Ψ_k Newsletter

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

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Contents

1 Editorial

In this issue of the Psi-k Newsletter we have a letter from the Psi-k chairman, followed by a "Call for Psi-k Workshop Proposals for 2010". In the subsequent sections there is a number of workshop reports and announcements of workshops/conferences as well as available positions. In particular, we turn readers' attention to the "KKR and Spectroscopy Hands-on Course", taking place in Munich on 24-26 June, 2009.

The abstracts of newly submitted or recent papers can be found just before the scientific highlight of the month. The latter is by M. Fechner[1], I.V. Maznichenko[2], S. Ostanin[1], A. Ernst[1], J. Henk[1], I. Mertig (*Halle, Germany*) on **"Ab initio Study of Magnetoelectricity in Composite Multiferroics "**.

For details, please check the table of content of the newsletter.

The *Uniform Resource Locator* (URL) for the Psi-k webpage is:

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

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

The email address for contacting us and for submitting contributions to the Psi-k newsletters is

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

For distributing Psi-k related information to the whole Psi-k community, please use the Psi-k Portal accessed from the above web page.

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

2 General News

2.1 Letter from the Psi-k Chairman

The new Psi-k: This is the second year of our new Psi-k organisation as a "Company limited by guarantee", registered in England and Wales with Company No. 06440198 and with the office at Daresbury. Our application as charity has been approved last year (Charity No.1126308, Name: Psi-k), so that we do not have to pay taxes. Thus we are a legally independent, non-profit, science organisation, funded only by financial contributions of the larger and financially strong Psi-k groups in Europe. Our funding amounts to a reasonable sum, but is not really sufficient for our large community and our many activities. Thus if you are able to sponsor Psi-k, we ask you for a reasonable membership fee. From smaller groups also small donations of about 1,000 - 2,000 Euro are welcome. Please contact me in this context.

This year we have an extremely large number of activities, with a considerable part jointly funded with CECAM. The poster "Psi-k Workshops 2009" lists 28 activities and is available on the Psi-k Website. If you haven't done yet, please download it and advertise in your institution.

Psi-k Activities in 2010: The call for Psi-k Workshop Proposals in 2010 is now being published (see below). We want to remind you that our big event is the Psi-k 2010 Conference in Berlin 12.-15. Sept. 2010

See: http://www.fhi-berlin.mpg.de/th/Meetings/psik_2010/

This is the showcase conference of Psi-k, organised every 5 years. We expect around 800 participants and in particular you! Please mark the dates in your calendar.

In order not to interfere with this big Psi-k Conference, the Scientific Advisory Committee agreed to avoid organizing competing workshops from April 15 to November 15, 2010. Well justified exceptions might be possible. Contrary to workshops, we welcome tutorials and summer schools during the whole year.

Forward Look and Computational Science Committee (CSEC): The ESF Forward Look "European Computational Science Forum: The 'Lincei Initiative'" has been successfully completed. The plan for the next step is to set up a "Computational Sciences Expert Committee (CSEC)" at the ESF. CSEC is supposed to be an advisory board and a pressure group for scientific computing in Europe. One of the aims is to convince national agencies and EU to provide funding for code development and support for users, for training and collaborations. CSEC should include all computational sciences, at least in principle.

The proposal for CSEC has been submitted to the ESF and the ESF Governing Council will decide on this in October. The final decision will very much depend on the support of our members. If you think you can help, please contact me.

Relation Psi-K - CECAM: The importance of CECAM is strongly increasing. The program for 2009 (see the CECAM website) lists 29 Workshops, 7 Tutorials and 6 Sponsored Events, in total 42 activities, many more than in any previous year. Please note, that CECAM now also funds tutorials, which were previously funded by EU contracts. Most interesting for you is the fact that the "Sponsored Events" refer to workshops, summer schools and tutorials, which are sponsored by CECAM, but which do not take place at Lausanne, Zrich or at the CECAM nodes. Thus CECAM is willing to sponsor activities anywhere in Europe, another dramatic change.

Thus there is a strong overlap of interests between Psi-k and CECAM, and it is for this reason that a recent Psi-k Board Meeting in Dresden was also attended by Wanda Andreoni, Director of CECAM and at the same time member of the Board of Psi-k. The aim is that Psi-k should collaborate and co-operate closely (and not compete) with CECAM and that Psi-k supports the development of CECAM as a Europe-wide organisation for computational sciences. It was envisaged that in the future Psi-k might fund fewer workshops and events and might supply more funding to the fewer selected activities. Such a change cannot be done abruptly and needs to be discussed at the next meeting of the scientific advisory committee (SAC) in November. Helpful for such a decision could be, that CECAM will sponsor activities, workshops, etc., anywhere in Europe, i.e. also at "your university", if "you" submit a fundable proposal.

"Psi-k Research Conference","Psi-k Summer School" and "Psi-k Graduate School"

Concerning the co-operation with CECAM the following decisions were taken at the Psi-k Board Meeting:

1. Psi-k should organise, in co-operation with and co-sponsored by CECAM, a series of annual "Psi-k Research Conferences" on varying topics, based on the model of Gordon Conferences in the US or the ESF-funded Euresco Conferences in the 90's. These conferences would be characterized by invited talks only and by lots of time for discussions. Due to the big Psi-k Conference in 2010, we intend to start this series in 2011.
2. Analogously Psi-k should organise in co-operation with CECAM a series of annual "Psi-k Summer Schools" on varying topics. This way we could extend the previous successful Psi-k Summer Schools which were largely funded by the EU project "Psi-k Training", which unfortunately expires in 2010.
3. Finally, a "Psi-k Graduate School" could annually be co-sponsored with CECAM. Again this was a successful activity of the "Psi-k Training" programme.

These series would become flagship projects for Psi-k and CECAM. However all such Psi-k proposals have to be approved for funding by the CECAM council and this requires very good and competitive proposals of our members.

With best regards,

Your chairman

Peter Dederichs

2.2 Call for Psi-k Workshop Proposals for 2010

Herewith we ask for proposals for workshops, small conferences, hands-on tutorials and summer schools in the field of ab-initio calculations to be held in 2010 and to be partially funded by the new Psi-k network.

The deadline for Psi-k proposals is Friday, October 2, 2009.

Our big activity in 2010 is the Psi-k 2010 Conference in Berlin, 12.-15. September 2010 (http://www.fhi-berlin.mpg.de/th/Meetings/psik_2010/). This is the showcase of Psi-k, organized every five years.

In order not to interfere with this big Psi-k conference, we will (and can) only support a reduced number of workshops, and in particular no workshops from April 15 to November 15, 2010. Well justified exceptions might be possible. Contrary to workshops, we welcome tutorials and summer schools during the whole year.

How to submit a proposal: You need to login to the Psi-k Portal, accessed from the Psi-k web pages (http://www.psi-k.org). First you will have to create an account (if you do not have it already). For this please use your e-mail address as userid. After the successful creation of an account you will end up in the PSI-K workspace. Click on the 'Workshop Proposal' button, and then click on the number 1 (left column) of the 'Call For Workshop Proposal List' to view its details, including the option to submit a proposal.

Then to submit a proposal for a workshop, click the 'Submit Workshop Proposal' button:

Fill in all form fields correctly and then you will be able to preview your proposal as a pdf-file by clicking on 'Preview(PDF)' button. If the preview button does not produce a pdf-file please check carefully that all input fields have been filled in, valid dates are used (format dd/mm/2009-dd/mm/2009) and budget (Euros) is provided. You can then make any changes to your proposal or 'Submit' your proposal as it is.

To view any proposals you have already submitted, first go to the relevant proposal page then click on the 'Show My Proposal(s)' button. You can view or modify your proposal, or download it as a pdf-file.

Collaboration with CECAM: As in the past years we strongly encourage joint CECAM/ Psi-k Workshops as well as joint tutorials about electronic structure calculations. The collaboration with CECAM is working very well and has effectively increased our funding substantially. Also for joint CECAM/Psi-k Workshops we ask you to avoid as much as possible the above dates before and after the Psi-k Conference.

The deadline for CECAM proposals has not been fixed yet. It is likely to be considerably earlier than our deadline.

The importance of CECAM, which is now located at Lausanne, is strongly increasing. This year

CECAM organizes and/or co-sponsors a total of 42 activities, many more than in previous years (see the CECAM website). Please notice that CECAM now also funds tutorials. In addition "Sponsored Events" are included in the program, i.e. workshops, tutorials or schools, which do not take place at CECAM in Lausanne, at Zürich or at other CECAM nodes.

Funding for US participants: Very often the workshops have an American co-organizer, who can bring in additional support for US participants by funding from NSF or other agencies. European organizers can also apply for support of US participants from:

U.S. Office of Naval Research Global (http://www.onrglobal.navy.mil) European Office of Aerospace Research and Development (http://www.london.af.mil)

With best regards,

Peter Dederichs and Walter Temmerman

(Chair and Vice-chair, Psi-k)

3 Psi-k Activities

"Towards Atomistic Materials Design"

3.1 Reports on Psi-k Supported Workshops

3.1.1 Report on 14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

Trieste (Italy)

January 8-10th, 2009

The Abdus Salam International Centre for Theoretical Physics (ICTP)
Psi-k Network
International School for Advanced Studies (SISSA)
INFM-DEMOCRITOS National Simulation Center
Centre Européen de Calcul Atomique et Moléculaire (CECAM)
International Center for Materials Research (ICMR)

Organizers: Francesco Mauri, Ralph Gebauer, and David Vanderbilt

http://users.ictp.it/~cm/TotalEnergy2009.html

This workshop was the 14th in a very successful series of worshops, held every two years at the ICTP in Trieste, Italy. The workshop is devoted to exposing recent advances in computational condensed matter physics and materials science, based on realistic calculations of the electronic structure of complex systems. It was held this year on 8-10 January 2009, with three full days of oral presentations, and poster sessions on the evenings of 8 and 9 January. Attendance at the workshop has grown over the years, so that this year there were 230 participants, including 23 presenters of oral talks and 155 poster presenters.

This year the workshop focused on several specific scientific themes:

- Many-body, quantum-chemistry, and quasiparticle techniques for studying complex materials
- Separable representations of the dielectric function and related quantities
- Thermal and electrical transport at the nanoscale
- Graphene and BN-based nanostructures

- FeAs-based superconductors
- Simulations of properties of complex materials systems, including electrochemical reactions, catalysis, DNA, and momentum distributions in water

There were two special events at the workshop. The first was the award of the 2008 ICTP Prize, which this year went to two condensed-matter theorists, at the beginning of the morning session on January 9. ICTP Director K.R. Sreenivasan began with some remarks about the history and role of ICTP, and then announced the two prize winners: Zhong Fang, of the Center for Quantum Simulation Sciences, CAS, Beijing, China, and Abhishek Dhar of the Raman Research Institute, Bangalore, India. Dr. Fang then gave his prize talk on "LDA+Gutzwiller Method for Correlated Electron Systems." Unfortunately, Dr. Dhar was unable to attend the workshop and so could not present his prize talk on the "Green-Kubo Formula for Heat Conduction in Open Systems."

The second special event was a special session on the morning of January 10 to honor the upcoming 60th birthday of Steven Louie, of UC Berkeley, and to recognize his seminal contributions to quasiparticle methods and their application to nanostructures. To mark this event, Prof. Alex Zettl, also of UC Berkeley and a long-time colleague of Louie's, presented a keynote talk on "Exploiting the Electronic, Thermal, and Mechanical Properties of Carbon and BN Nanostructures," in which he highlighted some of Louie's contributions.

