orbital and spin ground state of transition metal phthalocyanines
- 10:30 Coffee
- 10:45 Paolo Giannozzi (Udine): Theoretical design of phthalocyanine-inorganic semiconductor systems for new hybrid materials
- 11:30 Ulrich Schwarz (Dresden): Clash of cultures? Under pressure, experiment meets theory
- 12:15 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Concept and spin magnetism)

- 14:00 FPLO-8, an all-purpose DFT code (Klaus Koepernik)
- 15:00 Fixed spin moment method (Michael Kuz'min)
- 15:45 Task III: FSM calculation
- 16:00 Coffee
- 16:30 Task III: FSM calculation, continued
- 17:30 Break

Evening session: Workshop DFT meets Experiment, contributed talks

- 17:45 Ismaila Dabo (Marne-la-Vallée): First-principles simulation of electrochemical systems at fixed applied voltage
- 18:05 Ruijuan Xiao (Dresden): Density functional investigation of the dielectric constant for bilayer graphene.
- 18:25 Kemal Özdoğan (Gebze): A comparative study of ferromagnetism in quinternary Heusler alloys: Super cell, virtual crystal approximation and coherent potential approximation
- 18:45 End of session

Wednesday, August 27

Morning session: Workshop DFT meets Experiment, invited talks

- 9:00 Arkady Mikhaylushkin (Linköping): Structural properties of $Fe_{1-x}Ni_x$ compressed and heated to the Earth's core conditions
- 9:45 Alexander Tsirlin (Moscow): Unraveling magnetic interactions in low-dimensional spin-1/2 systems
- 10:30 Coffee
- 10:45 Ferenc Tasnádi (Linköping): Piezoelectric tensor of $B_{0.125}Al_{0.875}N$ in the special quasirandom structure model
- 11:30 Markus Gruner (Duisburg-Essen): Large scale ab initio calculations of functional magnetic materials
- 12:15 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Relativity and correlations)

- 14:00 Four component code (Manuel Richter)
- 14:45 Task IV: Evaluation of orbital moments and magnetic anisotropy
- 15:30 Coffee
- 16:00 LSDA+U method (Klaus Koepernik)
- 16:45 Task V: LSDA+U calculation
- 18:00 Break

Evening session: Workshop DFT meets Experiment, contributed talks

- 18:15 Katrin Koch (Dresden): Electronic structure of AFe_2As_2 and RFeAsO- a comparative study
- 18:35 Miriam Schmitt (Dresden): A joined experimental and theoretical study of the J_1-J_2 Heisenberg square lattice model compounds A_2CuTO_6 (A = Sr, Ba; T = Te, W)
- 18:55 End of session
- 19:30 Workshop Dinner

Thursday, August 28

Morning session: Workshop DFT meets Experiment, invited and contributed talks

- 9:00 Clemens Laubschat (Dresden): Dispersing 4f-states: LDA meets Anderson
- 9:45 Volker Blum (Berlin): Tackling biomolecular (secondary) structure with numeric atom-centered orbitals in the FHI-aims code framework
- 10:30 Coffee
- 10:45 Helmut Eschrig (Dresden): Electronic structure of superconducting iron-pnictides
- 11:30 Deepa Kasinathan (Dresden): Orbital order in low-dimensional spin 1/2 systems
- 11:50 Bothina Hamad (Amman): Exchange Coupling and Magnetic Properties of Fe/Ir Multilayers
- 12:10 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Large systems and molecules)

- 14:00 Approach to complex problems (Helge Rosner)
- 14:10 Evaluation of model parameters (Helge Rosner)
- 14:40 Task VII: Model parameters
- 15:30 Coffee
- 16:00 Task VII: Model parameters (cont.)
- 17:00 Molecules (Manuel Richter)
- 17:10 Task VI: Small molecule
- 17:40 Break

Evening session: Workshop DFT meets Experiment, contributed talks

- 18:00 Małgorzata Samsel-Czekała (Wrocław): Electronic and magnetic structure FPLO studies of U_2N_2 (N = P, As, S, Se) and U_2N_2 (N = Sb, Bi, Te) compounds having the highest Neel and Curie temperatures among uranium systems
- 18:20 Daniel Fritsch (Dresden): Magnetic properties of transition metal dimers
- 18:40 Closing

Friday, August 29

Departure or individual excursions

Posters will be displayed during the whole workshop, poster discussion is intended during the coffee breaks.

List of Participants

Volker Blum
Fritz-Haber-Institut Berlin, Faradayweg 4-6, Germany
blum@fhi-berlin.mpg.de

Igor Chaplygin
TU Dresden, Mommsenstrasse 13, Germany
Igor.Chaplygin@chemie.tu-dresden.de

Ismaila Dabo
ENPC-Université Paris-Est, 6-8 Avenue Blaise Pascal, France
daboi@cermics.enpc.fr

Steffen Danzenbächer
TU Dresden, Zellescher Weg 16, Germany
et@physik.phy.tu-dresden.de

Bernard Delley
Paul-Scherrer-Institut Villigen, WHGA/123, Switzerland
bernard.delley@psi.ch

Martin Diviš
Charles University Prague, Ke Karlovu 5, Czech Republik
divis@mag.mff.cuni.cz

Helmut Eschrig
IFW Dresden, Helmholtzstrasse 20, Germany
h.eschrig@ifw-dresden.de

Daniel Fritsch
IFW Dresden, Helmholtzstrasse 20, Germany
d.fritsch@ifw-dresden.de

Paolo Giannozzi
University Udine, Viale delle Scienze 208, Italy
p.giannozzi@fisica.uniud.it

Anna Go
University of Białystok, Lipowa 41, Poland
annago@alpha.uwb.edu.pl

Jerzy Goraus
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
goraus@cpfs.mpg.de

Markus Gruner
University of Duisburg-Essen, Lotharstrasse 1, Germany
me@thp.uni-duisburg.de

Robert Grzimek
Philipps-Universität Marburg, Biegenstrasse 10, Germany
grzimek@students.uni-marburg.de

Bothina Hamad
University of Jordan Amman, Amman 11942, Jordan
b.hamad@ju.edu.jo

Sayed Javad Hashemifar
Isfahan University of Technology, 84156 Isfahan, Iran
jhashemifar@gmail.com

Oleg Janson
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
janson@cpfs.mpg.de

Hem Kandpal
University Frankfurt, Max-von-Laue-Str. 1, Germany
kandpal@itp.uni-frankfurt.de

Deepa Kasinathan
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
dkasinathan@student.physics.ucdavis.edu

Alexander Kerkau
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
Alexander.Kerkau@cpfs.mpg.de

Martin Knupfer
IFW Dresden, Helmholtzstrasse 20, Germany
m.knupfer@ifw-dresden.de

Katrin Koch
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
Katrin.Koch@cpfs.mpg.de

Klaus Koepernik
IFW Dresden, Helmholtzstrasse 20, Germany
k.koepernik@ifw-dresden.de

Iryna Kondakova
Institut Material Science NAS Kiev, 41 prospect Nauky, Ukraine
ikondakova@gmail.com

Thomas Kroll
IFW Dresden, Helmholtzstrasse 20, Germany
t.kroll@ifw-dresden.de

Kurt Kummer
TU Dresden, Zellescher Weg 16, Germany
kurtkummer@googlemail.com

Michael D. Kuz'min
IFW Dresden, Helmholtzstrasse 20, Germany
m.kuzmin@ifw-dresden.de

Clemens Laubschat
TU Dresden, Zellescher Weg 16, Germany
laubschat@physik.tu-dresden.de

Alberto Marmodoro
University of Warwick, Coventry CV4 7AL, England
A.Marmodoro@warwick.ac.uk

Arkady Mikhaylushkin
Linköping University, SE 581 83 Link"oping, Sweden
arkady@ifm.liu.se

Carsten Neise
IFW Dresden, Helmholtzstrasse 20, Germany
c.neise@ifw-dresden.de

Ulrike Nitzsche
IFW Dresden, Helmholtzstrasse 20, Germany
u.nitzsche@ifw-dresden.de

Pavel Novák
Institute of Physics ASCR Prague, Cukrovarnicka 10, Czech Republic
novakp@fzu.cz

Ingo Opahle
University Frankfurt, Max-von-Laue-Str. 1, Germany
opahle@itp.uni-frankfurt.de

Alim Ormeci
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
ormeci@cpfs.mpg.de

Kemal "Ozdoğan
Gebze Institute of Technology, No: 101 41400 Cayirova, Turkey
kozdogan@gyte.edu.tr

Volker Pankoke
FZ Dresden-Rossendorf, Bautzner Landstrasse 128, Germany
v.pankoke@fzd.de

Warren Pickett
UC Davis, One Shields Avenue, USA
wepickett@ucdavis.edu

Rodica Plugaru
National Institute for Research and Development in Microtechnologies Bucharest, Erou Iancu Nicolae street 126A, Romania
rodica.plugaru@imt.ro

Neculai Plugaru
Instituto de Ciencia de Materiales de Aragón and Departamento de Física de la Materia Condensada Zaragoza, Pedro Cerbuna 12, Spain
plug@unizar.es

Manuel Richter
IFW Dresden, Helmholtzstrasse 20, Germany
m.richter@ifw-dresden.de

Helge Rosner
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
rosner@cpfs.mpg.de

Sanjubala Sahoo
University of Duisburg-Essen, Lotharstrasse 1, Germany
sanjub@thp.uni-duisburg.de

Małgorzata Samsel-Czekała
Institute of Low Temperature and Structure Research PAS Wrocław, Okólna 2, Poland
m.samsel@int.pan.wroc.pl

Miriam Schmitt
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
schmitt@cpfs.mpg.de

Stephan Sch"onecker
IFW Dresden, Helmholtzstrasse 20, Germany
s.schoenecker@ifw-dresden.de

Ulrich Schwarz
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
schwarz@cpfs.mpg.de

Liudmila Siurakshina
Joint Institute for Nuclear Research Dubna, Joliot-Curie 6, Russia
siurak@mpipks-dresden.mpg.de

Najmeh Soltani
Ferdowsi University of Mashhad, Vakilabad Boulevard, Iran
naj23s@yahoo.com

Yevgen Syvachenko
Joint Institute for Nuclear Research Dubna, Joliot-Curie 6, Russia
sivachenko@gmail.com

Ferenc Tasnádi
Linköping University, SE 581 83 Linköping, Sweden
tasnadi@ifm.liu.se

Alexander Tsirlin
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
tsirlin@cpfs.mpg.de

Torsten Weissbach
TU Dresden, Zellescher Weg 16, Germany
weistl@physik.phy.tu-dresden.de

Mirosław Werwiński
Inst. Molecular Phys. PAS Poznań, Mariana Smoluchowskiego 17, Poland
werwinski@ifmpan.poznan.pl