The large attendance of the workshop led to some changes in the mechanics. Oral talks were given in the Main Lecture Hall of the Leonardo da Vinci Building as in past years, but in a break with past practice, the poster sessions were moved to the Lower Level of the Adriatico Guest House, where food and drinks were provided on buffet tables in order to avoid queues. Posters were organized and arranged by topic. On 8 January the general theme was "Theory and Methods" and the subtopics were Density-Functional Theory beyond LDA, Time Dependent DFT, Many-Body Techniques for Real Materials, Quantum Monte Carlo, Ab-initio Molecular Dynamics, Large Scale and Multiscale Simulations, Activated Processes, Electronic and Thermal Transport, Response to External Fields, Simulations in Realistic Environments, and Other Methods. On 9 January the general theme was "Applications" and the subtopics were Nanoscience, Biochemistry and Biomaterials, Magnetism and Spintronics, Geophysics, Functional Materials, Surfaces, Spectroscopies, Catalysis and Electrochemistry, Chemical Reactions and Kinetics, Materials Design, and Other Applications. Attendees seemed to feel that this format was very successful.

The workshop was cosponsored by ICTP and several other institutions: the International School for Advanced Studies (SISSA), the INFM DEMOCRITOS National Simulation Center, the International Center for Materials Research (ICMR), the Psi-k Network, and the Centre Européen de Calcul Atomique et Moléculaire (CECAM). The organizers and participants of the workshop warmly thank these institutions for their support for the workshop.

Programme

	Thursday, 8 January 2009
8:00	Registration and administrative formalities
8:50	Welcoming Remarks
	SESSION 1: Many-body Techniques for Real Materials
9:00	*Bridging the size gap between density-functional and many-body perturbation theory* Geoffrey Stenuit - CNR-INFM Democritos, Trieste, Italy
9:35	*Efficient evaluation of dielectric matrices for ab-initio calculations of excited state properties and correlation energies* Giulia Galli - UC Davis, USA
10:10	*Efficient and accurate calculation of exact exchange and RPA correlation energies in ACFD theory* Huy-Viet Nguyen - Hanoi National University of Education, Viet Nam, and SISSA Trieste
10:45	Coffee Break + Registration
11:30	*Correlation in electronic excitations* Lucia Reining - Ecole Polytechnique, Palaiseau, France
12:05	*Electron correlation in graphene: band structure and electron-phonon interaction from GW* Claudio Attaccalite - U. del Pais Vasco, San Sebastian, Spain
12:40	Lunch break
	SESSION 2: Simulations of Structural Properties
14:40	*First-principles electrochemistry* Ismaila Dabo - INRIA and Université Paris-Est, France
15:15	*Ab-initio random structure searching: A window on structure space* Chris Pickard - St. Andrews, UK
15:50	Coffee Break + Registration
16:35	*Quantum Monte Carlo simulations of behavior at extreme conditions* Ron Cohen - Carnegie Institution, USA
	POSTER SESSION 1
17:30	Poster setup
18:30	Poster session / free discussions

	Friday, 9 January 2009
	SESSION 3: 2008 ICTP Prize Ceremony
8:50	Welcoming remarks and Presentation of the Award K.R. Sreenivasan - ICTP Director
9:35	*LDA+Gutzwiller method for correlated electron systems* Zhong Fang - Center for Quantum Simulation Sciences, CAS, Beijing, China
10:10	Coffee Break
	SESSION 4: Thermal and Electronic Transport
10:55	*Thermal transport at the nanoscale* Davide Donadio - UC Davis, USA
11:30	*First-principles studies of single-molecule junction conductance: Links, length, and switching* Jeff Neaton - Molecular Foundry, LBNL, Berkeley, USA
12:05	Lunch
	SESSION 5: Quantum Chemistry
14:40	*Fermion Quantum Monte Carlo in slater determinant spaces: A game of life, death and annihilation* Ali Alavi - Cambridge, UK
15:15	*Explicitly correlated ab initio methods for metals* Beate Paulus - Freie Universität Berlin, Germany
15:50	Coffee Break
16:30	*Constrained DFT for electron transfer and reaction barrier heights* Troy Van Voorhis - MIT, Cambridge, USA
17:10	*Efficient first-principles van der Waals density functional forces* Jose Soler - Universidad Autónoma de Madrid, Spain
	POSTER SESSION 2
17:45	Poster setup
18:30	Poster session / free discussions

	Saturday, 10 January 2009
	SESSION 6: Carbon Nanostructures
8:50	Introduction of Keynote Speaker
9:00	*Exploiting the Electronic, Thermal, and Mechanical Properties of Carbon and BN Nanostructures* Keynote talk in honor of STEVEN LOUIE's 60th birthday Alex Zettl - UC Berkeley, USA
9:50	*Band offsets from many-body perturbation theory* Gian-Marco Rignanese - Univ. Catholique de Louvain, Belgium
10:25	*Energy gaps in graphene superstructures* Young-Woo Son - KIAS, Seoul, Korea
11:00	Coffee Break
	SESSION 7: Large-scale and Multi-scale Simulation
11:45	*Towards an error-controlled multi-scale catalysis modeling* Karsten Reuter - FHI-MPG, Berlin, Germany
12:20	*Computational investigation of DNA derivatives for nano-electronics* Rosa di Felice - INFM-CNR, Modena, Italy
12:55	Lunch
	SESSION 8: Functional Materials
14:40	*DFT studies of FeAs superconductors* Lilia Boeri - MPI-FKF, Stuttgart, Germany
15:15	*Hydrogen superconductivity and other superconductors* Gianni Profeta - Università degli Studi dell'Aquila, Italy
15:50	Coffee Break
16:35	*Ab-initio pseudopotential calculations of the orbital magnetization* Davide Ceresoli - MIT, Cambridge, USA
14:40	*Quantum protons in hydrogen bonded systems* Roberto Car - Princeton U., Princeton, USA
17:45	Concluding Remarks

The full list of participants and the abstracts of the presentations at this workshop can be downloaded from the Psi-k Portal (192 pages), accessed from the Psi-k webpage `http://www.psi-k.org`**.**

3.1.2 Report on Workshop Magnetism in Complex Systems

Vienna University of Technology, Vienna, Austria

16.-18. April 2009

Ψ_k, Austrian Ministry of Science and Research, TU-Wien

Peter Mohn and Jürgen Hafner

http://www.cms.tuwien.ac.at/

Our workshop was intended to cover both the theoretical and the experimental aspects of magnetism. To this end we invited speakers and participants from both sides of the gap and finally 50 scientists met in Vienna in order to learn from each other. The experimental side covered basic questions like how to measure magnetic properties (Hilscher) and the thermodynamic aspects of magnetism (Michor). Two lectures gave emphasis to EMCD (Stöger-Pollach, Leifer). Spectroscopic methods were respresented by one lecture about the determination of magnetic structures from neutron scattering (Rotter) and one lecture about spin resolved PES (Dedkov). Finally Havela gave an overview about the magnetism of heavy elements, followed by a respective theoretical account by Shick. The theoretical part started with an introduction into magnetism within the LDA (Mohn) and about DMFT and results for various applications (Held). Post DFT methods and the application of hybrid functionals were covered by two lectures by Franchini and Kresse. Szunyogh gave an introduction into relativistic effects and Eriksson reported about ab-initio spin dynamics. Following these more methodological lectures applications were presented which covered Verwey transitions (Blaha), magnetism on grain boundaries (Sob), magnetism from non-magnetic elements (Arita), Magnetic nanostructures on surfaces (Lounis), and in low dimensional systems (Eyert). The field of magnetism in biological systems was covered by a lecture about magnetic ordering in porphyrin molecules (Panchmatia). Turek reported about spin-polarized transport and Kudrnovsky about DMS. The magnetism of small aggregates was discussed for Mn-nanostructures (Zeleny) and transition-metal dimers and ad-atoms (Blonski). Finally Khmelevskyi tried to remove the aura of micraculousity from the old and ever new Invar problem. All participants were invited to present their own work so that we ended up with 10 posters, which had to be presented as a micro-poster-presentation to the full audience (micro-poster-presentation means that any poster has to be introduced within 3 minutes by showing not more that 2 slides, just enough to raise the interest). The social part of the program included all lunches and coffee breaks as well as the conference dinner. Although Vienna has also a high touristic appeal, the meeting remained very well attended until the very end and was regarded as highly interesting and useful to all participants.

PROGRAMME

Thursday, 16.April 2009

8.30 Registration

9.00-9.05 Hafner: Welcome address

9.05-9.50 Mohn: Magnetism and electronic structure (LDA).

9.50-10.35 Hilscher: Basic aspects of magnetic measurements.

10.35-11.00 Coffee break

11.00-11.45 Michor: Thermodynamic measurements in magnetic systems; specific heat, dilatometry, and alike

11.45-12.30 Šob: Magnetism on grain boundaries.

12.30-13.30 Lunch

13.30-14.15 Stöger-Pollach: Detection of magnetic properties on the nanometer scale.

14.15-15.00 Leifer: Probing the electronic nanocosmos in the electron microscope: Measurements in semiconductor quantum structures and magnetic materials.

15.00-15.30 Coffee break

15.30-16.15 Blaha: Magnetic and charge order phase transition in $YBaFe_2O_5$ (Verwey transition)

16.15-17.00 Dedkov: Spin-resolved photoelectron spectroscopy of magnetic objects: Principles and recent applications.

Friday, 17.April 2009

9.00-9.45 Held: Dynamical Mean Field Theory (DMFT) and applications.

9.45-10.30 Franchini: Magnetism in metal oxides by post-DFT methods.

10.30-11.00 Coffee break

11.00-11.45 Kresse: Hybrid functionals: Dilute Magnetic Semiconductors.

11.45-12.30 Lounis: Magnetic Nanostructures on Surfaces.

12.30-13.30 Lunch

13.30-14.15 Arita: Theoretical materials design of ferromagnets comprising non-magnetic elements.

14.15-15.00 Szunyogh: Spin-orbit induced phenomena in nanomagnetism.

15.00-15.30 Coffee break

15.30-16.15 Havela: 5f magnetism and its specific features.

16.15-17.00 Shick: Electronic structure and spectral properties of actinides: f-electron challenge.

17.00-17.45 Panchmatia: Substrate induced magnetic ordering and switching of the metal centre in porphyrin molecules, for application in Spintronics.

18.00-19.00 Poster micro presentation followed by postersession.

19.15- Conference Dinner

Saturday, 18.April 2009

9.00-9.45 Eriksson: Atomistic spin-dynamics.

9.45-10.30 Rotter: Magnetic neutron scattering.

10.30-11.00 Coffee break

11.00-11.45 Turek: Spin-polarized transport properties of bulk and layered systems.

11.45-12.30 Kudrnovsky: Electronic, magnetic, and tranport properties of diluted magnetic semiconductors: (Ga,Mn)As as a case study.

12.30-13.30 Lunch

13.30-14.15 Eyert: Magnetism in low-dimensional systems; From frustration to complex order.

14.15-15.00 Zeleny: Noncollinear magnetism in Mn nanostructures.

15.00-15.30 Coffee break

15.30-16.15 Blonski: Magnetic anisotropy of transition-metal dimers and isolated adatoms on non-magnetic substrates.

16.15-17.00 Khmelevskyi: Theory of magnetostriction in Invar materials.

NOTE *Most of the presentations can be dowloaded as ppt or pdf from the www-page given above!*

POSTER PRESENTATIONS

Ali Al-Zubi: Complex magnetism of Fe monolayers on hexagonal substrates.

Giovanni Barcaro, Alessandro Fortunelli and Falko Netzer: Theoretical analysis of the Kondo effect in Cobalt atoms adsorbed on Cu surfaces.

Katarzyna A. Kacprzak, Lauri Lehtovaara, Jaako Akola, Olga Lopez-Acevedo, Hannu Häkkinen: Electronic structure effects of a palladium impurity in a thiolate protected gold cluster.