Ulrich Wiesenh"utter
IFW Dresden, Helmholtzstrasse 20, Germany
u.wiesenhuetter@ifw-dresden.de

Julia Wildeboer
MPI-CPfS Dresden, Nöthnitzer Str. 40, Germany
juliawildeboer@web.de

Jochen Wosnitza
FZ Dresden-Rossendorf, Bautzner Landstra"se 128, Germany
j.wosnitza@fzd.de

Ruijuan Xiao
IFW Dresden, Helmholtzstrasse 20, Germany
r.xiao@ifw-dresden.de

Erik Ylvisaker
UC Davis, One Shields Avenue, USA
eylvisaker@physics.ucdavis.edu

Hongbin Zhang
IFW Dresden, Helmholtzstrasse 20, Germany
h.zhang@ifw-dresden.de

3.1.3 Report on Workshop Computational Magnetism and Spintronics (CCMS08 = CompMag2008)

Max-Planck-Institute for the Physics of Complex Systems Dresden, Germany

November 03-07, 2008

Sponsors

MPI-PKS, psi-k.org, and ESF

Organizers

Olle Eriksson – University of Uppsala, Sweden,

Ingrid Mertig and Peter Zahn – Martin-Luther-Universität Halle, Germany

`http://www.mpipks-dresden.mpg.de/~ccms08`

Summary

The workshop was organized at the Max-Planck-Institute for the physics of complex systems in Dresden. Financial support of the Max-Planck-Institute, the psi-k.org network and the ESF Activity 'Towards Atomistic Materials Design' is kindly acklowledged. The workshop was attended by about 90 scientist from 22 countries from Europe and overseas. They presented new theoretical developments and methods, and actual experimental results in 30 talks. Nearly all participants took the chance to present their own results on 52 posters. This provided an inspiring atmosphere for discussions and lively exchange of ideas, which were centered at computer simulations of known, as well as brand new spintronics phenomena. This includes the understanding of the magnetic order and dynamics of nanostructures, spin dynamics under the influence of magnetic and electrical fields,

the currently discovered Spin Hall effect, and the behavior of electrons in graphene. The addressed topics of the invited talks were, in addition a full list is given below:

- Spin Hall Effect (Stern, Buhmann, Jin, Bruno)
- Graphene (Katsnelson, Józsa, Louie, Nieminen, Kelly)
- Multiferroics (Picozzi, Alexe, Ederer, Garcia, Ravindran, Dörr)
- Electronic correlation effects (Schulthess, Temmermann, Lichtenstein)
- Magnetic structures and spin dynamics (Blügel, Wulfhekel, Nordström)
- Diluted magnetic semiconductors (Sanyal, Sato)
- Spin dependent transport (Turek, Ebert, Györffy, Heiliger, Resta, Tosatti)

The intense interaction of experiment and theory will boost the field for the future. The workshop is the second in the series CompMag, which started 2006 in Jülich. It should provide a European forum for the development of computational solid state physics with special emphasis on magnetism. The next meeting of the series will be organized by Stefan Blügel in Jülich in the spring of 2010.

Programme

Monday, November 3

09:00 - 09:20	Opening by Roderich Moessner and the Organizers
09:20 - 10:00	Nathaniel Stern *Imaging electrical spin generation and the spin Hall effect in semiconductors*
10:00 - 10:40	Hartmut Buhmann *Spin Hall effects in HgTe quantum well structures*
11:10 - 11:50	Xiaofeng Jin *Anomalous Hall effect in ultrathin Fe films*
11:50 - 12:30	Jairo Sinova *Anomalous Hall transport in spin-orbit coupled systems: Merging Keldysh, Kubo and Boltzmann approaches*
14:00 - 14:40	Balazs L. Gyorffy *Spin-currents and charge-currents induced torques in relativistic quantum mechanics*
14:40 - 15:20	Ilja Turek *Ballistic torkances in non-collinear spin valves*
15:20 - 16:00	Patrick Bruno *Hall effects, generalized Einstein relation, and Berry phase*
16:30 - 17:30	CCMS08-Colloqium Qian Niu

Berry phase effects on spin and charge transport

Tuesday, November 4

09:00 - 09:40 Hubert Ebert
A first-principle description of the TAMR in semiconductor/ferromagent heterostructures

09:40 - 10:20 Christian Heiliger
Bias dependence of spin transfer torque in MgO based tunnel junctions: Ab initio calculations

11:00 - 11:40 Csaba Józsa
Spin injection and transport phenomena in graphene

11:40 - 12:20 Mikhail Katsnelson
Defects in graphene: Electronic structure, magnetism, scattering mechanisms

14:00 - 15:30 Poster session I

16:00 - 16:40 Steven G. Louie
Computational study of the electronic, magnetic, transport and optical properties
of carbon nanostructures

16:40 - 17:20 Risto Nieminen
Defect-associated magnetism in nanostructured carbon

17:20 - 18:00 Paul Kelly
Graphene and graphite as perfect spin filters

18:00 - 18:40 Raffaele Resta
Orbital magnetization in solid state physics

Wednesday, November 5

09:00 - 09:40 Walter Temmerman
Disordered Local Moment Picture of Strongly Correlated 3d and 4f systems

09:40 - 10:20 Thomas Schulthess
Intricacies of electronic structure calculations in cuprates and other strongly correlated electron systems

11:00 - 11:40 Marin Alexe
Controlling ferromagnetism with an electric field

11:40 - 12:20 Silvia Picozzi
Multiferroic manganites

14:00 - 15:30 Poster session II

16:00 - 16:40 Claude Ederer
Toroidal moments and magneto-electric coupling: The case of $BiFe0_3$ vs. $FeTi0_3$

16:40 - 17:20 Vincent Garcia
Intrinsic and artificial multiferroic tunnel junctions for spintronics

17:20 - 18:00 Ponniah Ravindran
Giant magnetoelectric effect from density functional calculations

Thursday, November 6

09:00 - 09:40 Wulf Wulfhekel
Inelastic tunneling spectroscopy as a tool to study magnetic excitations

09:40 - 10:20 Stefan Blügel
Homochiral magnetic structures at surfaces

11:00 - 11:40 Lars Nordström
Spin dynamics; from a fine to coarse spatial resolution

11:40 - 12:20 Erio Tosatti
Magnetic phenomena, spin orbit effects, and electron transport in nanowire contacts, particularly in Platinum

14:00 Leaving for the guided city tour and the visit of Panometer Dresden (http://www.panometer.de)

Friday, November 7

09:00 - 09:40 Alexander Lichtenstein
Electronic structure and magnetism of correlated materials

09:40 - 10:20 Biplab Sanyal
First principles theory of diluted magnetic semiconductors

11:00 - 11:40 Kazunori Sato
Control of spinodal decomposition in dilute magnetic semiconductors and computational materials design for semiconductor spintronics

11:40 - 12:20 Kathrin Dörr
Reversible strain experiments on strongly correlated oxide films

12:20 - 12:30 Closing

List of poster presentations

1 Donat Adams
Theoretical study of the pressure induced spin collapse in $LuFeO_3$ orthoferrite

2 Emmanuel Arras
Computational investigation of the atomic structure of Mn-rich nanocolumns : Comparison with possible GeMn ordered compounds

3 Pio Baettig
Why are Garnets not Ferroelectric? – A Theoretical Investigation of Y3Fe5O12

4 Swarnali Bandopadhyay
Circulating currents in multichannel mesoscopic ring

5 Cyrille Barreteau
Anisotropic Magneto Resistance in iron atomic contacts

6 Lars Bergqvist
odoping with Li interstitials in Mn-doped GaAs

7 Orkidia Bilani-Zeneli
Strain-sensitive oxide films on piezoelectric substrates

8 Karel Carva
Out-of-plane spin-transfer torques and spin-mixing conductances: first-principles study

9 Stanislav Chadov
LSDA+DMFT study of locally correlated heusler compounds

10 Sudip Chakraborty
Ab-initio study of oxygen encapsulated manganese doped silicon quantum dots

11 Francesco Cricchio
Magnetism in strongly correlated actinides compounds

12 S. N. Dolia
Magnetism in spintronics materials Zn1-xMnxO

13 Manuel dos Santos Dias
A simple model for the magnetic structure of nanoclusters near a surface

14 Vaclav Drchal
TB-LMTO method for embedded clusters

15 Engin Durgun
Spintronic properties of silicon nanowires and graphene nanoribbons functionalized with transition metal atoms

16 Dmitry Fedorov
Relativistic treatment of the spin relaxation time in nonmagnetic metals

17 Jonas Fransson
Detection of spin reversal and nutations through current measurements

18 Daniel Fritsch
Magnetic anisotropy of homonuclear transition metal dimers

19 Martin Gmitra
First-principles calculations of spin-orbit coupling effects in Fe/GaAs interfaces

20 Oscar Grånäs
Spin and orbital polarizations in correlated systems

21 Martina Hentschel
Quantum spin Hall effect in graphene

22 Mighfar Imam
Strain-Stabilised magnetic surface alloys

23 Daungruthai Jarukanont
Spin-polarized current through organic molecules

24 Muthukumar Kaliappan
Density Functional Theory Prediction of the Different Binding Sites for Ce in C78, C80 and C82 Cages - Insights Through Electronic Structure

25 Hiroshi Katayama-Yoshida
Colossal thermoelectric cooling power by adiabatic spin entropy expansion in nano superstructures

26 Sergeii Khmelvskyi
Temperature induced Longintuginal Spin Fluctuations in Fe and Ni: First-principle approach

27 Angela Klautau
Magnetism of 3d nanostructures on Pt(111): A first principles study

28 Roman Kovacik
Construction of model Hamiltonians for complex oxides using maximally localized Wannier functions

29 Anjali Kshirsagar
Vacancy induced Magnetism in GaN / Magnetsism in II-VI semiconductor materials: Bulk vs nanostructures

30 Mukul Laad
Quantitative description of half-metals: An LDA+DMFT perspective

31 Samir Lounis
Playing dominos with finite magnetic wires

32 Frantisek Máca
Magnetism without magnetic impurities in oxides ZrO2 and TiO2

33 Alessio Meyer
Ab initio periodic simulation of the magnetic structure of garnets

34 S.Hossein Mirhosseini
Electron correlations effects on interface and surface properties

35 Natalia Ostrovskaya
Numerical simulation of current-driven torque dynamics in three-layered magnetic structures

36 Martin Rohrmüller
Ab initio g-tensor calculation for paramagnetic surface states in c-Si:H-based solar cells

37 Andrea Salguero
Orbital order in Mn2V2O4

38 Leonid Sandratskii
Thermal magnetic properties of the Ni sublattice in half-metallic NiMnSb

39 Lakshmi Sankaran
Spin transport in graphene nano-ribbons

40 Ersoy Sasioglu
Spin-wave dynamics from many-body perturbation theory using Wannier functions

41 Haldun Sevincli
Electronic and Magnetic Properties of TM-Atom Adsorbed Graphene and Graphene Nano-Ribbons

42 Mahavir Sharma
Magnetic and electrical transport properties of Ce substituted perovskite oxides $La_{1-x}Ce_xMnO_3$

43 Dinesh Kumar Shukla

Thin film growth of multiferroic BiMn2O5 using pulsed laser ablation and its charecterization