Alessio Meyer and R. Dovesi: Magnetic interactions in $Ca_3Y_2G_3O_{12}$ garnets from first principles (Y= Cr, Fe; G= Si, Ge).

Robert Hammerling: High magnetic multipole moments from ab-initio calculations.

Josef Redinger and Peter Mohn: An interface between two non-magnetic metals turns magnetic: The case of YCo_2 (111)/Cu(111).

Lucas Fernández Seivane, Diego Carrascal and Jaime Ferrer: Magnetism and magnetic anisotropies of small structures containing 5d atoms.

A. Uldry, M. Samaras, R. Iglesias, M. Victoria, W. Hoffelner: From Iron-Chromium to Steel.

Andrei Reyes-Huamantinco, Andrei Ruban, Peter Puschnig, and Claudia Ambrosch-Draxl: Temperature dependence of the stacking fault energy in the Fe-22.5at% Mn alloy: An ab-initio study.

V. Drchal, J. Kudrnovsky, and I. Turek: Electronic, magnetic, and transport properties of semi-Heusler (Cu,Ni)MnSb alloys.

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3.1.3 Workshop on Quantum Theory of Solids, QTS-5

Aarhus University, Aarhus, Denmark
May 18-20, 2009

Organized by: N. E. Christensen and A. Svane

The workshop took place on Monday-Wednesday May 18-20 at the Aarhus University conference center. The aim of the workshop was to bring together research experts in correlation effects in solids. Physics covered by the talks include superconductivity, phonons, magnetism, electron localization, excitons, van der Waals interactions, ferro- and thermo-electrics, and scintillators. Techniques being discussed included dynamical mean field theory, self-interaction corrections, hybrid functionals, renormalized band theory, GW, Bethe-Salpeter equations, LDA+U, and disordered local moments, and systems considered included oxides and oxide surfaces, iron pnictides, fullerenes, Heusler alloys, semiconductors, and rare-earth and actinide compounds. The talks stimulated a lot of discussion and debates, which went far into the coffee and lunch breaks.

Program

	Monday 18/5
8:15-8:30	N. E. Christensen, *Opening of Meeting*
8:30-9:10	O. Gunnarsson, *Electron-phonon coupling in correlated systems*
9:10-9:50	E. K. U. Gross, *Ab-initio theory of Superconductivity*
9:50-10:30	S. Savrasov, *Electronic and exchange interactions in superconducting pnictides*
10:30-11:00	Coffee
11:00-11:40	W. R. L. Lambrecht, *Electronic structure, magnetism and phonons in RE nitrides, Gd pnictides and Eu chalcogenides*
11:40-12:20	A. Postnikov, *Impurity vibration modes in semiconductors*
12:20-13:30	Lunch
13:30-14:10	O. K. Andersen, *pd Wannier functions, bands and magnetism in FeAs materials*
14:10-14:50	J. Kudrnovsky, *Electronic, magnetic, and transport properties of (Cu,Ni)MnSb Heusler alloys*
14:50-15:10	Coffee
15:10-15:50	L. Errico, *Fe doped* TiO_2 *and* SnO_2*: Local structure and magnetic behaviour*
15:50-16:30	B. Hammer, *Modeling the surface reactivity of bulk-reduced rutile* TiO_2
16:30-17:10	S. Satpathy, *Electronic structure of the perovskite oxide interfaces*
17:20-19:00	Poster Session

Tuesday 19/5

8:30- 9:10	M. van Schilfgaarde, *Magnetic exchange interactions in the quasiparticle self-consistent GW approximation*
9:10- 9:50	M. Lüders, *The flavours of SIC*
9:50-10:30	W. M. Temmerman, *Disordered local magnetic moments in 3d-monoxides and heavy 4fs*
10:30-11:00	Coffee
11:00-11:40	S. Biermann, *Electronic correlations from a dynamical mean field perspective*
11:40-12:20	R. C. Albers, *DMFT Electronic Structure Calculations: Fact or Fiction*
12:20-13:30	Lunch
13:30-14:10	O. Eriksson, *Data Mining electronic structures for new materials*
14:10-14:50	M. Gatti, *Understanding correlations in* VO_2 *from first principles*
14:50-15:10	Coffee
15:10-15:50	P. M. Oppeneer, *Electronic structure of* URu_2Si_2 *and correlated Pu materials*
15:50-16:30	C. Ambrosch-Draxl, *Strongly bound electron-hole pairs*
16:30-17:10	R. Laskowski, *BSE and LDA+U calculations for delafossites and ZnO*
17:10-17:50	V. Antonov, *Electronic structure and x-ray magnetic circular dichroism in* $CeFe_2$
18:30	Bus departure for conference dinner

Wednesday 20/5

8:30- 9:10	G. Zwicknagl, *Heavy quaiparticles, instabilities and co-operative phenomena in f-electron systems*
9:10- 9:50	P. Hyldgaard, *Van der Waals interactions in sparse matter*
9:50-10:30	M. Alouani, *Tunneling magnetiresistance of Fe/MgO/Fe junctions*
10:30-11:00	Coffee
11:00-11:40	J. Frantti, *Polarisation rotation in ferroelectrics*
11:40-12:20	L. Nordström, *Polarisations of transition metals*
12:20-13:30	Lunch
13:30-14:10	E. A. Kotomin, *Hybrid functional calculations of point defects in perovskites*
14:10-14:50	K. Köpernik, *Recent applications of LSDA+U: An analysis of the method*
14:50-15:10	Coffee
15:10-15:50	L. Petit, *Large scale predictive calculations of materials properties*
15:50-16:30	G. K. H. Madsen, *Electronic structure theory of thermoelectric materials*
16:30-17:10	A. Svane, *Actinides: Total energy and GW calculations*

List of Participants

R. C. Albers (Los Alamos)	M. Alouani (Strasbourg)	C. Ambrosch-Draxl (Loeben)
O. K. Andersen (Stuttgart)	V. Antonov (Stuttgart)	S. Biermann (Palaiseau)
N. E. Christensen (Aarhus)	O. Eriksson (Uppsala)	L. Errico (La Plata)
J. Frantti (Helsinki)	Y. Fujoka (Helsinki)	M. Gatti (Palaiseau)
I. Gorczyca (Warsaw)	E. K. U. Gross (Berlin)	O. Gunnarsson (Stuttgart)

B. Hammer (Aarhus)	P. Hyldgaard (Chalmers)	H. H. Kristoffersen (Aarhus)
K. Köpernik (Dresden)	E. Kotomin (Stuttgart)	J. Kudrnovsky (Prague)
W. R. L. Lambrecht (Cleveland)	R. Laskowski (Wien)	M. Lüders (Daresbury)
G. K. H. Madsen (Aarhus)	J. Martinez (La Plata)	L. Nordström (Uppsala)
D. L. Novikov (East Hartford)	P. M. Oppeneer (Uppsala)	L. Petit (Aarhus)
A. Postnikov (Metz)	S. Sathpathy (Colombia)	S. Savrasov (Davis)
M. van Schilfgaarde (Tempe)	J. Stausholm-Møller (Aarhus)	A. Svane (Aarhus)
Z. Szotek (Daresbury)	W. Temmerman (Daresbury)	G. Zwicknagl (Braunschweig)

See details of program and abstracts of contributions on the Psi-k portal or on:
http://www.phys.au.dk/qts5/

3.2 Announcements of Psi-k Supported Workshops

3.2.1 KKR and Spectroscopy – Hands-on Course 2009

Ludwig-Maximilians-Universität München

June 24-26, 2009

Psi-k, German Federal Ministry of Education and Research

H. Ebert and W.M. Temmerman

http://olymp.phys.chemie.uni-muenchen.de/ak/ebert/workshops/2009/KKRHOC2009/

The purpose of this workshop is to teach theoreticians and experimentalists the use of the Munich SPR-KKR band structure and spectroscopy program package. There will be interactive computer sessions guided by tutors in the morning where people can gain experience and become familiar with the program package on how to calculate among other things: ground state properties of solids and surfaces, alloys, impurities, etc. as well as spectroscopic properties (XAS, EXAFS, XMO, XRS, XES, VB-XPS, CL-XPS, MCP, APS, AES, etc.). In the afternoon there will be lectures given by experts in the field. The code will be available free of charge after signing a license agreement.

List of speakers:

J. Honolka, H. Ebert, W. M. Temmerman, G. Fecher, P. H. Dederichs, O. Šipr, W. Wurth, J. Fink and E. Engel.

Attendance fee: 70 Euros

4 General Workshop/Conference Announcements

4.1 Workshop on Nanomagnetism, Spin-Electronics and Quantum Optics (NSEQO 2009)

First Announcement

Rio de Janeiro, Brazil, November 11-13, 2009

`http://www.cbpf.br/~nseqo`

GENERAL INFORMATION

Venue

NSEQO2009 will be held at the Brazilian Center for Physics Research (CBPF), Rio de Janeiro, located within walking distance from the Sugar Loaf, and near the famous beaches of Copacabana and Ipanema.

Aim of the Conference

This interdisciplinary workshop is organized in the framework of the 2009 year of France in Brazil. It will focus on areas of research that have been the topics of long-established collaborations between France and Brazil. It will include some of the most prominent scientists in the field, in particular, Prof. A. Fert, recent Nobel Prize winner. The workshop will also celebrate the 60th anniversary of the foundation of the CBPF (Centro Brasileiro de Pesquisas Fsicas).

The workshop will bring together scientists in the field of Nanomagnetism, Spin Electronics and Quantum optics from different parts of the world. It is hoped that the workshop will also stimulate new collaborations between France and Brazil.

Workshop Format

The workshop will essentially consist of invited presentations. It will include oral sessions and one poster session. To favor fruitful exchanges between the participants from different areas, the sessions themselves will preserve the interdisciplinary character of the whole workshop.

Topics

Contributions are invited in the following areas:

- Giant magnetoresistive and giant magnetoimpedance materials

- Micromagnetism, magnetization processes and magnetic viscosity at the nanoscale

- Nanostructures, surfaces and interfaces

- Cavity quantum electrodynamics
- Correlated photons and light beams
- Cold atoms

Working language

The working language of the Workshop is English.

Organizing Committee

A. P. Guimarães (CBPF, Brazil) Chair
J.-E. Wegrowe (École Polytechnique, France) Co-chair
D. Givord (Institut Néel, France)
G. Cernicchiaro (CBPF, Brazil) Secretary
L. C. Sampaio (CBPF, Brazil) Treasurer

Quantum Optics Program Committee/Brazil

Vanderley Bagnato (USP-SC)
Sebastião de Pádua (UFMG)
Paulo H.S. Ribeiro (UFRJ)
José Tabosa (UFPE)

Nanomagnetism and Spin-Electronics Program Committee/Brazil

Antonio Azevedo (UFPE)
Mario Baibich (UFRGS)
Roberto Bechara Muniz (UFF)
Waldemar Macedo (CDTN)
Jean-Yves Bigot (IPCMS, Strasbourg)
Jean Dalibart (LKB, ENS, Paris)
Elisabeth Giaccobino (LKB, Jussieu, Paris)
Dominique Givord (Institut Néel, Grenoble)
Frédéric Petroff (Unité de Physique CNRS/Thalès, Palaiseau)

Invited Speakers/France

A. Aspect (LCFIO, Orsay)
A. Barthélémy (Unité de Physique CNRS-Thalès, Palaiseau)
A. Bramati (LKB, Jussieu)
J.Y. Bigot (IPCMS, Strasbourg) (confirmed)
C. Chappert (IEF, Orsay) (confirmed)
B. Chatel (LCAR, Toulouse) (confirmed)
M. Dyakonov (LPTA, Montpellier) (confirmed)
A. Fert (Unité de Physique CNRS-Thalès, Palaiseau) (confirmed)

J.C. Garreau (PhLam, Villeneuve d'Ascq)
S. Haroche (Collège de France et LKB, ENS)
W. Wernsdorfer (Institut Néel, Grenoble)

Invited Speakers/Brazil (confirmed)

J. d'Albuquerque e Castro (UFRJ, Rio de Janeiro)
L. Andrade (IPEN, São Paulo)
V. Bagnato (USP, São Carlos)
A. Z. Khoury (UFF, Niteri)
C. Monken (UFMG, Belo Horizonte)
M. Nussenzveig (UFRJ, Rio de Janeiro)
S. M. Rezende (UFPE, Recife)
P. S. Ribeiro (UFRJ, Rio de Janeiro)
L. C. Sampaio (CBPF, Rio de Janeiro)

Abstracts

The instructions for the preparation and submission of abstracts will be available in the forthcoming announcements.