44 Nirpendra Singh
Collinear and non-collinear Magnetism in Samarium orthoferrites

45 Ivetta Slipukhina
Ab initio study of the electronic and magnetic properties of Mn5Ge3Cx compounds

46 Rudolf Sykora
Influence of spin-orbit interaction on ballistic conductances in magnetic multilayers

47 Zdzislawa Szotek
Application of SIC-LSD to novel functional materials

48 Laszlo Szunyogh
Domain wall formation and spin-wave spectra in ultrathin magnetic films: Fe monolayer on W(001)

49 Grigory Tkachov
Spin-polarized tunneling through randomly transparent magnetic junctions: Reentrant magnetoresistance approaching the Julliere limit

50 Yoshitaka Uratani
Magnetic anisotropic properties in multiferroic $PbVO_3$ and $BiCoO_3$ from first-principles

51 Oleg Yazyev
Structure, magnetic properties and spin transport of magnetoresistive junctions based on epitaxial graphene and h-BN

52 Igor Maznichenko
Electronic and magnetic properties of doped ZnO

List of speakers

Marin Alexe	Halle, DE
Stefan Blügel	Jülich, DE
Patrick Bruno	Grenoble, FR
Hartmut Buhmann	Würzburg, DE
Kathrin Dörr	Dresden, DE
Claude Ederer	Dublin, IR
Vincent Garcia	Paris, FR
Balazs L. Gyorffy	Bristol, GB
Christian Heiliger	Giessen, DE
Xiaofeng Jin	Shanghai, CN
Csaba Józsa	Groningen, NL
Mikhail Katsnelson	Nijmegen, NL
Paul Kelly	Twente, NL

Alexander Lichtenstein	Hamburg, DE
Steven G. Louie	Santa Barbara
Risto Nieminen	Helsinki, FI
Lars Nordström	Uppsala, SE
Silvia Picozzi	L'Aquila, IT
Ponniah Ravindran	Oslo, NO
Raffaele Resta	Trieste, IT
Biplab Sanyal	Uppsala, SE
Kazunori Sato	Osaka, JP
Thomas Schulthess	Zurich, CH
Jairo Sinova	College Station, US
Nathaniel Stern	Santa Barbara, US
Walter Temmerman	Daresbury, GB
Erio Tosatti	Trieste, IT
Ilja Turek	Prague, CZ
Wulf Wulfhekel	Karlsruhe, DE

List of participants

Donat Jozsef Adams	Marin Alexe
Emmanuel Arras	Pio Baettig
Swarnali Bandopadhyay	Cyrille Barreteau
Lars Bergqvist	Orkidia Bilani-Zeneli
Stefan Blügel	Patrick Bruno
Hartmut Buhmann	Karel Carva
Stanislav Chadov	Sudip Chakraborty
Francesco Cricchio	Peter H. Dederichs
S. Dolia	Kathrin Dörr
Manuel dos Santos Dias	Vaclav Drchal
Engin Durgun	Hubert Ebert
Claude Ederer	Olle Eriksson
Dmitry Fedorov	Jonas Fransson
Daniel Fritsch	Vincent Garcia
Martin Gmitra	Martin Gradhand
Oscar Grånäs	Balazs L. Gyorffy
Christian Heiliger	Martina Hentschel
Tilina Herath	Mighfar Imam
Daungruthai Jarukanont	Xiaofeng Jin
Csaba Jozsa	Muthukumar Kaliappan
Hiroshi Katayama-Yoshida	Mikhail Katsnelson
Paul Kelly	Sergii Khmelvskyi

Angela Klautau
Mukul Laad
Steven G. Louie
Frantisek Máca
Igor Maznichenko
Alessio Meyer
Cesar A. M. Martinez
Qian Niu
Silvia Picozzi
Raffaele Resta
Andrea Salguero
Lakshmi Sankaran
Saeed Sarkarati
Kazunori Sato
Haldun Sevincli
Dinesh Kumar Shukla
Jairo Sinova
Nathaniel Stern
Zdzislawa Szotek
Walter Temmerman
Grigory Tkachov
Ilja Turek
Wulf Wulfhekel
Peter Zahn

Roman Kovacik
Alexander Lichtenstein
Samir Lounis
Alberto Marmodoro
Ingrid Mertig
Seyed H. Mirhosseini
Risto Nieminen
Natalia Ostrovskaya
Ponniah Ravindran
Martin Rohrmüller
Leonid Sandratskii
Biplab Sanyal
Ersoy Sasioglu
Thomas C. Schulthess
Mahavir Sharma
Nirpendra Singh
Ivetta Slipukhina
Rudolf Sykora
Laszlo Szunyogh
Jan Thöne
Erio Tosatti
Yoshitaka Uratani
Oleg Yazyev

3.2 Reports on Collaborative Visits

3.2.1 Report on a Collaborative Visit of Pietro Vidossich (CoSMoLab, Parc Científic de Barcelona, Spain) to the Physical Chemistry Institute, University of Zurich

From October 13. to 17. 2008 I visited the group of Professor Juerg Hutter at the Physical Chemistry Institute, University of Zurich. Scope of the visit was to be trained in the usage of the CP2K program developed in Professor Hutter's group.

CP2K [1] (freely available at http://cp2k.berlios.de), based on the QUICKSTEP algorithm [2], is an efficient numerical code for accurate density functional calculations showing linear scaling with system size, thus able to tackle systems of up to thousands of atoms.

During my staying, with the help of Dr. Teodoro Laino, I worked on the setup of QM/MM simulations [3] of myeloperoxidase (MPO), a heme protein of the human innate immune system [4]. The interest in MPO lies in the fact that it is the only human peroxidase able to oxidize chloride to hypochlorous acid at an appreciable rate [4]. MPO active site contains a heme group covalently attached to the protein chain by three bonds: a sulfonium ion linkage between a methionine and one heme vinyl group; two ester bonds between two heme methyl groups and an aspartate and a glutamate. The ester bonds are present also in the other members of the human peroxidase family, whereas the heme-Met linkage appears unique to MPO. Indeed, mutagenesis studies [4] have show that variants lacking this bond have lost chloride oxidation activity. Calculations are aimed at the elucidation of the effect of these linkages on the electronic structure of the resting state and of the high redox intermediate known as Compound I (formally an iron(V)-oxo species).

The visit was very successful, and preliminary calculations were run on the facilities of the Barcelona Supercomputing Center without any problem. I am very grateful to the network for its support, which made my trip to Zurich possible. Pietro Vidossich

[1] VandeVondele, J; Krack, M; Mohamed, F; Parrinello, M; Chassaing, T; Hutter, J. Comput. Phys. Commun. 167, 103-128 (2005).
[2] Lippert, G; Hutter, J; Parrinello, M. Mol. Phys. 92, 477-487 (1997).
[3] Laino, T; Mohamed, F; Laio, A; Parrinello, M. J. Chem. Theory Comput. 1, 1176-1184 (2005).
[4] Zederbauer, M; Furtmller PG; Jakopitsch, C; Smulevich, S; Obinger, C; Nat. Prod. Rep. 24, 571-584 (2007).

4 General Workshop/Conference Announcements

4.1 Quantum Monte Carlo and the CASINO program IV

International Summer School

Sun 2nd August - Sun 9th August 2009

Towler Institute, Vallico Sotto, Tuscany, Italy

http://www.vallico.net/tti/tti.html (MAIN WEBSITE)

http://www.tcm.phy.cam.ac.uk/∼mdt26/poster.png (POSTER)

The fourth international summer school in the series "Quantum Monte Carlo and the CASINO program" will take place during August 2009 at the TTI monastery in the Tuscan Apuan Alps in Italy, organized and hosted by members of Cambridge University physics department's Theory of Condensed Matter Group. The aim of the school is to give students a thorough introduction to quantum Monte Carlo as a method for performing high-quality calculations of the electronic structure of atoms, molecules, and materials. The course is designed for young quantum chemists or theoretical physicists who have no previous experience with this technique, though anyone interested is welcome to take part.

The monastery is a unique venue where the community spirit and magnificent location have inspired memorable workshops in the past. It is a delightful 16th century building incorporating an ancient church, and is situated in the isolated but spectacular setting of the Tuscan mountain village of Vallico Sotto. The Institute is fully equipped with relevant presentation and computer technology, and all accommodation is on-site. As with all events at the Institute, formal lectures are restricted to the mornings, and participants are given the freedom and space to think and to contemplate and discuss the issues at hand. In addition to hands-on exercises, a programme of healthy recreational activities will be organized in the afternoons, and it is hoped that by following this strict regime, together with breathing clean mountain air and by preparing and sampling fine Tuscan cuisine, the participant will be able to return home mentally and physically refreshed as well as better informed.

Describing the complex behaviour of materials at the atomic level requires a sophisticated description of the correlated motion of the electrons. Quantum Monte Carlo (QMC) is an increasingly popular and explicitly many-body method with the unusual capability of yielding highly accurate results whilst also exhibiting a very favourable scaling of computational cost with system size. Over the last eighteen years, the Cambridge group have

been researching QMC methods and we have created a powerful, general computer program - CASINO - to carry out the calculations. The school will focus both on the basic theory of QMC and on more advanced practical techniques, and will include a thorough introduction to the CASINO program. A background in density functional theory or similar is normally thought to be useful.

Instructors will include the main authors of the CASINO program (Dr. Mike Towler, Dr. Neil Drummond and Dr. Pablo Lopez Rios) and possibly others.

Participants would normally need to book a flight to Pisa airport from where onward transportation will be arranged (though other destinations are possible). Details of previous schools - including photographs - are available under the PUBLIC EVENTS link on the TTI web site.

Interested students should email Mike Towler (mdt26 at cam.ac.uk) for registration and further details.

NB: TTI IS AVAILABLE FOR HOSTING EVENTS THROUGHOUT THE SUMMER - PLEASE ASK

4.2 Quantum Monte Carlo in the Apuan Alps V

International Conference

Sat 25th July - Sat 1st August 2009

Towler Institute, Vallico Sotto, Tuscany, Italy

http://www.vallico.net/tti/tti.html (MAIN WEBSITE)

http://www.tcm.phy.cam.ac.uk/∼mdt26/tti_c_poster_2009.png (POSTER)

Continuing the series of alternative and very informal meetings at this venue, the Cambridge University Theory of Condensed Matter group is organizing a fifth international conference to discuss the development and application of the continuum quantum Monte Carlo method in condensed matter physics and quantum chemistry. The conference will take place in our 16th Century monastery in the mediaeval high mountain village of Vallico Sotto (in the Tuscan Apuan Alps near the beautiful Italian city of Lucca).

The normal format for these events involves formal presentations being restricted to the mornings, with the afternoons left free for relaxed discussion and participation in fun activities. For the young and vigorous, we organize mountain walks, caving and other healthy outdoor exercise, whilst the unfit and elderly might enjoy artistic tours, city visits, and gentle country strolls, with all participants reuniting in the evening for excellent Tuscan dinners in local restaurants.

This year's workshop will involve up to 35 people, all accommodated on site. Given the limited space most speakers will be specifically invited, but anyone who feels that they have something to contribute and who wishes to attend the event is most welcome to contact the organizers (Mike Towler: mdt26 at cam.ac.uk) for further details. There is no charge either for attendance at the conference or accommodation.

NB: TTI IS AVAILABLE FOR HOSTING EVENTS THROUGHOUT THE SUMMER - PLEASE ASK

5 General Job Announcements

Ph. D. Position in Solid State Theory
Vienna University of Technology, Vienna, Austria

We announce an opening for a Ph.D. position in theoretical solid state physics with a focus on electronic correlations and computational materials science. Possible topics are:

- Merging bandstructure calculations (Wien2K/VASP) with dynamical mean field theory (for details see http://arxiv.org/abs/cond-mat/0511293; http://www.psi-k.org/newsletters/News_56/newsletter_56.pdf)
- Dynamical vertex approximation for magnons and quantum criticalit (http://arxiv.org/abs/cond-mat/0603100)
- Thermoelectrics (http://arxiv.org/abs/0806.2506)
- Nanostructured quantum dots (http://arxiv.org/abs/0811.2697)

We are looking for an excellent Ph.D. candidate who takes delight in solid state theory and numerical methods and offer professional supervision and a seminal research topic. The position is part of the interdisciplinary graduate school functional materials (http://funmat.tuwien.ac.at, gross salary $\sim$ EUR 1.700, 14 times per year) so that openness to cooperate with experimental physicists is expected. The Ph.D. work will profit from an international research environment including cooperations with Japan (Tokyo), India (Kolkata), and the US.

Contact and questions:
Prof. K. Held (held@ifp.tuwien.ac.at;http://www.ifp.tuwien.ac.at/cms).

Deadline: December 31, 2008

Applications including admission form, CV and up to two letters of recommendation (for details see http://funmat.tuwien.ac.at) shall be sent by e-mail in PDF form with "Functional Materials" in the subject line to pers1@zv.tuwien.ac.at AND sekretariat@ifp.tuwien.ac.at.

6 Abstracts

Efficient calculation of the Coulomb matrix and its expansion around $\mathbf{k} = \mathbf{0}$ within the FLAPW method

Christoph Friedrich[a], Arno Schindlmayr[b], Stefan Blügel[a]
[a] *Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[b] *Department Physik, Universität Paderborn, 33095 Paderborn, Germany*

Abstract

We derive formulas for the Coulomb matrix within the full-potential linearized augmented-plane-wave (FLAPW) method. The Coulomb matrix is a central ingredient in implementations of many-body perturbation theory, such as the Hartree-Fock and *GW* approximations for the electronic self-energy or the random-phase approximation for the dielectric function. It is represented in the mixed product basis, which combines numerical muffin-tin functions and interstitial plane waves constructed from products of FLAPW basis functions. The interstitial plane waves are here expanded with the Rayleigh formula. The resulting algorithm is very efficient in terms of both computational cost and accuracy and is superior to an implementation with the Fourier transform of the step function. In order to allow an analytic treatment of the divergence at $\mathbf{k} = \mathbf{0}$ in reciprocal space, we expand the Coulomb matrix analytically around this point without resorting to a projection onto plane waves. Without additional approximations, we then apply a basis transformation that diagonalizes the Coulomb matrix and confines the divergence to a single eigenvalue. At the same time, response matrices like the dielectric function separate into head, wings, and body with the same mathematical properties as in a plane-wave basis. As an illustration we apply the formulas to electron-energy-loss spectra (EELS) for nickel at different $\mathbf{k}$ vectors including $\mathbf{k} = \mathbf{0}$. The convergence of the spectra towards the result at $\mathbf{k} = \mathbf{0}$ is clearly seen. Our all-electron treatment also allows to include transitions from $3s$ and $3p$ core states in the EELS spectrum that give rise to a shallow peak at high energies and lead to good agreement with experiment.

(Submitted to Computer Physics Communications, Preprint at arXiv:0811.2363)
Contact person: c.friedrich@fz-juelich.de

Hybrid density functional theory applied to magnetite I: Crystal and electronic structures

Andrew D. Rowan and Charles H. Patterson
School of Physics, Trinity College Dublin, Dublin 2, Ireland

Abstract

The electronic structure and equilibrium structure of magnetite (Fe_3O_4) in the high temperature, cubic $Fd\bar{3}m$ and low temperature, monoclinic $P2/c$ unit cells have been computed using the Perdew-Wang generalized gradient approximation (GGA) to density functional theory (DFT) and the B3LYP hybrid density functional. The ground state for the GGA-DFT is an itinerant electron metallic state in the cubic unit cell and the ground state for the B3LYP functional is a charge ordered semiconducting state in the monoclinic unit cell. The electronic band gap for Fe_3O_4 in the $P2/c$ unit cell is 0.87 eV. The equilibrium structure predicted by the B3LYP functional for Fe_3O_4 in the $P2/c$ unit cell has been calculated with lattice parameters fixed at values obtained in recent x-ray diffraction work and with the lattice fully relaxed. Bond lengths obtained with lattice parameters fixed at experimental values are in excellent agreement with x-ray measurements [J.P. Wright, J.P. Attfield and P.G. Radaelli, Phys. Rev. B **66** 214422 (2002)]. The degree of charge order, measured as disproportionation of charge on octahedral B sites, is considerably less than unity and in reasonable agreement with values from resonant x-ray diffraction measurements. However, conduction electrons are found to be fully localized on B1 and B4 sites in orbitally ordered t_{2g} states. This shows that they are formally Fe^{2+} ions while Fe B2 and B3 sites are formally Fe^{3+} sites. Therefore Verwey's original conjecture regarding charge localization in Fe_3O_4 applies, even though the specific pattern of charge order is different. Electronic structure predictions for Fe_3O_4 by the B3LYP functional are compared with those by the DFT + Hubbard U method.

(Submitted to Phys. Rev. B)
http://www.tcd.ie/Physics/People/Charles.Patterson/publications.php
Contact person: Charles Patterson (Charles.Patterson@tcd.ie)

Hybrid density functional theory applied to magnetite II: Γ-point phonons and vibrational spectra

Charles H. Patterson
School of Physics, Trinity College Dublin, Dublin 2, Ireland L. V. Gasparov
Department of Chemistry and Physics, University of North Florida, St. John's Bluff Rd. South, Jacksonville, Florida 32224

Abstract

Generalized gradient and B3LYP hybrid density functional theory (DFT) approximations are used to calculate phonons at the Γ point of the Brillouin zone of magnetite (Fe_3O_4). DFT in a generalized gradient approximation (GGA), predicts an itinerant electron ground state for the cubic, $Fd\bar{3}m$ unit cell observed above the Verwey transition temperature, T_V, and the B3LYP hybrid DFT approximation predicts a charge ordered semiconducting state for the monoclinic $P2/c$ unit cell below T_V. Phonon frequencies predicted for these crystal structures are compared to frequencies from infra-red (IR) conductivity and Raman scattering experiments. The charge ordered state predicted by B3LYP is similar to that found in recent DFT-GGA + Hubbard-U calculations. Charge ordering causes symmetry breaking of force constants on symmetry lowering from the cubic $Fd\bar{3}m$ unit cell to the $P2/c$ unit cell. This produces frequency splitting of modes which are degenerate in the cubic unit cell and concentration of ion displacements in phonon eigenvectors on particular Fe octahedral B site chains, especially in the highest frequency bands. There is one unstable eigenmode in the B3LYP calculation of the vibrational spectrum of the $P2/c$ unit cell. It is suggested that this instabilty occurs because the $P2/c$ space group unit cell is an approximation to the actual Cc space group determined by x-ray scattering.

(Submitted to Phys. Rev. B)
http://www.tcd.ie/Physics/People/Charles.Patterson/publications.php
Contact person: Charles Patterson (Charles.Patterson@tcd.ie)

Interplay between structure and magnetism in hydride iron-vanadium systems

A. Lebon
LMB/UBO 6 avenue Victor Le Gorgeu, 29285 Brest Cedex, France

A. Mokrani
Institut des Matériaux Jean Rouxel, UMR CNRS 6502, Université de Nantes, 2 rue de la Houssinière, B.P. 44322 Nantes, France

A. Vega
Institut des Matériaux Jean Rouxel, UMR CNRS 6502, Université de Nantes, 2 rue de la Houssinière, B.P. 44322 Nantes, France

Abstract

The structural and electronic properties of dimers, bulk and alloys of Fe and V upon loading with hydrogen have been investigated using the density-functional method SIESTA. We have calculated the hydrogen induced modifications of both the geometrical structure and the magnetic properties which have been found to be closely related to each other. The general trends derived from our results are in good agreement with those found in the experimental characterizations of hydrogen-loaded Fe/V multilayer systems. In particular, we have found that hydrogen prefers a V environment when inserted in the alloy systems at high concentration, it occupies octahedral positions leading to a strong anisotropic expansion of the lattice accompanied by an increase of the local Fe magnetic moments. We have found that the main trends obtained in the extended systems were already present in the most stable geometrical- and spin-isomers of the free-standing FeVH clusters.

(Physical Review B 78, 184401 (2008))
Contact person: A. Lebon (Alexandre.Lebon@univ-brest.fr)

Ionic relaxation contribution to the electronic reconstruction at the n-type $LaAlO_3/SrTiO_3$ interface

R. Pentcheva[a] and W. E. Pickett[b]
[a] *Department of Earth and Environmental Sciences, University of Munich, Theresienstr. 41, 80333 Munich, Germany*
[b] *Department of Physics, University of California, Davis, CA 95616*

Abstract

Density functional theory calculations reveal that the compensation mechanism at the isolated n-type interface in $LaAlO_3/SrTiO_3$ superlattices involves both ionic and electronic degrees of freedom. Strong polar distortions screen the local electric field and reduce the band discontinuity across the interface. We find that the electronic reconstruction depends sensitively on whether structural optimization is performed within GGA (conventional exchange and correlation effects) or GGA+U (which includes strong intra-atomic interactions). For a structural optimization within GGA+U the excess charge is confined to the interface TiO_2-layer with a charge-ordered, orbitally-polarized arrangement of Ti^{3+} and Ti^{4+}. While the charge ordered phase represents the ground state, optimization within GGA leads to more pronounced lattice polarization, suppression of charge order (with remaining d_{xy}-orbital occupation in the interface layer) and a delocalization of the excess charge extending over a few $SrTiO_3$ layers.