Registration

Those interested in receiving the next announcements should fill in the registration form at the conference homepage at

`http://www.cbpf.br/~nseqo`

Participant - Early Registration US$ 170
Full Registration US$ 200

Student - Early Registration US$ 80
Full Registration US$ 100

Accommodation

There is an ample choice of Hotel accommodations around the Conference venue. Details will be available at the homepage. Reservations and queries should be made through the agency Metatron Viagens (metatron@rioturismo.com, Phone +55 (21) 2524-8773 and +55 (21) 2524-5851, http://www.rioturismoeventos.com)

Transportation

Rio de Janeiro is served by most major airlines.

Passport and Visa Requirements

Most participants will only need a valid passport. However, a tourist visa will be necessary for citizens of some countries. In this case, the visa can be obtained from the Brazilian Consulate. Participants should ask their travel agents whether or not nationals from their country require a visa.

Social activities

November 10 (Tuesday) 18:00 – Cocktail reception

November 12 (Thursday) 17:30 – Snacks and Brazilian Music at the Urca Hill.

Important Dates

May 15, 2009: Abstract submission opens

June 15, 2009: Deadline for abstract submission, pre-registration and application for support

August 15, 2009: Announcement of abstract acceptance

September 10, 2009: Deadline for early registration and lower fee and hotel rate

Publication

The submitted contributions will not be published. The abstracts will be available through the program book.

Contact

NSEQO 2009 / CBPF
Rua Dr. Xavier Sigaud, 150 - Urca
Rio de Janeiro - RJ - Brazil
CEP: 22290-180

Phone / Fax: +55 (21) 2141-7274

E-mail: nseqo@cbpf.br

We look forward to seeing you in Rio in November.

A. P. Guimarães

5 General Job Announcements

Ph. D. Position in theoretical spin transport/spin-injection in semiconductors

Department of Physics, University of York, York, UK

Public demand for increasingly faster and smaller electronic devices, such as computers, requires that more and even smaller transistors are packed on every chip. This has led to the birth of nanotechnology and, more recently of the nanotechnology field called 'spintronics'. Here not only the charge, but also the spin – another fundamental property of electrons and holes – is used to design device functionalities. Among the potential benefits of spintronics devices is the possibility of computers in which the same unit is used for computation and storage, of lower power consumption, of miniaturisation, and more generally the possibility of designing conceptually new devices which mix old functionalities with completely new ones.

The basis of spintronics is understanding the spin dynamics. Unfortunately key issues such as how to inject a current of spins in a semiconductor, how to sustain it across the interfaces of the different materials forming the devices, which materials/nanostructures are best and what lengths a current of spin can travel in a specific material are still open questions.

This project aims to master the principles underlying the spin dynamics, with particular attention to applications such as nanocircuits and their components. Objectives are to fully understand spin transport, diffusion and injection into semiconductors. These properties are fundamental for developing semiconductor and hybrid (metal/semiconductor) spintronics devices.

This is an EPSRC-funded studentship, with a stipend in line with EPSRC directions. The studentship is fully funded for EU nationals only.

We are looking for highly motivated students, possibly with a background in solid state physics and good computational skills.

For more details please contact Dr Irene D'Amico (`http://www-users.york.ac.uk/~ida500`), ida500@york.ac.uk.

For applications follow the instructions at

`http://www.york.ac.uk/depts/phys/jobvacs/phd_stsis.htm`

Applications will be accepted until the position is filled.

Post-Doc/Research Professor Positions in Computational Nano-Bio Physics (WCU)

KAIST, Daejeon, Korea

We, Prof. Yong-Hyun Kim's group at KAIST (see http://www.nrel.gov/cms/yong.html), invite applications for one or two theoretical postdoctoral/research professor positions, available immediately. Initial assignment is for a year, but renewable upon funding availability, performance, and mutual agreement up to a total of three years. Research direction will be, but not limited to, one of the followings:

(1) Computational design of energy storage materials: Hydrogen and battery
(2) Development of first-principles van der Waals potentials
(3) Molecular dynamics
(4) Proteins
(5) Carbon nanostructures

The starting salary will be KRW 30-45M/year depending on the qualification. Candidate should send curriculum vitae including research interest and a list of publications, and arrange two or three reference e-mail letters to:

Yong-Hyun Kim
yong.hyun.kim at kaist.ac.kr or yong.hyun.kim at nrel.gov

Graduate School of Nanoscience and Technology (WCU)
KAIST
Daejeon 305-701, Korea

International PhD Program and Post Doc Position
University of Salerno, Italy

a) Ph.D. Position in Nanoscience and Nanotechnology International PhD Program in Nanoscience and Nanotechnology at University of Salerno

From the point of view of learning and education the aim of the PhD Program is the development of professional skills suitable for the peculiar subject. Problems connected to scientific research in the field of Nanoscience and Nanotechnology are difficult to approach if one is confined in the classical Faculty and/or Department boundaries. These needings led to the creation of `NANO_MATES`, the Interdisciplinary Center for Nanoscience and Nanotechnology, promoting the present International PhD Program in Nanoscience e Nanotecnology. The program is coordinated by University of Salerno and Jacobs University Bremen Several positions will be available soon.

Research Topics:

The main scientific topics of the PhD program are outlined below:

-Nanostructured Materials:

Development of materials by syntesis and/or nanofabrication techniques: new bottom-up and top-down approaches; nanostructuration in biological systems.

-Characterization Techniques of Nanostructures

Application and development of techniques for characterization of nanostructured materials. Surface properties. Electric and electromagnetical properties. Optical properties. Functional Characterization.

-Simulations and Theory

Development and application of theoretical and simulation approaches for nanostructured materials and for novel devices based on nanostructured materials. Coarse-Graining and Multiscale simulations. -Novel Devices Development and characterization of new devices.

To have more information about the Program and the selection process contact the PhD coordinator Dr. Giuseppe Milano

e-mail: gmilano@unisa.it
webpage: http://www.molnac.unisa.it/
visit the PhD Program web page:

http://www.nanophd.unisa.it

b) An exceptional Post Doc candidate is required to carry out a research project in the group of Dr. Giuseppe Milano at University of Salerno

The project involves the development and application of new molecular simulation methods at atomistic and coarse-grained level to soft matter. Experience in modifying and writing Molecular Dynamics and/or Monte Carlo codes (not simply using packages) is required. The appointment is for one year with the possibility of a yearly renewalthereafter. The research group has good computational facilities, and friendly atmosphere. Computational facilities at Molnac include local workstations, two beowulf cluster, and access to large computer resources via membership at the main supercomputer centres in Europe. Please send a CV and names of 3 references to Dr. Giuseppe Milano (gmilano@unisa.it).

Dr. Giuseppe Milano
Assistant Professor
Dept. of Chemistry University of Salerno
Phone: +39 089 969567
Fax: +39 089 969603
e-mail: gmilano@unisa.it

Postdoctoral Position in Computational Materials Science
Nanoscience Center, University of Jyväskylä, Finland

Research area: Density functional / molecular dynamics simulations of amorphous semiconductor materials

The new materials modeling group of Dr Jaakko Akola at the Nanoscience Center (NSC, Univ. of Jyväskylä) is seeking a postdoctoral fellow. The position is funded by the Academy of Finland and is coupled to the Finnish-Japanese program on Functional Materials. The main emphasis will be on large scale density functional (DF) / molecular dynamics (MD) simulations of amorphous phase-change materials (PCMs) that are used as recording layers in optical recording (DVD-RAM, Blu-ray Disc, DVD-RW). The project involves close collaboration with Japanese experimental colleagues at SPring-8 (synchrotron facility), Yamagata University, and the research division at Panasonic. The extensive DF/MD simulations will be performed at the Finnish IT Center for Science (CSC) and Forschungszentrum Jülich, Germany, in collaboration with Dr Robert O. Jones (FZ Jülich).

Recording layers of contemporary digital versatile disk (DVD) media are based on PCMs, which utilize rapid and reversible phase transitions between the amorphous and crystalline phases of nanosized spots on a polycrystalline film. Differences between the optical contrast and electrical resistivity of the two phases allow one to identify the state. Many crystalline materials amorphize rapidly but the need for rapid recrystallization eliminates most of them for optical storage purposes. For scientists, the structure of the amorphous phase of PCMs poses the main problem and is difficult to tackle both experimentally and theoretically. I have worked on this topic with Dr R.O. Jones for several years by performing massively-parallel DF/MD simulations which mimic the experimental melt-quench process for amorphization (see, e.g., J. Akola and R.O. Jones, Phys. Rev. B **79**, 134118 (2009)). Recently, we have discovered that DF/MD simulations combined with the experimental x-ray diffraction and neutron scattering data of our Japanese partners can lead to a successful description of the amorphous phase, and this will comprise the core for future collaboration.

Applicants are expected to have a strong background in computational physics and/or chemistry, density functional methods, as well as programming experience. The starting date can be flexible during the fall 2009 or January 2010. The initial contract will be for one year but can be extended for another year upon mutual agreement.

Interested candidates should send their curriculum vitae, list of publications, and arrange to have one to three references sent to:

Jaakko Akola
Nanoscience Center, Department of Physics
P.O. Box 35
FI-40014 University of Jyväskylä
Finland

Further information can be obtained via email: jaakko.akola@phys.jyu.fi and under
`http://iffwww.iff.kfa-juelich.de/~jeakola/J.Akola.shtml`.

6 Abstracts

Structural phase transitions and fundamental band gaps of $Mg_xZn_{1-x}O$ alloys from first principles

I. V. Maznichenko[1], A. Ernst[2], M. Bouhassoune[2,3], J. Henk[2], M. Däne[1,4], M. Lüders[5], P. Bruno[2,6], W. Hergert[1], I. Mertig[1,2], Z. Szotek[5], W. M. Temmerman[5]

[1]*Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06099 Halle, Germany*

[2]*Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany*

[3]*Department Physik, Universitt Paderborn, 33095 Paderborn, Germany*

[4]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

[5]*Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK*

[6]*European Synchrotron Radiation Facility – BP 220, F-38043 Grenoble Cedex, France*

Abstract

The structural phase transitions and the fundamental band gaps of $Mg_xZn_{1-x}O$ alloys are investigated by detailed first-principles calculations in the entire range of Mg concentrations x, applying a multiple-scattering theoretical approach (Korringa-Kohn-Rostoker method). Disordered alloys are treated within the coherent potential approximation (CPA). The calculations for various crystal phases have given rise to a phase diagram in good agreement with experiments and other theoretical approaches. The phase transition from the wurtzite to the rock-salt structure is predicted at the Mg concentration of $x = 0.33$, which is close to the experimental value of $0.33 - 0.40$. The fundamental band gap, typically underestimated by the local density approximation, is considerably improved by the self-interaction correction. The increase of the gap upon alloying ZnO with Mg corroborates experimental trends. Our findings are relevant for applications in optical, electrical, and in particular in magnetoelectric devices.