(Physical Review B **78**, 205106 (2008))
Contact person: pentcheva@lrz.uni-muenchen.de

The f-electron challenge: localized and itinerant states in lanthanide oxides united by GW@LDA+U

Hong Jiang,[1] Ricardo I. Gomez-Abal,[1] Patrick Rinke,[1,2] and Matthias Scheffler[1,2]
[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*
[2] *University of California at Santa Barbara, CA 93106,USA*

Abstract

Many-body perturbation theory in the GW approach is applied to lanthanide oxides, using the local-density approximation plus a Hubbard U correction (LDA+U) as the starting point. Good agreement between the G_0W_0 density of states and experimental spectra is observed for CeO_2 and Ce_2O_3. Unlike the LDA+U method G_0W_0 exhibits only a weak dependence on U in a physically meaningful range of U values. For the whole lanthanide sesquioxide (Ln_2O_3) series G_0W_0@LDA+U reproduces the main features found for the optical experimental band gaps. The relative positions of the occupied and unoccupied f-states predicted by G_0W_0 confirm the experimental conjecture derived from phenomenological arguments.

(submitted to: Phys. Rev. Lett.)
Contact person: Patrick Rinke (rinke@fhi-berlin.mpg.de)

Manipulation and Control of Hydrogen Bond Dynamics in Absorbed Ice Nanoclusters

Heiko Gawronski,[1] Karina Morgenstern,[1] Javier Carrasco[1] and Angelos Michaelides[2,3]

[1] *Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany*

[2] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany*

[3] *Materials Simulation Laboratory, London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, United Kingdom*

Abstract

Inelastic electron tunneling is used to explore the dynamics of ice nanoclusters adsorbed on Ag(111). The diffusion of entire nanoclusters or internal hydrogen bond rearrangement can be selectively controlled by injecting electrons either directly into the clusters themselves or indirectly (indirect inelastic electron tunneling) into the substrate at distances of up to 20 nm from them; a reaction probability that oscillates with the tip-cluster lateral distance presents evidence that surface state electrons mediate the excitation. Density functional theory calculations reveal a strong sensitivity of the computed activation energies of the individual processes to the applied electrical field.

(appeared as: Phys. Rev. Lett. **101**, 136102 (2008))

Contact person: Angelos Michaelides (michaeli@fhi-berlin.mpg.de)

Thermodynamics of the Heusler alloy $Co_{2-x}Mn_{1+x}Si$: a combined density functional theory and cluster expansion study

B. Hülsen,[1] P. Kratzer,[2] and M. Scheffler[1]
[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany*
[2] *Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany*

Abstract

Previous studies indicated that intrinsic point defects play a crucial role for the density of states of ferromagnetic half-metals in the band gap region: At large concentrations, defect-derived bands might close the gap at the Fermi energy in the minority spin channel. In this work, structural disorder in the Co- and Mn-sublattices of the full Heusler alloy $Co_{2-x}Mn_{1+x}Si$ ($-1 \leq x \leq 2$) is investigated with a cluster expansion approach, parametrized using all-electron density functional theory calculations. By establishing two separate cluster expansions, one for the formation energy and one for the total spin moment, we are in a position to determine the stability of different configurations, to predict new (also half-metallic) ground states and to extend the known Slater-Pauling rule for ideally stoichiometric Heusler alloys to non-stoichiometric, Mn-rich compositions. This enables us to identify potentially half-metallic structures in the Mn-rich region. With the help of Monte Carlo simulations based on the cluster expansion, we establish theoretically that $Co_{2-x}Mn_{1+x}Si$ close to the stoichiometric composition ought to show a high degree of structural order in thermodynamic equilibrium. Hence, samples prepared with the correct stoichiometry should indeed be half-metallic after thermal annealing. Moreover, we predict that adding a small amount of Mn to stoichiometric Co_2MnSi allows to suppress the thermally activated formation of detrimental Co antisites. At Mn-rich compositions ($x > 1$), the ordered ground state structures predicted for zero temperature are found to be thermally unstable and to decompose into Co_2MnSi and Mn_3Si above room temperature.

(submitted to: Phys. Rev. B)
Contact person: Peter Kratzer (Peter.Kratzer@uni-duisburg-essen.de)

Exchange interactions and critical temperature of bulk and thin films of MnSi: A density functional theory study

M. Hortamani,[1,2] L. Sandratskii,[2] P. Kratzer,[1,3] I. Mertig[2,4] and M. Scheffler[1]
[1]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany*
[2]*Max-Planck-Instiutut für Mikrostrukturphysik, D-06120 Halle, Germany*
[3]*Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany*
[4]*Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany*

Abstract

Recent theoretical work [H. Wu et al., Phys. Rev. Lett. **92**, 237202 (2004); M. Hortamani et al., Phys. Rev. B **74**, 205305 (2006) M. Hortamani, Ph.D. thesis, Freie Universität, Berlin, 2006] predicted ferromagnetism at zero temperature in thin MnSi films of B2-type crystal structure on Si(100). The relevance of this finding for finite-temperature experiments needs to be clarified by further investigations, since bulk MnSi is a weak ferromagnet with an experimentally measured Curie temperature of only $T_c = 30$ K, and T_c is generally expected to be lower in thin films than in bulk materials. Here, we estimate T_c of such MnSi films using a multiple-sublattice Heisenberg model with first- and second-nearest-neighbor interactions determined from density functional theory calculations for various collinear spin configurations. The Curie temperature is calculated either in the mean-field approximation MFA or in the random-phase approximation RPA. In the latter case we find a weak logarithmic dependence of T_c on the magnetic anisotropy parameter, which was calculated to be 0.4 meV for this system. In stark contrast to the above mentioned rule, large Curie temperatures of above 200 K for a monolayer (ML) MnSi film and above 300 K for a two ML MnSi film with B2-type structure on Si(100) are obtained within the RPA, and even higher values in MFA. Complementary calculations of MnSi bulk structures and thin unsupported MnSi films are performed in order to analyze these findings. We find that bulk MnSi in the cubic B2 structure is paramagnetic, in contrast to MnSi in the B20 ground-state structure in agreement with the Stoner criterion. In a tetragonally distorted B2 structure, the Mn atoms gradually develop a spin magnetic moment, passing through a low-spin and a high-spin state. However, the ferromagnetism of the MnSi/Si(100) films cannot be explained by tetragonal distortions alone, since the distorted B2 bulk structure is found to order antiferromagnetically. Comparison of the calculations of supported and unsupported films suggests that the reduced coordination of Mn atoms near surfaces and interfaces is crucial for the ferromagnetic ground state of the films. The coordination number of the Mn atoms in B2-type MnSi films on Si(100) constitutes a borderline case, where the spin magnetic moments of Mn are still large despite their sixfold coordination to Si, but the $sp-d$ hybridization with Si states gives rise to a sizable ferromagnetic coupling of the Mn spins. We conclude that the Curie temperatures predicted from the Heisenberg Hamiltonian make thin MnSi films an interesting subject for further experimental investigation of spintronics materials.

(submitted to: Phys. Rev. B)
Contact person: Peter Kratzer (Peter.Kratzer@uni-duisburg-essen.de)

Azobenzene-functionalized alkanethiols in self-assembled monolayers on gold

R. Schmidt, W. Freyer, D. Brete, T. Gießel, C. Gahl, M. Weinelt

Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

Erik McNellis, Karsten Reuter

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany

Abstract

Self-assembled monolayers (SAMs) of 4-trifluoromethyl-azobenzene-4'-methyleneoxy- alkanethiols ($CF_3-C_6H_4-N=N-C_6H_4-O-(CH_2)_n-SH$ on (111)-oriented poly-crystalline gold films on mica were examined by X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS). The spectra are analyzed with the help of density-functional-theory calculations of the isolated molecule. Only one doublet is detected in the sulphur 2p spectra of the investigated SAMs, consistent with a thiolate bond of the molecule to the gold surface. The C 1s XP spectra and the corresponding XAS π^* resonance exhibit a rich structure which is assigned to the carbon atoms in the different chemical surroundings. Comparing XPS binding energies of the azobenzene moiety and calculated initial-state shifts reveals comparable screening of all C 1s core holes. While the carbon 1s XPS binding energy lies below the π^*-resonance excitation-energy, the reversed order is found comparing core ionization and neutral core excitation of the nitrogen 1s core-hole of the azo group. This surprising difference in core-hole binding energies is interpreted as site-dependent polarization screening and charge transfer among the densely packed aromatic moieties. We propose that a quenching of the optical excitation within the molecular layer is thus one major reason for the low trans to cis photo-isomerization rate of azobenzene in aromatic-aliphatic SAMs.

(appeared as: Appl. Phys. A **93**, 267 (2008))
Contact person: Erik McNellis (mcnellis@fhi-berlin.mpg.de)

Surface energy and surface proton order of ice Ih

Ding Pan,[1,2] Li-Min Liu,[2,3,4,5] Gareth A. Tribello,[4,5,6] Ben Slater,[4,5,6]
Angelos Michaelides[2,3,4,5] and Enge Wang[1,2]

[1]*Institute of Physics, Chinese Academy of Sciences, P.O.Box 603, Beijing 100190, China*

[2]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany*

[3]*London Centre for Nanotechnology, University College London, London WC1H 0AJ, UK*

[4]*Materials Simulation Laboratory, University College London, London WC1H 0AJ, UK*

[5]*Department of Chemistry, University College London, London WC1H 0AJ, UK*

[6]*Davy Faraday Research Laboratory, Kathleen Lonsdale Building, Gower Street, University College London, London WC1E 6BT, UK*

Abstract

Ice Ih is comprised of orientationally disordered water molecules giving rise to positional disorder of the hydrogen atoms in the hydrogen bonded network of the lattice. Here, we arrive at a first principles determination of the surface energy of ice Ih and suggest that the surface of ice is significantly more proton ordered than the bulk. We predict that the proton order–disorder transition, which occurs in the bulk at ∼72 K, will not occur at the surface at any temperature below surface melting. An order parameter which defines the surface energy of ice Ih surfaces is also identified.