(Submitted to Phys. Rev. B)

Contact person: aernst@mpi-halle.de

Groundstate electronic structure of actinide monocarbides and mononitrides

L. Petit, A. Svane
Department of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark
Z. Szotek, W. M. Temmerman
Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK
G. M. Stocks
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Abstract

The self-interaction corrected (SIC) local spin-density approximation (LSD) is used to investigate the groundstate valency configuration of the actinide ions in the actinide monocarbides, AC (A = U, Np, Pu, Am, Cm), and the actinide mono-nitrides, AN. The electronic structure is characterized by a gradually increasing degree of f-electron localization from U to Cm, with the tendency towards localization being slightly stronger in the (more ionic) nitrides compared to the (more covalent) carbides. The itinerant band-picture is found to be adequate for UC and acceptable for UN, whilst a more complex manifold of competing localized and delocalized f-electron configurations underlies the groundstates of NpC, PuC, AmC, NpN, and PuN. The fully localized $5f$-electron configuration is realized in CmC (f^7), CmN (f^7), and AmN (f^6). The observed sudden increase in lattice parameter from PuN to AmN is found to be related to the localization transition. The calculated valence electron densities of states are in good agreement with photoemission data.

(Submitted to Phys. Rev. B)
Contact person: lpetit@phys.au.dk

First-principles study of the effect of Fe impurities in MgO at geophysically relevant pressures

Donat J. Adams
Department of Materials Sciences, Laboratory of Crystallography, ETH Zürich, Switzerland
Walter M. Temmerman and Zdzislawa Szotek
STFC, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U. K.

Abstract

The self-interaction corrected local spin density (SIC-LSD) formalism and the standard GGA treatment of the exchange-correlation energy have been applied to study the collapse of the magnetic moment of Fe impurities in MgO. The system $Mg_{1-x}Fe_xO$ is believed to be the second most abundant mineral in the Earth's lower mantle and is therefore geophysically relevant. We confirm the experimentally found increase of the critical pressure upon iron concentration. Our calculations using standard GGA for a fixed Fe concentration show that different arrangements of Fe atoms can remarkably shift the transition pressure of the HS-LS transition. This could explain the experimentally found broad transition regions. Our results indicate that the HS-LS transition in $Mg_{1-x}Fe_xO$ is first order. We find that SIC-LSD fails to predict the divalent Fe configuration as the lowest energy configuration and discuss possible reasons for it.

(Submitted to Phys. Rev. B)
Contact person: donat.adams@cea.fr

Robustness of "cut and splice" genetic algorithms in the structural optimization of atomic clusters

Vladimir A. Froltsov and Karsten Reuter
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4–6, D-14195 Berlin (Germany)

Abstract

We return to the geometry optimization problem of Lennard-Jones clusters to analyze the performance dependence of "cut and splice" genetic algorithms (GAs) on the employed population size. We generally find that admixing twinning mutation moves leads to an improved robustness of the algorithm efficiency with respect to this *a priori* unknown technical parameter. The resulting very stable performance of the corresponding mutation+mating GA implementation over a wide range of population sizes is an important feature when addressing unknown systems with computationally involved first-principles based GA sampling.

(published as: Chem. Phys. Lett. **473**, 363 (2009))
Contact person: Karsten Reuter (reuter@fhi-berlin.mpg.de)

Oxygen adsorption structures on Ag(111)

Joachim Schnadt,[1,2] Jan Knudsen,[2] Xiao Liang Hu,[3] Angelos Michaelides,[3]
Ronnie T. Vang,[2] Karsten Reuter,[4] Zheshen Li,[5] Erik Laegsgaard,[2]
Matthias Scheffler,[4] and Flemming Besenbacher[2]

[1]*Division of Synchrotron Radiation Research, Department of Physics, Lund University, Box 118, 221 00 Lund, Sweden*

[2]*Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, University of Aarhus, Building 1521, Ny Munkegade, 8000 Aarhus C, Denmark*

[3]*London Centre for Nanotechnology and Department of Chemistry, University College London, London WC1E 6BT, UK*

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

[5]*Institute for Storage Ring Facilities at the University of Aarhus (ISA), Building 1525, Ny Munkegade, 8000 Aarhus C, Denmark*

Abstract

The oxidized Ag(111) surface has been studied by a combination of experimental and theoretical methods, scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS), and density functional theory (DFT). A large variety of different surface structures is found, depending on the detailed preparation conditions. The observed structures fall into four classes: (a) individually chemisorbed atomic oxygen atoms, (b) three different oxygen overlayer structures, including the well-known $p(4\times4)$ phase, formed from the same Ag_6 and Ag_{10} building blocks, (c) a new $c(4\times8)$ structure not previously observed, and (d) at higher oxygen coverages structures characterized by stripes along the high-symmetry directions of the Ag(111) substrate. Our analysis provides a detailed explanation of the atomic-scale geometry of the Ag_6/Ag_{10} building block structures, and the $c(4\times8)$ and stripe structures are discussed in detail. The observation of many different and co-existing structures implies that the O/Ag(111) system is characterized by a significantly larger degree of complexity than previously anticipated, and this will impact our understanding of oxidation catalysis processes on Ag catalysts.

(submitted to: Phys. Rev. B)

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

Exploring the random phase approximation: applicaton to CO adsorbed on Cu(111)

Xinguo Ren[1], Patrick Rinke[1,2], Matthias Scheffler[1,2,3]

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

[2]*Materials Department, University of California, Santa Barbara, CA 93106, USA*

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Abstract

The adsorption of CO on the Cu(111) surface is investigated in the random-phase approximation (RPA) as formulated within the adiabatic connection fluctuation-dissipation (ACFD) theorem. The RPA adsorption energy is obtained by adding a "local XC correction", that is extrapolated from cluster calculations of increasing size, to the PBE value for the extended system. In comparison to density functional theory calculations with the generalized gradient functionals PBE and AM05 and the hybrid functionals PBE0 and HSE03, we find a hierarchy of improved performance from AM05/PBE to PBE0/HSE03, and from PBE0/HSE03 to RPA, both in terms of the absolute adsorption energy as well as the adsorption energy difference between the atop and hollow fcc sites. In particular the very weak atop site preference at the PBE0/HSE03 level is further stabilized by about 0.2 eV in the RPA. The mechanism behind this improvement is analyzed in terms of the *GW* density of states, that gives a spectral representation en par with the RPA formalism for the total energy.

(submitted to: Phys. Rev. B)

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A metal-free, polymeric photocatalyst for hydrogen production from water under visible light

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Abstract

The production of hydrogen from water using a catalyst and solar energy is an ideal future energy source, independent of fossil reserves. For an economical use of water and solar energy, catalysts that are sufficiently efficient, stable, inexpensive, and capable of harvesting light are required. Here, we show that an abundant material, polymeric carbon nitride, can produce hydrogen from water under visible-light irradiation in the presence of a sacrifacial donor. Contrary other conducting polymers semiconductors, carbon nitride is chemically and thermally stable and does not rely on complicate device manufacturing. The results represent an important first step towards photosynthesis in general where artificial conjugated polymer semiconductors can be used as energy transducers.

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Two-step mechanism for low temperature oxidation of vacancies in graphene

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Abstract

We have studied the oxidation of vacancies in graphene by *ab-initio* atomistic thermodynamics to identify the dominant reaction mechanisms. Our calculations show that the low temperature oxidation occurs via a two step process: vacancies are initially saturated by stable O-groups, such as ether (C-O-C) and carbonyl (C=O). The etching is activated by a second step of additional O_2 adsorption at the ether groups, forming larger O-groups, such as lactone (C-O-C=O) and anhydride (O=C-O-C=O), that may desorb as CO_2 just above room temperature. Our studies show that the partial pressure of oxygen is an important external parameter that affects the mechanisms of oxidation and that allows us to control the extent of etching.

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Atomic processes in molecular beam epitaxy on strained InAs(137): A density-functional theory study

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Abstract

The atomic processes in molecular beam epitaxy of InAs on the InAs(137) surface are investigated by means of first-principles total-energy calculations. We consider layer-by-layer growth on InAs(137) facets as a typical process during the evolution of shallow InAs islands in the Stranski- Krastanov growth mode of InAs on GaAs that is exploited for the self-assembly of heteroepitaxial quantum dots. From the calculated energetics we conclude that a growth scenario where an As_2 molecule adsorbs on a single In adatom, followed by capture of another In adatom, is most likely. Moreover, our calculations of the potential-energy surface for In adatoms on the InAs(137) surface show that In adatoms are highly mobile. Surface diffusion on InAs(137) is found to be almost isotropic with energy barriers < 0.3 eV for adatom hopping. Aiming at an understanding of the growth processes at the strained side facets of quantum dots, we extend our calculations to isotropically strained InAs(137) facets. It is found that the compressive strain present on side facets of shallow InAs islands on GaAs leads to a considerable lowering of the binding energy of In adatoms. The height of diffusion barriers is found to be less affected by the strain. Most importantly, the intermediate species consisting of an In adatom plus an adsorbed As_2 molecule is destabilized by compressive strain in excess of -5%. This finding leads us to the conclusion that layer growth on InAs(137) facets ceases in highly strained regions of InAs islands on GaAs, in line with the observed shape evolution of such islands.

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Long-Range Magnetic Interactions Induced by the Lattice Distortions and the Origin of the E-type Antiferromagnetic Phase in the Undoped Orthorhombic Manganites

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Abstract

With the increase of the lattice distortion, the orthorhombic manganites $R\mathrm{MnO_3}$ (R= La, Pr, Nd, Tb, and Ho) are known to undergo the phase transition from the layered A-type antiferromagnetic (AFM) state to the zigzag E-type AFM state. We consider the microscopic origin of this transition. Our approach consists of the two parts. First, we construct an effective low-energy model for the manganese 3d-bands and derive parameters of this model from the first-principles electronic structure calculations. Then, we solve this model in the Hartree-Fock approximation (HFA) and analyze the behavior of the interatomic magnetic interactions. We argue that the nearest-neighbor interactions decrease with the increase of the distortion and at certain stage start to compete with the longer range (particularly, second- and third-neighbor) AFM interactions in the orthorhombic **ab**-plane, which trigger the formation of the E-phase. The origin of these interactions is closely related to the orbital ordering, which takes place in the distorted orthorhombic structure. The model is able to capture the main experimental trends and explain why $\mathrm{LaMnO_3}$ develops the A-type AFM order and why it tends to transform to the E-type AFM order in the more distorted compounds. Nevertheless, the quantitative agreement with the experimental data crucially depends on other factors, such as the magnetic polarization of the oxygen sites as well as the correlation interactions beyond HFA.

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Enhanced effective mass in doped $SrTiO_3$ and related perovskites

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Abstract

The effective mass is one of the main factors determining the Seebeck coefficient and electrical conductivity of thermo-electrics. In this ab-initio LDA-GGA study the effective mass is estimated from the curvature of electronic bands by one-band-approximation and is in excellent agreement with experimental data of Nb? and La? doped $SrTiO_3$. It is clarified that the deformation of $SrTiO_3$ crystals has a significant influence on the bandgap, effective electronic DOS- mass and band- mass, but the electronic effect due to the eg- band flattening near the Gamma-point due to Nb -doping up to 0.2 atthe effective mass; this can be explained by the different surroundings of A- and B-sites in perovskite. Substitution with other elements such s Ba on the A-site and V on the B-site in $SrTiO_3$ increases the effective mass as well.

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Density functional study of elastic and vibrational properties of the Heusler-type alloys Fe_2VAl and Fe_2VGa

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Abstract

The structural and elastic properties as well as phonon-dispersion relations of the Heusler-type alloys Fe_2VAl and Fe_2VGa are computed using density-functional and density-functional perturbation theory within the generalized-gradient approximation. The calculated equilibrium lattice constants agree well with the experimental values. The elastic constants of Fe_2VAl and Fe_2VGa are predicted for the first time. From the elastic constants the shear modulus, Young's modulus, Poisson's ratio, sound velocities and Debye temperatures are obtained. By analyzing the ratio between the bulk and shear modulii, we conclude that both Fe_2VAl and Fe_2VGa are brittle in nature. The computed phonon-dispersion relation shows that both compounds are dynamically stable in the $L1_2$ structure without any imaginary phonon frequencies. The isomer shifts of Fe in the two compounds are discussed in terms of the Fe s partial density of states, which reveal larger ionicity/less hybridization in Fe_2VGa than in Fe_2VAl. For the same reason the Cauchy pressure is negative in Fe_2VAl but positive in Fe_2VGa.

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Manuscript available from: svane@phys.au.dk

High pressure structural study of fluoro perovskite $CsCdF_3$ upto 60 GPa: A combined experimental and theoretical study

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Abstract

The structural behaviour of $CsCdF_3$ under pressure is investigated by means of theory and experiment. High-pressure powder x-ray diffraction experiments were performed up to a maximum pressure of 60 GPa using synchrotron radiation. The cubic $Pm\bar{3}m$ crystal symmetry persists throughout this pressure range. Theoretical calculations were carried out using the full-potential linear muffin-tin orbital method within the local density approximation and the generalized gradient approximation for exchange and correlation effects. The calculated ground state properties – the equilibrium lattice constant, bulk modulus and elastic constants – are in good agreement with experimental results. Under ambient conditions, $CsCdF_3$ is an indirect gap insulator with the gap increasing under pressure.

(Phys. Rev. B: submitted)

Manuscript available from: svane@phys.au.dk

7 SCIENTIFIC HIGHLIGHT OF THE MONTH: *Ab initio* Study of Magnetoelectricity in Composite Multiferroics

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Abstract

The coexistence of magnetism and ferroelectricity in the same crystalline phase of a so called multiferroic material involves the opportunity of magneto-electric coupling. Magnetoelectric coupling, however is highly attractive since it offers magnetization switching by an electric field or polarization switching by a magnetic field. Since this phenomenon, in principle, allows to store information in nanometer-sized memories with four logic states, the issues of multiferroics (MF) are of prime interest. Studies based on density functional theory have significantly contributed to this rapidly developing field of single-phase MF (see, Ψ_k Scientific Highlight 92 by S. Picozzi and C. Ederer and references therein). In such multiferroics, however, the electric polarization and magnetization interact weakly with each other while ferromagnetism disappears far below room temperature. A more robust scenario of magnetoelectricity might occur in artificial MF composed of ferromagnetic thin films which are grown epitaxially on a ferroelectric substrate. Inaccessible by conventional synthesis, composite multiferroics exhibit specific properties which are superior to those of customary materials. In the study of composite multiferroics, the results of *ab initio* calculations, reported by Tsymbal's group from Nebraska University after 2006, have shown an extremely promising direction for the next years. Although these calculations go ahead of experiment they explore the trends and basic physics of magnetoelectrics. Here, on the basis of first-principles calculations we predict that epitaxial ultrathin Fe films deposited on TiO_2-terminated (001) surface of $ATiO_3$ perovskites (A = Pb, Ba) exhibit an unexpected change in their magnetic structure with increasing Fe-film thickness. The magnetic order changes from strongly ferromagnetic for the single-monolayer-Fe system to ferrimagnetic with almost vanishing magnetization upon deposition of a second Fe layer. Ferromagnetic order is restored for thicker Fe films. This effect can be understood in terms of hybridization of electronic states and structural relaxation. Additionally, we study the effect of iron oxidation on the magnetoelectric coupling at the $Fe_2/ATiO_3(001)$ interface. The simulated oxygen coverage ranged between 0.5 and 2.0 adsorbed O atom per Fe atom, using a slab geometry. The magnetic properties of the Fe layer are gradually degraded with increasing O coverage for $c > 1.5$. However, the change in magnetization which is induced by the electric polarization reversal remains robust for all energetically favorable compositions. For instance, we show that the surface oxidation of composite MF cannot destroy the switchable magnetoelectricity.

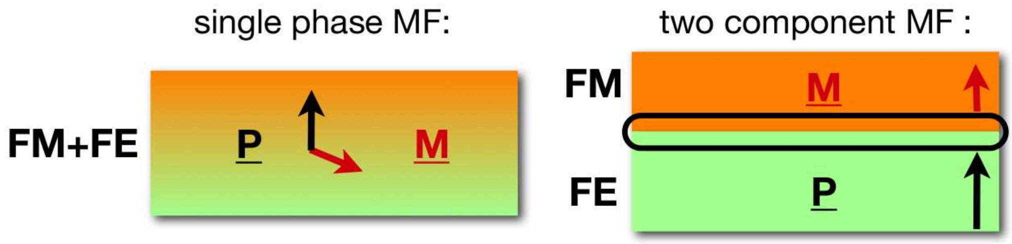

Figure 1: Single-phase and composite multiferroics are sketched in the left and right panels, respectively. In the single-phase MF, its magnetoelectricity is the volume effect while for composite multiferroic, in contrary, the ME coupling is confined to the interface area.

1 Introduction

When any two of all four primary ferroic properties, i. e., ferroelectricity, ferromagnetism, ferroelasticity, and ferrotoroidicity coexist in a so called multiferroic material (MF), its symmetry must be restricted dramatically [1]. In the absence of space-inversion and time-reversal symmetry, the occurrence of ferroelectricity and magnetism in the same phase of an MF allows the observation of both a switchable electric polarization, $\boldsymbol{P}$, and a switchable magnetization, $\boldsymbol{M}$. In principle this phenomenon allows to store information in nanometer-sized memories with four logic states [2–4].

Although some single-phase MFs, such as $BiFeO_3$ and RMnO$_3$ (R rare earths), were known since mid of the seventies [5], the search for novel multiferroics is not finished yet. Moreover, their classification has been revised [6] since 2003 when the type-II class of magnetic MF has been established. For instance, in $TbMnO_3$ ferroelectricity is caused by a particular type of magnetic order, which exists only at low temperature. In multiferroics, no matter what its class, an applied electric field, $\boldsymbol{E}$, displacing the magnetic ions, affects the magnetic exchange coupling or, vice versa, the external magnetic field, $\boldsymbol{H}$, induces the electric polarization: $P_i \sim \alpha_{ij} H_j$, where α is the magnetoelectric tensor and $i, j = x, y, z$. According to Landau theory, the linear magnetoelectric (ME) contribution to the Gibbs free energy is $E_i \alpha_{ij} H_j$. If α is sufficiently strong then $\boldsymbol{M}$ can be easily modified by $\boldsymbol{E}$. It should be kept in mind that magnetoelectricity is a volume effect for which the induction of $\boldsymbol{M}$ depends linearly on $\boldsymbol{E}$. In a type-I single-phase MF, $\boldsymbol{P}$ and $\boldsymbol{M}$ interact weakly and, therefore, α is marginal there. Besides, all multiferroics possess a hierarchy of phase transformations [7], in which ferromagnetism disappears far below room temperature. In a type-II MF, the magnitude of $\boldsymbol{P}$ is never large, which precludes strong magnetoelectricity. Obviously, the quest for fundamentally new multiferroics requires a better understanding of the mechanisms which mediate the ME coupling.

Ab initio calculations based on density functional theory (DFT) predict that a voltage of about 30 meV, applied across a $SrRuO_3/SrTiO_3$ interface, without magnetic cations, can induce a net magnetic moment [8]. Since the space-inversion symmetry is broken between the two unlike terminations, the ME effect results entirely from spin accumulation at the interface. The effect might be enhanced by the use of materials with higher spin polarization. Indeed, a more robust scenario of magnetoelectricity occurs in epitaxially grown two-phase MF consisting of ferroelectric and ferromagnetic components. The ME effect is mediated by strain across the biferroic interface. Inaccessible by conventional synthesis, the MF composites exhibit specific properties which are superior to those of customary materials. *Ab initio* studies suggest that the interface bonding is the source of strong ME coupling in Fe/BaTiO$_3$(001) [9,10]. The interfacial Ti atoms show an induced magnetic moment of about $0.3\,\mu_\mathrm{B}$. Moreover, for the two opposite directions of $\boldsymbol{P}$ ($P_\downarrow$ and $P_\uparrow$), there are rather noticeable differences of 0.1–0.2μ_B in the magnetic moments of Fe and Ti at the interface. This is a very promising phenomenon, which is entirely confined to the ferroelectric/ferromagnetic interface and which differs from the volume ME effect. The interface ME effect defines the change in magnetization at the coercive field E_c: $\mu_0 \Delta M \approx \alpha E_c$. α of about $2 \cdot 10^{-10}\,\mathrm{Gcm^2/V}$ estimated for Fe/BaTiO$_3$(001) from first principles, is two orders of magnitude larger than that predicted for SrRuO$_3$/SrTiO$_3$.

Epitaxial growth of the two-pase MF thin films of high quality continues to be very challenging. A 30 nm thick Fe(001) film has been grown recently on a ferroelectric BaTiO$_3$(001) substrate [11]. For this MF, the interface ferromagnetic resonance mode is characterized by a large out-of-plane magnetic anisotropy comparable to and of opposite in sign to the shape anisotropy, the latter favoring an in-plane easy axis for thick film interiors. The trends of magnetic anisotropy detected for Fe/BaTiO$_3$ are in a good agreement with corresponding *ab initio* calculations [10, 12]. In the case of one Fe monolayer (ML), DFT predicts that perpendicular anisotropy is favored to in-plane anisotropy by 0.72 meV (0.54 meV) per Fe atom for $P_\downarrow$ ($P_\uparrow$) [10]. Although the spin reorientation transition under switching of $\boldsymbol{P}$ is not found from first principles, the ME coupling alters the magnetocrystalline anisotropy energy by about 50 %. The magnetic order of Fe/BaTiO$_3$ can be tuned by the Fe layer thickness to ferrimagnetic with almost zero $\boldsymbol{M}$ upon deposition of a second Fe ML [10]. Ferromagnetic order is restored for Fe films thicker than 3 ML, for which the shape anisotropy energy favors in-plane alignment of $\boldsymbol{M}$ [12].

Recently, Niranjan *et al.* [13] modeling different Fe$_3$O$_4$/BaTiO$_3$(001) interfaces within DFT, have found that ME coupling is stronger for the O-deficient type of the Fe$_3$O$_4$ interface. This suggests that the presence of oxygen or oxygen vacancies at the biferroic interface plays an important role. The temperature dependent magnetization curves of epitaxial magnetite films grown on BaTiO$_3$(001) demonstrate [14] a strong perpendicular magnetic anisotropy, which is modified by the piezoelectric response of the substrate.

2 Magnetoelectric coupling in Fe/BTO

In the following we give a detailed example of the magnetoelectric coupling at an interface. For that reason we present results obtained from first-principles calculations [10]. A perfect model system for a multiferroic interface is an ATiO$_3$ (A = Ba or Pb) substrate covered with iron layers 3. Both materials are not only ferroic separately at room temperature but also as a two-component compound. The polarization of the FE substrates ranges from $26\,\mu\mathrm{C/cm^2}$ for BTO to $75\,\mu\mathrm{C/cm^2}$ for PTO; iron has a magnetic moment of $2.25\,\mu_\mathrm{B}$. More importantly, the in-plane lattice constants of the [001] surfaces of the substrates match nearly perfectly with that of iron. The mismatch $(a_\mathrm{sub} - a_\mathrm{Fe})/a_\mathrm{sub}$ is below 3 % and allows epitaxial growth of the interface, as has recently been shown experimentally [11].