(Published in: Phys. Rev. Lett. 101, 155703 (2008))

Contact person: Angelos Michaelides (angelos.michaelides@ucl.ac.uk)

On the accuracy of DFT exchange-correlation functionals for H bonds in small water clusters II: The water hexamer and van der Waals interactions

Biswajit Santra,[1] Angelos Michaelides,[2] Martin Fuchs,[1] Alexandre Tkatchenko,[1] Claudia Filippi[3,4] and Matthias Scheffler[1]

[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany*

[2] *Materials Simulation Laboratory, London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, United Kingdom*

[3] *Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, NL-2300 RA Leiden, Netherlands*

[4] *Faculty of Science and Technology and MESA+Research Institute, University of Twente, P.O. Box 217, 7500 AE Enschede, Netherlands*

Abstract

Second order MøllerPlesset perturbation theory at the complete basis set limit and diffusion quantum Monte Carlo are used to examine several low energy isomers of the water hexamer. Both approaches predict the so-called prism to be the lowest energy isomer, followed by cage, book, and cyclic isomers. The energies of the four isomers are very similar, all being within 1015 meV/H_2O. These reference data are then used to evaluate the performance of several density-functional theory exchange-correlation (xc) functionals. A subset of the xc functionals tested for smaller water clusters [I. Santra *et al.*, J. Chem. Phys. **127**, 184104 (2007)] has been considered. While certain functionals do a reasonable job at predicting the absolute dissociation energies of the various isomers (coming within 1020 meV/H_2O), none predict the correct energetic ordering of the four isomers nor does any predict the correct low total energy isomer. All xc functionals tested either predict the book or cyclic isomers to have the largest dissociation energies. A many-body decomposition of the total interaction energies within the hexamers leads to the conclusion that the failure lies in the poor description of van der Waals (dispersion) forces in the xc functionals considered. It is shown that the addition of an empirical pairwise (attractive) C_6R^{-6} correction to certain functionals allows for an improved energetic ordering of the hexamers. The relevance of these results to density-functional simulations of liquid water is also briefly discussed.

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Contact person: Angelos Michaelides (angelos.michaelides@ucl.ac.uk)

O- and H- induced surface core level shifts on Ru(0001): Prevalence of the additivity rule

S. Lizzit,[1] Y. Zhang,[2] K. L. Kostov,[3] L. Petaccia,[1]
A Baraldi,[4,5] D. Menzel[2,6] and K. Reuter[2]

[1]*Sincrotrone Trieste, Strada Statale 14 Km 163.5, 34012 Trieste, Italy*

[2]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany*

[3]*Institute of General and Inorganic Chemistry, Bulgarian Academy of Science, 1113 Sofia, Bulgaria*

[4]*Physics Department and Center of Excellence for Nanostructured Materials, University of Trieste, via A Valerio 2, 34127 Trieste, Italy*

[5]*Laboratorio Nazionale TASC INFM-CNR, in AREA Science Park, 34012 Trieste, Italy*

[6]*Physik-Department E20, Technische Universität München, 85748 Garching, Germany*

Abstract

In previous work on adsorbate-induced surface core level shifts (SCLSs), the effects caused by O atom adsorption on Rh(111) and Ru(0001) were found to be additive: the measured shifts for first layer Ru atoms depended linearly on the number of directly coordinated O atoms. Density-functional theory calculations quantitatively reproduced this effect, allowed separation of initial and final state contributions, and provided an explanation in terms of a roughly constant charge transfer per O atom. We have now conducted similar measurements and calculations for three well-defined adsorbate and coadsorbate layers containing O and H atoms: (1×1)-H, (2×2)-(O+H), and (2×2)-(O+3H) on Ru(0001). As H is stabilized in fcc sites in the prior two structures and in hcp sites in the latter, this enables us to not only study coverage and coadsorption effects on the adsorbate-induced SCLSs, but also the sensitivity to similar adsorption sites. Remarkably good agreement is obtained between experiment and calculations for the energies and geometries of the layers, as well as for all aspects of the SCLS values. The additivity of the next-neighbor adsorbate-induced SCLSs is found to prevail even for the coadsorbate structures. While this confirms the suggested use of SCLSs as fingerprints of the adsorbate configuration, their sensitivity is further demonstrated by the slightly different shifts unambiguously determined for H adsorption in either fcc or hcp hollow sites.

(to appear as invited paper in: J. Phys. Cond. Matter: Special Heinz issue (2009))
Contact person: Dietrich Menzel (dietrich.menzel@ph.tum.de) and Karsten Reuter (reuter@fhi-berlin.mpg.de)

First-principles statistical mechanics approach to step decoration at surfaces

Yongsheng Zhang and Karsten Reuter
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany

Abstract

Using a first-principles parameterized lattice-gas Hamiltonian we study the adsorbate ordering behavior at atomic steps of a Pd(100) surface exposed to an oxygen environment. We identify a wide range of gasphase conditions comprising near atmospheric pressures and elevated temperatures around 900 K, in which the step is decorated by a characteristic O zigzag arrangement. For catalytic processes like the high-temperature combustion of methane that operate under these conditions our approach thus provides first insight into the structure and composition at a prominent defect on the working surface

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Contact person: Karsten Reuter (reuter@fhi-berlin.mpg.de)

Fingerprints for spin-selection rules in the interaction dynamics of O_2 at Al(111)

Christian Carbogno,[1] Jörg Behler,[2] Axel Groß,[1] and Karsten Reuter[3]
[1] *Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany*
[2] *Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany*
[3] *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany*

Abstract

We performed mixed quantum-classical molecular dynamics simulations based on first-principles potential-energy surfaces to demonstrate that the scattering of a beam of singlet O_2 molecules at Al(111) will enable an unambiguous assessment of the role of spin-selection rules for the adsorption dynamics. At thermal energies we predict a sticking probability that is substantially less than unity, with the repelled molecules exhibiting characteristic kinetic, vibrational and rotational signatures arising from the non-adiabatic spin transition.

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Contact person: Karsten Reuter (reuter@fhi-berlin.mpg.de)

Linear-scaling total-energy calculations calculations with the tight-binding Korringa-Kohn-Rostoker Green-function method

Rudolf Zeller
Institut für Festkörperforschung, Forschungszentrum Jülich GmbH,
D-52425 Jülich, Germany

Abstract

A complex-energy broadening scheme with quartic dependence on the broadening parameter is presented for Green function density-functional electronic-structure calculations. The scheme is applied in a recently developed linear-scaling algorithm based on the tight-binding Korringa-Kohn-Rostoker Green function method where it leads to considerable computational saving compared to the standard Fermi-Dirac broadening with quadratic dependence. The linear-scaling algorithm is applied for total-energy and spin-moment calculations for large supercells and the advantages of the quartic broadening scheme are discussed.

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Contact person: ru.zeller@fz-juelich.de

7 SCIENTIFIC HIGHLIGHT OF THE MONTH: "Harnessing the power of modern package management tools for a large Fortran-90-based project: the mutation of ABINIT"

Harnessing the power of modern package management tools for a large Fortran-90-based project: the mutation of ABINIT

Y. Pouillon[1,2,3], X. Gonze[1]

[1] European Theoretical Spectroscopy Facility (ETSF),
Université Catholique de Louvain - Louvain-la-Neuve - Belgium

[2] Universidad del País Vasco (UPV/EHU) - Donostia-San Sebastián - Spain

[3] European Theoretical Spectroscopy Facility (ETSF) - Donostia-San Sebastián - Spain

Abstract

ABINIT is a Fortran 90 free software application that allows the atomic-scale simulation of properties of matter, thanks to Density Functional Theory and Many-Body Perturbation Theory. It is used by more than thousand individuals, who enjoy the wide spectrum of properties that ABINIT allows to compute easily. Several dozen developers contribute to ABINIT from different parts of the world. In 2004, it was perceived that a change of the paradigm for source and package management was needed, in order to benefit from standard package management tools. Thus started a noticeable mutation of ABINIT.

Although the restructuration of the Fortran 90 source directories was needed, the biggest clarification arose from understanding the different kinds of people linked to ABINIT, *i.e.* end-users, developers and maintainers, and the parts of the package they should have access to or control of. Previously, everyone was modifying the source and build system, while further advances required more specialisation in the community, e.g. the management of external libraries, in growing number, which has to be done by skilled maintainers. To address the issues raised by Fortran compilers, and because the ABINIT developers are mostly scientists, it was decided to provide support beyond the GNU Autotools (nowadays the paradigm for binary/package generation) by developing a new build system on top of it. While building ABINIT is now much simpler for end-users, we have had to deal carefully with the additional complexity encountered by developers and maintainers. We discuss the issues that appeared during the mutation.

All these efforts now guarantee further extensibility and maintainability of ABINIT, and have nicely improved its visibility in different communities, with the integration of the packages into the Debian, Gentoo and Ubuntu Linux distributions. Being generic and portable, the new build system might be used in the future by other projects as well.

7.1 Introduction

ABINIT is a feature-full software package for the atomic-scale simulation of molecules and materials, based on Density Functional Theory (DFT) and Many-Body Perturbation Theory (MBPT). Though it is tuned to perform best on periodic systems like crystals, ABINIT is nevertheless able to deal with surfaces and molecules. Not only does it provide valuable information on the geometries of all these systems, it gives access to their electronic, dynamical and dielectric properties as well. Providing 16 tutorials and a lot of help, its companion website, `http://www.abinit.org/`, lets the newcomer step-in smoothly and discover progressively all of its features.

Started in 1997, on the basis of a legacy code, ABINIT has been being written by scientists for scientists, and delivered under the terms of the GNU General Public License (GPL) since 2000. Enjoying the freedom, openness and conviviality found within the project, several dozen developers have joined the community, bringing unexpected contributions as well. ABINIT counts now more than 1000 registered users and an average of 45 regular contributors from all around the world. In addition to its 500,000 lines of Fortran 90 contained in a thousand files, ABINIT features also about 600 automatic tests. For details about the scientific use of ABINIT, we refer the reader to Refs. [1, 2].

From the very start of the ABINIT project, many software engineering concepts were kept in mind, especially those related to portability, self-testing and self-documentation. As an example, every source file provides a header describing the purpose of the routine it contains, as well as its arguments, and other useful information, that may be processed by RoboDOC[1] to generate the HTML documentation for the source code[2]. Yet, despite the rigour that has been the basis of its development, ABINIT has not been originally designed to handle properly extensive code reuse. Its structure was quite intermixed and no much care was taken about packaging standards. Beyond the quite easily handled BLAS/LAPACK library for linear algebra operations, and the — already more difficult to address — MPI library for parallelism, the demand expanded a lot from 2004.

Indeed, that year, the NANOQUANTA Network of Excellence (NoE), consisting in 10 research teams sponsored by the European Union (EU) was launched. One major goal of NANOQUANTA was the integration of the software developed within the network into an unified distribution of which ABINIT is a major component. The interoperability with several other codes guarantees that many kinds of complex calculations can be smoothly performed. Such efforts continue and expand within the European Theoretical Spectroscopy Facility (ETSF)[3]. As a consequence, it was needed to link ABINIT with NetCDF[4] for architecture-independent data exchange, XMLF90 for CML input/output, and the Nanoquanta exchange-correlation library, a C-based library

[1] RoboDOC home page: `http://www.xs4all.nl/~rfsber/Robo/robodoc.html`.
[2] See `http://www.abinit.org/package/robodoc/masterindex.html`.
[3] Website of the ETSF: `http://etsf.eu/`
[4] NetCDF home page: `http://www.unidata.ucar.edu/software/netcdf/`

coming from the Octopus code [3], providing routines that any DFT-based code may benefit from. These have been joined recently by a NetCDF-based platform-independent data-exchange library named ETSF I/O [4,5]. The latter implements the file format we described in the October 2007 highlight of this newsletter (#83). ABINIT has also been chosen as a basis by another EU-sponsored endeavour, codename BigDFT[5], the purpose of which is to eliminate the bottlenecks limiting the applicability of DFT to "large systems", i.e. containing more than 10000 atoms. Last but not least, the possibility of quantum transport calculations through the use of Wannier90 [6] started not much later afterwards.

As a consequence, 2004 became a turning point. When the support for external libraries became somewhat problematic, it felt obvious that the growth would soon become unmanageable if no action were undertaken quickly. Although very portable, the home-made build system was rather monolithic, e.g. with two shell-scripts generating a primitive Makefile for each directory containing the Fortran 90 routines, and was only able to handle Fortran properly. Its limits with respect to external libraries were obvious for some compilers and architectures.

As most users are running ABINIT in Unix-like environments, and because of the free-software-oriented philosophy of the development model, it has been decided to bring the code as close as possible to the GNU Coding Standards. Thus started an extensive and in-depth mutation of the whole package which is now reaching its final steps. Between its 4.4 and 5.0 versions, ABINIT underwent a series of preparatory minor modifications: enforcement of the strict programming rules, already known within the ABINIT developer community as the "abirules"; large enhancements within the subroutine headers, in particular addition of intents for all arguments; decompression of the sources into a *abinit-<version>* directory, instead of the current directory; complete restructuring of the source directory tree; adoption of a decentralised Version Control System (VCS): Bazaar[6]. While these preliminary steps were quickly addressed by a few selected developers within a small amount of time, the complete rewriting of the build system that followed, nicknamed "breaking the monolith", required many more efforts and a much broader culture in software programming and management. The former "monolith" was broken into many pieces, improving the distinction between the three levels of contributors along: end-users, developers, and maintainers (see Fig. 1).

7.2 Developing software in scientific environments

Before fully entering into the details, and in order to facilitate the understanding of our approach, let start with an overview of the situation. The ABINIT developer community is mostly made of physicists and chemists. As such, the typical ABINIT contributors do not have a very extended culture in computer programming, which means that in most cases their development expertise is limited to Fortran 90. Furthermore, since most ABINIT developers are hired to carry out scientific research, they cannot devote too much time in taking a software engineer's point of view. Another essential point to account for is the lack of comfort accompanying High-

[5]See `http://www-drfmc.cea.fr/sp2m/L_Sim/BigDFT/index.html` for details.
[6]See `http://bazaar-vcs.org/` for details

Performance Computing (HPC) environments. Working in a HPC environment may indeed imply a lot of constraints: restricted access, the need of a custom MPI installation for parallelism, unavailability of recent versions for software like Python and the Autotools, necessity for very specific skills, to cite the most obvious ones. In some cases, security issues linked with the potential military applications of the results finish to make things very involved.

All this means that the build system has to take care of as many aspects as possible, far beyond what standard source management tools provide, and hide as much complexity as possible to the end-user. In particular, its interface has to be minimalistic and clear. One precision: by using "source management", we mean everything related to the build and distribution of the source code; other aspects, like version control, also play a major role in this respect, but will not be discussed here. Only maintainers should have to modify the build system, and that is why we have opted for a configuration-file-based approach for users and developers. Before everything else, we have defined minimum software requirements: Perl, Python, GNU Make or equivalent, GNU M4, GNU Autoconf, GNU Automake, and GNU Libtool, the three last ones forming the so-called "GNU Autotools". Perl and Python were chosen for performance and clarity, and they definitely constitute too large packages for us to provide any support for them. However, we were able to find a version combination of the Autotools which can be installed in a user's home directory, in case it would not be possible for them to have recent versions installed system-wide[7]. Alternative systems have been thought about as well, but they do not provide sufficient support for Fortran 90. The GNU Autotools are the only ones able to conciliate the growth of ABINIT with the preservation of its portability, both by the high number of their features and because of their ubiquity among the Free Software community.

7.3 The build system

The new build system of ABINIT constitutes a software layer above the Autotools. Let us first examine important characteristics of these.

One of the fundamental concepts of the Autotools has lead our way: the end-user does not have to care about the build system, in particular **it is not necessary to have the Autotools installed to build the source code**. A distributed source tree is fully autonomous and contains both the data and the code to be built out-of-the-box, by end-users, through the well-established '`configure; make; make install`' trilogy.

On the other hand, the developers and the maintainers have to install the Autotools on their development platforms, because the build system has to be kept synchronised with the source code, which means that some files (*e.g.* the *configure* script) have to be regenerated on a regular basis. To make an analogy between an Autotools-based build system and a scientific code, we can say that:

[7] One of us (Y.P.) wrote an installer script taking care of everything, and made the software bundle available on the ABINIT web site. See `http://www.abinit.org/gnu/` for details.

- the *configure.ac* is the source code of the main program;
- the M4 macros are the libraries (like BLAS, LAPACK, NetCDF, etc.);
- the *configure* script is the compiled code, Autoconf being the compiler;
- the *Makefile.am* files are the input data;
- the *Makefile.in* files are the preprocessed input data, Automake being the preprocessor;
- the *Makefile* files are the output data coming out from *configure*;
- the *make* program is a post-processor;
- distributing an Autotools-ready source package is like distributing a ready-to-use scientific code along with some example input data.

In order to facilitate future enhancements, improve modularity and simplify the build system, the physical and logical structures of the source directory tree have been first aligned, *i.e.* the directory tree has been split into 9 blocks (see Fig. 1), with corresponding global configuration files when necessary. In addition to these global files, one or two other local configuration files can be found in each of the core source libraries, as well as in some external libraries (see Fig. 2):

- *abinit.src* (A1), that lists the source files of a library, identifying Fortran modules, and controlling which files will be part of the libraries; this lets developers easily try and compare different ways to implement a feature;
- *abinit.amf* (A2), containing additions to *Makefile.am* files, such as explicit dependencies between object files, or lists of extra files to put in the source tarball; this is necessary when the build process cannot be fully automated.

Apart from the *configure.ac* file which has to be located in the top source directory, the whole build system is concentrated in one "pluggable" directory we have called *config/*. It contains the global configuration files mentioned above, as well as the scripts generating the files required to build ABINIT. These scripts take care of the pre-build stage shown in Fig. 2. Even if it cannot cover all situations, this design is both very flexible and extensible, and still usable by a relatively unexperienced developer, provided that the corresponding documentation is available.

Taking care of the build system itself has been attributed exclusively to the maintainers, in order to set the developers free from learning the internals of the Autotools and provide a better overall stability. As such, the developers of the code can be seen as the end-users of the build system, while the maintainers of the code are the developers of the build system. This also means that regular communication during the whole development process has become a key aspect, which was not the case in the version 4 of ABINIT. In other words, the developers now concentrate on the source code, while the maintainers provide source code management services.

Most of the issues we have to face when building ABINIT come from the Fortran compilers. In particular, their user interfaces are not-at-all standardised, and the compilation of Fortran modules produces the very annoying *.mod* files. These are binary, which means that, contrary to C header files, they are not platform-independent. Much worse, they are incompatible from one compiler to the other and may obey various conflicting naming conventions. Another painful issue is that a few compilers do not use the *'-I'* option to look for modules.

Needless to say, dealing nicely with such a situation is way beyond the average software-engineering skills of most scientists, and the Autotools do not provide any solution in this case. We have thus addressed these issues by providing compiler-vendor auto-detection, "tricks", and default optimisation flags for most Fortran compilers, at least those used within the ABINIT community. By "tricks", we mean workarounds one has to apply to have a Fortran compiler working properly, *e.g.* where to apply specific flags to obtain 64-bit objects.

Most build parameters are only machine-dependent, (*i.e.* not version-specific), and change quite rarely. Then it is very convenient for both users and developers to store them into config files. In order to have ABINIT built seamlessly on several machines sharing the same home directory — which is a relatively common situation in HPC environments, we have named these config files *$HOME/.abinit/build/<hostname>.ac*, i.e. the name of the machine plus an 'ac' extension to tell that the file is meant to be read by Autoconf's *configure* script.

One very delicate point is MPI support, both as it is critical for HPC and because there is no standard neither for its structure nor for its location. After a few failed attempts, we finally decided to push towards maximum flexibility, providing as many options as possible. Even if these options have to be set manually, it will typically be done every other year. It is possible either to let the build system auto-detect natively MPI-capable Fortran compilers or to use command-line parameters, e.g. specifying a prefix for the MPI installation. As time goes by, a more and more comprehensive database of examples is made available as well, saving developers' and users' time more and more efficiently.

7.4 Using the build system

End-users do not need know what the build system is, since they are not supposed to modify the sources. They may even ignore that it exists at all, as they will mostly download a tarball and build the code once in a while. For them, the mutation of ABINIT only means enhanced comfort. What they only have to know is that the build of ABINIT now follows the well-established '`configure; make; make install`' trilogy, and that they should store critical information into a config file. In most situations, once the latter has been set and proved to lead to reliable binaries, one may forget anything about the build parameters for quite a while. A fully documented template is provided with the source code of ABINIT to facilitate the setting of these parameters.

For developers, the new build system of ABINIT introduces the concept of a **pre-build stage**,

necessary to ensure a permanent consistency between the source tree itself and the metadata used to build it. The front-end script *makemake* performs all required steps that make the build of ABINIT possible (see Fig. 2):

1. Update the source tree according to the latest information available. Some routines are written by scripts and depend on the contents of other source files, like *e.g.* the routine checking the names of input variables. The most important and time-consuming part is dedicated to the parsing of all ABINIT source files and the subsequent generation of the Fortran interfaces for all the routines.

2. Update parts of the build system in order to follow accurately the evolution of the ABINIT source tree. This critical step consists in the writing of M4 macros by the build system itself. For instance, command-line options for the configure script are declared and a parser is written so that their validity and consistency can be checked at configure-time. Another example is the declaration of all the makefiles, which vary in number and location with time.

3. Generate prototype makefiles for Automake. Each of these files describes in a compact way how to build the contents of a directory. They highly depend on the auxiliary config files found in many source directories.