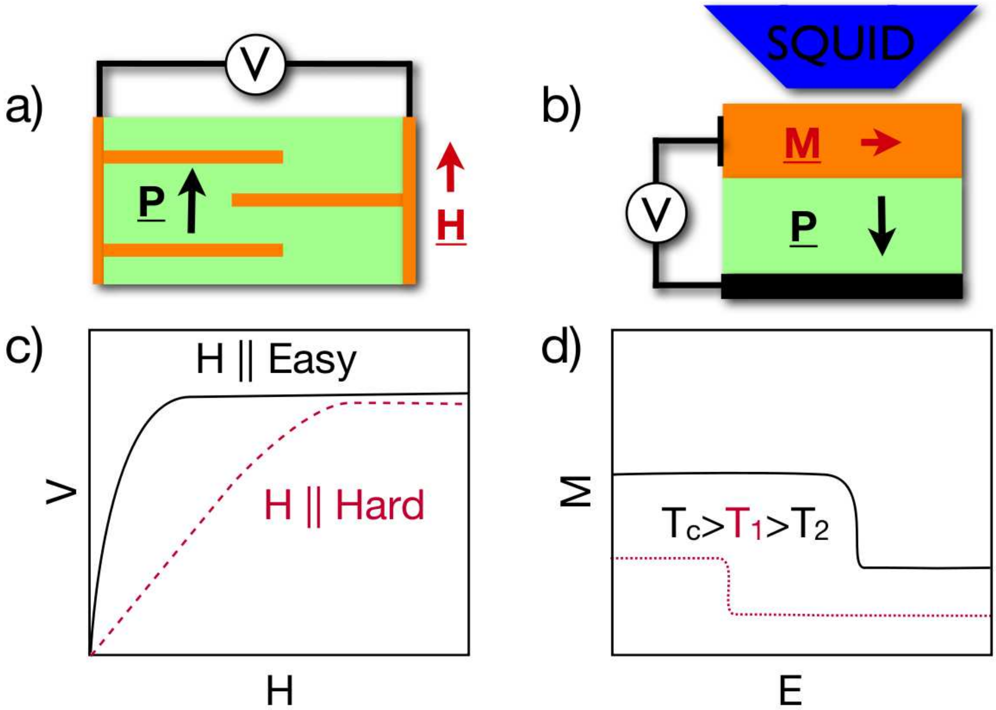

Figure 2: The schemes a and b in the upper panel show experimental setups for determining the ME coupling at biferroic interfaces. The figures below show the corresponding results of the measurements. In a) Ni contacts are embedded in a $BaTiO_3$ matrix and an applied magnetic field gives rise to a voltage change. In b) a $La_{1/3}Sr_{2/3}MnO$ film is deposited on top of a $BaTiO_3$ surface. SQUID allows the detection of the film magnetization under an applied bias. A detailed discussion of both experiments is given in [2, 15].

To treat the interplay between geometric, electronic and magnetic properties in the best way we use a multi-code approach. The geometric relaxations and magnetic properties are obtained by the Vienna Ab-initio Simulation Package (VASP) [16]. A cross-check of the magnetic structure obtained by VASP was done with the scalar-relativistic Korringa-Kohn-Rostoker (KKR) [17] method; the magnetocrystalline anisotropy was additionally computed with a relativistic layer-KKR code [18]. In all codes the local spin-density approximation (LSDA) to density-functional theory (DFT) is used. Further various quantities were carefully compared among the three computer codes to obtain consistent results. Reliability is achieved by numerous convergence tests.

At the atomic scale both materials are combined via the Fe/TiO_2 interface. The TiO_2 termination of the FE substrate was chosen since it is energetically preferable [19]. The same arguments hold for the positions of the Fe atoms which prefer to sit above the oxygen atoms. To model the change of the polarization direction the structural properties of the FE substrate have to be considered. Within the tetragonal phase the polarization of the $ATiO_3$ is caused by the displacement of the atoms along the [001] axis. It can be defined as $\delta \equiv z(\text{cation}) - z(\text{O})$. For the considered systems there exist two distinguished scenarios for the atomic displacements. If the displacement in the FE substrate is positive the polarization points towards the interface; if it is negative, the polarization points away from the interface. Both situations mimic the state after polarization switching, that is in remanence. We denote the two states corresponding their polarization directions as $P_\uparrow$ and $P_\downarrow$. For our calculation they are modeled by considering two different supercells. Both consist of 5 unit cells of $ATiO_3$ (A = Ba or Pb) covered with L monolayers of iron and separated by 2 nm of vacuum. They differ in δ, which was set to the positive bulk value for the $P_\uparrow$ state and negative for $P_\downarrow$. The structural relaxation concerns the three top layers of the $ATiO_3$ and the Fe layer until the forces are less than 5 meV/Å.Å

The magnetic and ferroelectric properties are shown in Fig. 3. On the left-hand side of Fig. 3 the unit cell of $Fe_2/TiO_2/PbTiO_3(001)$ with $P_\uparrow$ is shown. For the distance between the TiO_2 and Fe at the interface we obtained—after structural relaxation independently on the iron thickness and polarization direction—a value of $a \approx 1.8$ Å. Further compression of the surface area of $ATiO_3$, which could suppress ferroelectricity, was not found. The only structural detail which is sensitive to the number of iron layers is the distance between the first and second iron layer. In case of two layers (not shown in the figure) this distance is about 1.05 Å whereas for thicker layers it is about 1.2 Å. Later we will explain the change in the magnetic ordering caused by the structural relaxation. A detailed overview of the structure is given in [10].

At the right-hand side of Fig. 3 the two order parameters at the interface of $Fe_2/TiO_2/PbTiO_3(001)$ are shown. The unit-cell resolved polarizations were calculated by $P_i = \delta \cdot q_{\text{Born}}$, where q_{Born} is the Born effective charge. At first glance, it is clearly visible that the largest interference of the two ferroic properties is found in the TiO_2 layer. In particular there the magnetization changes sign when the polarization is turned. A change of the polarization due to the vicinity of the iron was not observed. Similarly the iron moments are only mildly influenced by the change of the polarization direction. The total change of magnetization $\Delta M = M(P_\downarrow) - M(P_\uparrow)$ for this system is about $1\,\mu_B$. This change will be explained by a detailed analysis of the hybridization

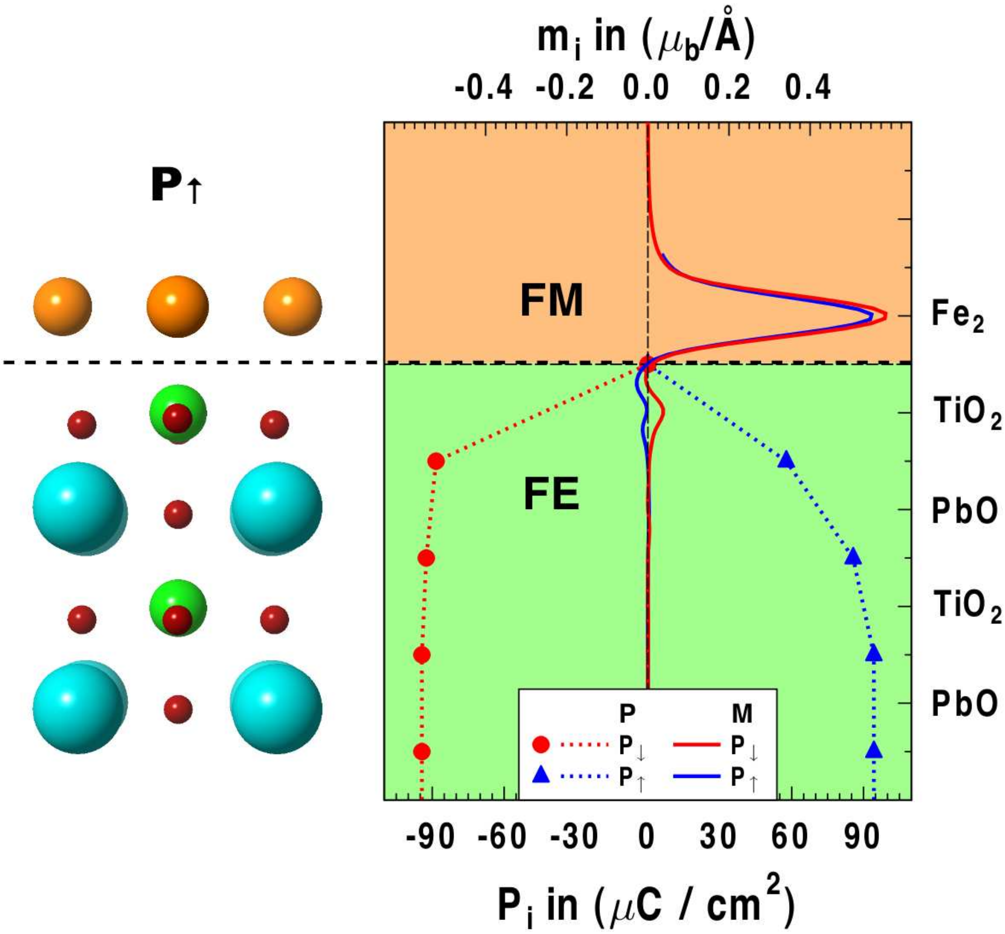

Figure 3: The unit cell of biferroic $Fe_2/TiO_2/A TiO_3(001)$ (A = Ba, Pb) with a 2 nm thick vacuum layer is sketched as a side view. On the right-hand side the order parameters at the interface for 1 ML Fe on top of PTO are shown. The layer resolved polarization is plotted as a dotted line, whereas the magnetization is represented by a solid line. The two colors correspond to the states $P_\uparrow$ (blue) and $P_\downarrow$ (red). The largest change of the magnetization was obtained within the TiO_2 plane next to the interface.