4. Run the Autotools in order to make the source tree autonomous and distributable. This step gathers all hand-written and script-written M4 macros into one file (running *aclocal*) and uses them in various places when creating the configure script (running *autoconf*). It also creates a C header input file (runing *autoheader*) that will store all preprocessing options later when processed by the *configure* script. Last but not least, it transforms the prototype makefiles into input data for the *configure* script (running *automake*).

Let's now have a look at the pre-configuration stage also described in Fig. 2. By having the ABINIT build system partly writing itself we suppress the need for developers to edit *configure.ac*, which is the most delicate part of any autotools-based build system. Moreover, having everything grouped under one command and performed systematically ensures that the source tree will always be in a consistent state. When developers add, move or delete a file or a directory, they have to update the corresponding metadata and run the *makemake* script. In case of a file, they mostly have to change one line in the *abinit.src* file (A1) found in the same directory; in the case of a new pre- or post-processing program, they have to edit the *config/specs/binaries.cf* (D1) file as well; for a directory containing a library, editing *config/specs/corelibs.cf* (D2) will be necessary. To facilitate the process, all these files are self-documented.

Providing the *configure.ac* script as well as a set of hand-made useful M4 macros is under the responsibility of the maintainers, who are the only ones who should edit the other global config files, as it will likely have consequences on the behaviour of the whole build system. Adding support for a new platform, compiler, or plug-in are also maintainer tasks, since such operations involve writing or modifying M4 macros, as well as editing the *configure.ac* script. Therefore, in contrast to what was happening until ABINIT 4, some communication is now necessary when

performing a certain number of actions, and this is precisely where the mutation of the code has involved a mutation of the community: roles have become specified more clearly and protocols have had to be defined.

7.5 Outcome

At present, several lessons have been drawn from the mutation. First, it is not yet possible to provide full auto-detection: the *<hostname>.ac* file is needed on most platforms, especially to deal with MPI. Now that there is a Fortran 90 compiler in the GNU Compiler Collection (GCC), the support of Fortran 90 by the GNU Autotools is greatly improving and the user interfaces of the Fortran compilers will hopefully tend to unify. This is however far from being the case for MPI, as system administrators are completely free to install it as they wish. Second, the jump from a home-made build system the developers were used to, towards a sophisticated build system based on the Autotools has generated some temporary frustration within the developer community. Indeed, the GNU Autotools generate automatically a large number of files defying human readability. During the transition, when the documentation on the new build system was still inexisting, most developers would try to solve their build-time problems by reading and hacking these files, which is both a nightmare for everybody and also the wrong way to proceed. Now, after a few years of practice, this issue has completely disappeared but took a long time to be eliminated. Third, while the usual developers could read, understand and modify the former build system according to their needs, a full handle of the new one is now only possible for maintainers. Though it is frustrating for some of the expert developers to lose the full understanding of the package they had previously, this is the price for the continued growth and complexification of the ABINIT package, as the Autotools are invisibly taking care of countless details. A good deal of the challenge is in the shift from independent individual contributions towards partnerships, and from control to mastery, with a particular emphasis on the critical importance of ***communicating before hacking***.

But one of the nicest results of this big mutation is that ABINIT has attracted the attention of several software packagers, who have also contributed in an interesting way to the improvement of its overall quality. ABINIT is now distributed with the Debian, Gentoo and Ubuntu Linux distributions, though no request or effort has been made on our side. This unexpected acknowledgment by the Free Software community is very encouraging and has a lot of nice side-effects. On one hand, the visibility and availability of the software are greatly improved, publicity is made for the related projects, and the user base expands faster. On the other hand, it puts an additional pressure on the developers and maintainers to produce higher-quality code and documentation. In any case, having standard packages available is a neat feature when it comes to deploy the software on a bunch of machines for schools or lectures.

Along with the 5.6 version of ABINIT, the new build system has reached a good level of quality and robustness. Its user interface is now frozen and most of the upcoming bug fixes and improvements will only appear as minor changes to end-users. We have successfully tested the automatic generation of Fortran 90 interfaces for all the subroutines and functions contained

in ABINIT, which was an extremely critical step. This has put a definitive end to the era of quick-and-very-dirty developments. In order to have the build system fitting the needs of both users and developers, we have allowed as many degrees of freedom as possible. As a bonus to our efforts, the set of Python scripts forming the new build system might be used by other intermixed C/C++/Fortran 90/Python software projects; actually the build systems of BigDFT and ETSF I/O have already imported some of our ideas.

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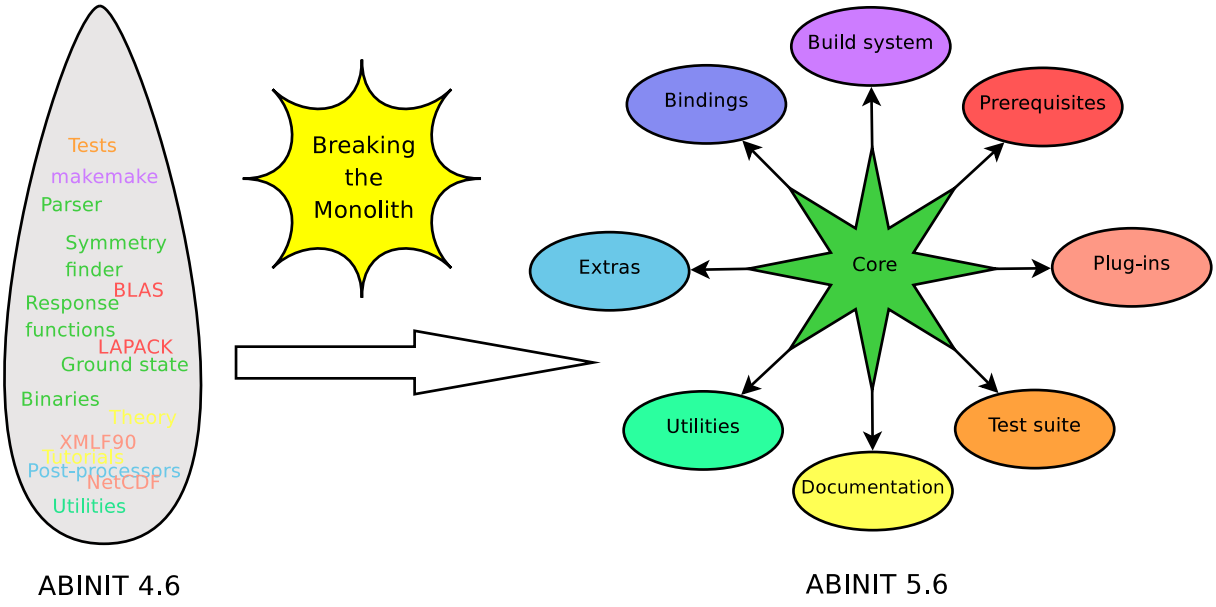

Figure 1: Overall view on the mutation of ABINIT, based on the restructuring of the code and the implementation of a new build system, providing better modularity and extensibility.

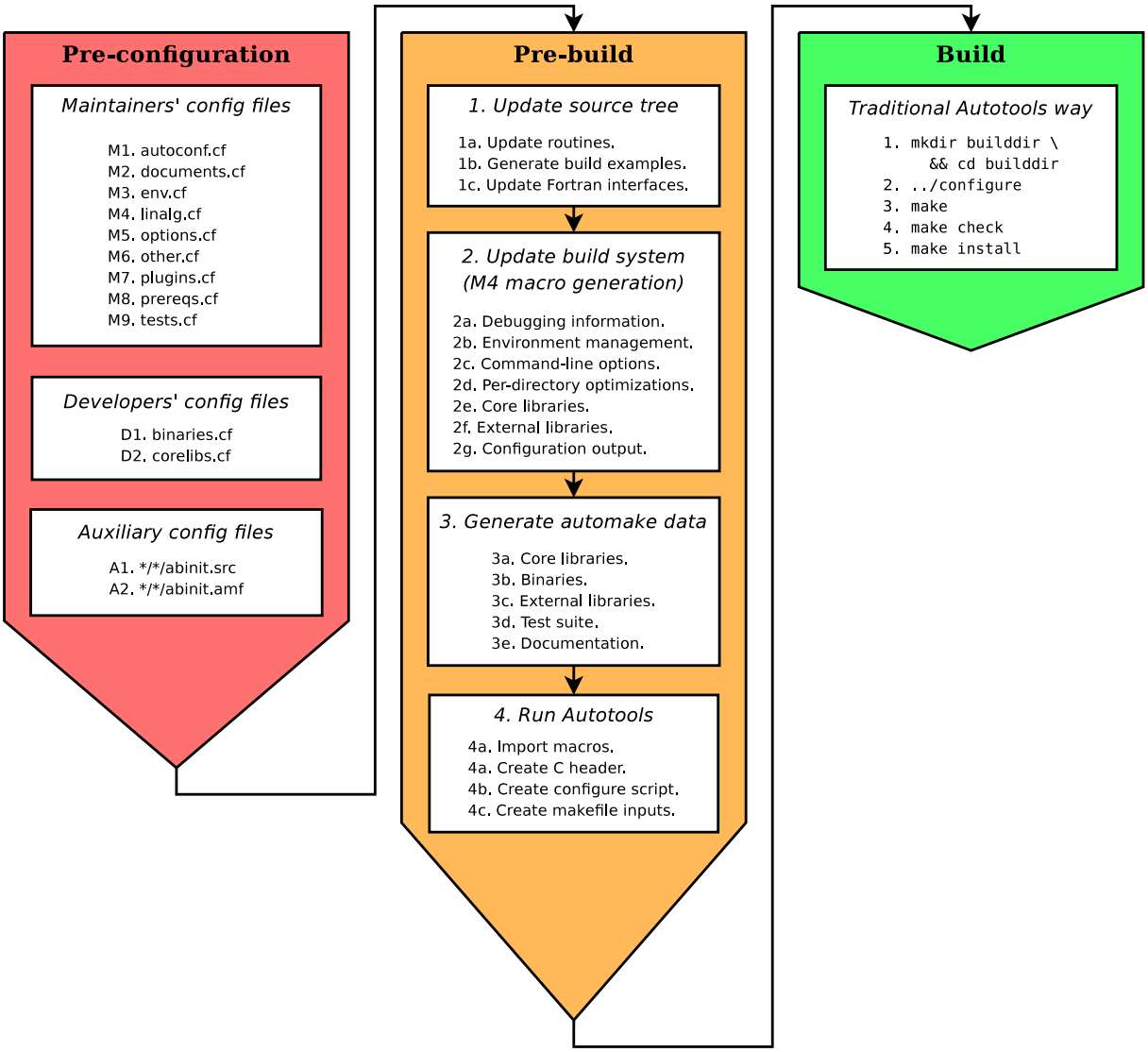

Figure 2: Steps involved in a build of ABINIT. As many files are generated automatically, the process requires different classes of contributors to operate at different steps and to co-operate with one another.