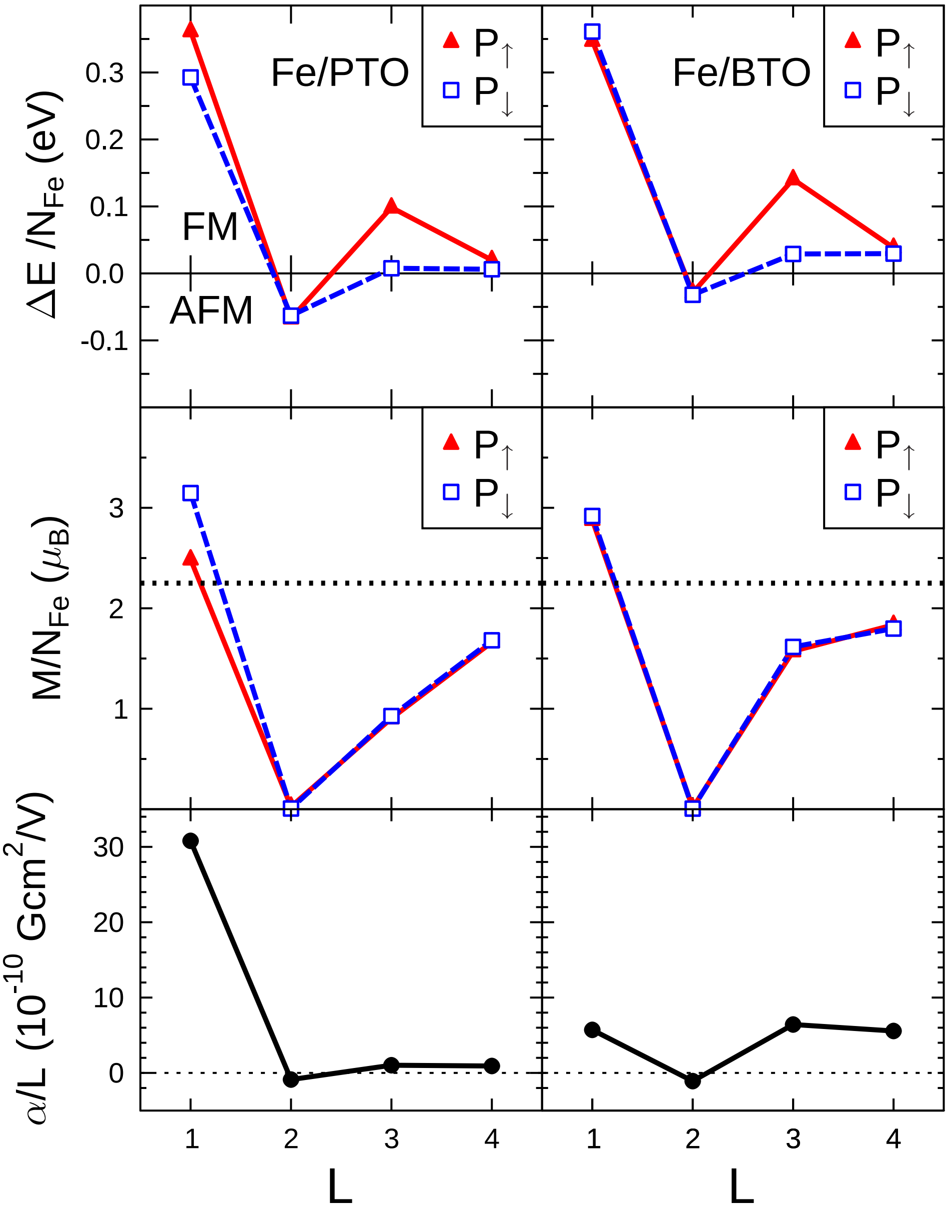

Figure 4: Magnetism of $(\mathrm{Fe}_2)_L/\mathrm{ATiO}_3(001)$ for PbTiO_3 (PTO) and BaTiO_3 (BTO) versus Fe-film thickness L. In the top panel the total-energy difference $\Delta E \equiv E_{\mathrm{AFM}} - E_{\mathrm{FM}}$ of the antiferrimagnetic (AFM) and ferromagnetic (FM) configurations are normalized with respect to the number N_{Fe} of Fe atoms in the film unit cell. In the middle panel the magnetization per Fe atom for the lowest-energy configuration is plotted. Here, the dotted line indicates the magnetic moment of Fe bulk. The magnetoelectric coupling coefficient α of $(\mathrm{Fe}_2)_L/\mathrm{ATO}(001)$ (A = Ba, Pb) is plotted versus the Fe-film thickness L in the lower panel.

of Fe, Ti and O atoms at the interface in Section 2.1.

For all substrates and Fe-film thicknesses, total energies of two magnetic configurations were computed: ferromagnetic (FM) and antiferrimagnetic (AFM) ordering was considered. The top panel in Fig. 4 shows the energy difference $\Delta E = E_{\mathrm{AFM}} - E_{\mathrm{FM}}$ between these two configurations. For both substrates we obtained for 1ML Fe ferromagnetic order of the iron independently of the polarization direction. Adding a second layer changes the ordering substantially. Here, an antiferromagnetic ordering seems to be preferred. But the constrained self-consistent calculations did not converge towards a complete AFM configuration; forcing the top layer to be antiferromagnetic the layer beneath always shows ferromagnetic order with suppressed moments. Consequently the preferred order for $L = 2$ is antiferrimagnetic. Deposition of a third Fe layer restores the ferromagnetic order. In almost all cases, the relation of $E_{\mathrm{FM}} < E_{\mathrm{AFM}}$ is obtained. An exception is $L = 2$ for which it was not possible to reach an antiferromagnetic solution but an antiferrimagnetic instead. Thus, the magnetic order of the two-phase multiferroics can be tuned by the Fe-film thickness independently of the perovskite substrate. Strain and electric polarizability are of minor importance for the ordering.

The middle panel of Fig. 4 shows the magnetization of the interface as a function of the iron layer thickness. The magnetization is normalized to the number of iron atoms to allow comparison of the results. The two curves within the figures correspond to the two polarization states, and their difference is the change of magnetization under polarization reversal. For 1 ML iron on PTO there exists a large magnetization which is mainly carried by the magnetic moments of iron $m_{\mathrm{Fe}} \approx 3\,\mu_{mathrmB}$. A difference of about $1\,\mu_{\mathrm{B}}$ between the two polarization directions is obvious in the case of Fe on PTO. This is in contrast to the BTO substrate where this difference is tiny ($\Delta M = 0.05\,\mu_{\mathrm{B}}$). With two layers of iron the magnetization drops down to almost zero due to the change of the abovementioned magnetic order. Further, the two curves lie on top of each other. Upon adding more layers ferromagnetic order is stabilized and the magnetization increases. For more layers the magnetization converges towards the bulk value of iron (dashed line).

Based on the change of the magnetization the surface magneto-electric coefficient is calculated. It is defined as $\alpha_{\mathrm{surf}} = \Delta M/(E_c \cdot A)$, where A is the surface area and E_c is the coercive field needed to switch the polarization. Using the experimental values of E_c for BTO (10 kV/cm) and PTO (33 kV/cm), the coupling coefficients were calculated and plotted as a function of the number of iron layers in the lower panel of Fig. 4. Since the ΔM is largest for Fe on PTO, the largest coupling is obtained for this system. Interestingly the coefficient for PTO decays with increasing number of iron layers. This is in contrast to BTO where α_{surf} stays nearly constant. An exception is the case $L = 2$ for which the value approaches zero for both substrates. Theoretical studies of superlattices of BTO and Fe show that this value is also valid for thick Fe films [9]. To compare these values we consider values obtained for a $SrRuO_3/SrTiO_3$ interface. *Ab initio* calculations based on the density functional theory (DFT) predict that a voltage of about 30 meV/e, applied across the interface without magnetic cations, can induce a net magnetic moment [8]. This leads to an α_{surf} two orders of magnitude smaller than that predicted for the Fe/PTO system.

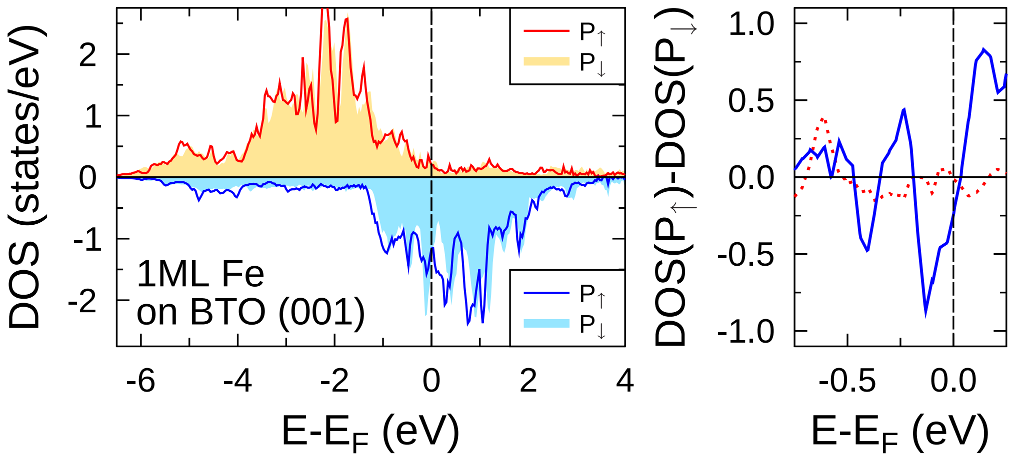

Figure 5: Electronic structure at the surface of $(Fe_2)_1/BaTiO_3(001)$. The left panel shows the spin-resolved density of states (DOS) for Fe/BTO. The right panel gives the difference between the spin-resolved DOS for $P_\uparrow$ and $P_\downarrow$ close to the Fermi energy E_F (majority: red, dotted; minority: blue, solid).

2.1 Microscopic origin of ME coupling

From the preceding it is evident that the magnetic moments of the Fe film are changed in a complex manner by the interface. To achieve insight into the mechanism, we illustrate in Fig. 5 the spin-polarized electronic properties at the Fe/BTO interface. A switching effect is mainly seen for the minority electrons around the Fermi energy. This effect is much more obvious in the difference between the two densities for the two polarizations. The effect is clearly dominating for minority electrons whereas there are only minor changes for majority electrons. This could be attributed to a hybridization of the Fe *d*-minority states with the Ti *d*-states which leads to an induced moment on the Ti site oriented opposite to the iron moments. Since the Ti atom is closer to the Fe atoms in the $P_\uparrow$ state the hybridization is stronger for this configuration. Consequently the induced Ti moment is larger. For $P_\downarrow$ the opposite is the case and a smaller Ti moment can be observed. It turns out that it this moment which causes the difference of the total magnetization between the two polarization states.

Because of the larger displacement of the atoms this effect is even more pronounced in Fe/PTO (confer the right-hand side of Fig. 3). In contrast to BTO an additional large induced moment on the oxygen could be observed in the $P_\downarrow$ case. The O moment is aligned parallel with the iron moments. Switching to $P_\uparrow$ causes in induced moment on Ti antiparallel to the iron moments which then induces a moment on the lower oxygen. The larger displacement and the additionally induced moment causes the sizable change of $1\,\mu_B$.

The change of the minority charge distribution in real space is shown in Fig. 6 for Fe on BTO. Considering the right-hand-side panel, it is obvious that most of the minority charge is pushed into the interstitial region between the iron atoms under polarization switching. This charge originates mainly from the Ti atom, as is evident from the side view, and is responsible for the

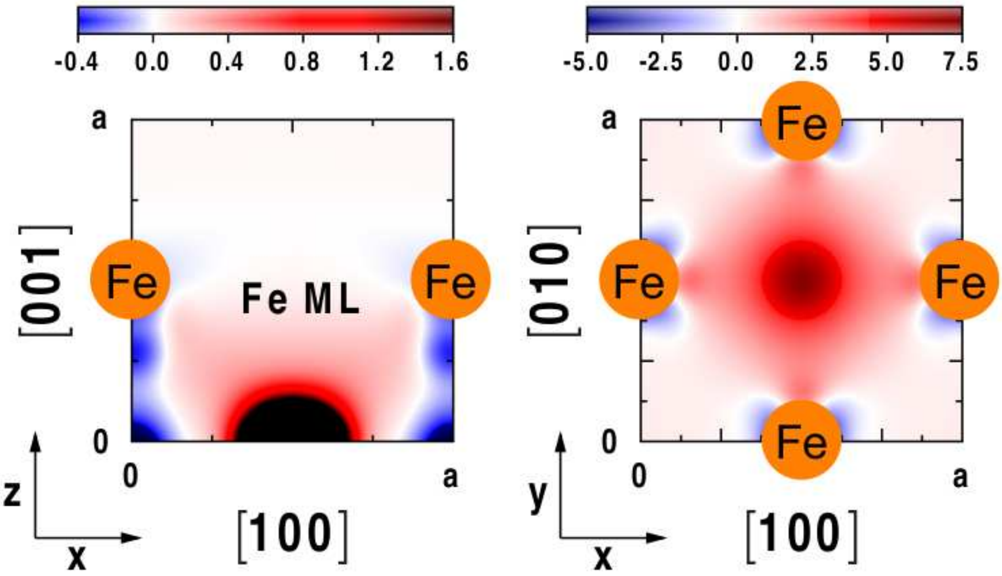

Figure 6: (Color) Charge redistribution of minority-spin electrons at the interface of $(Fe_2)_1$/BTO(001) upon reversal of the electric polarization $\boldsymbol{P}$ with respect to the surface normal. The difference of the charge densities for $P_\uparrow$ and $P_\downarrow$ is depicted in a perpendicular (left) and an in-plane cut through the Fe atoms (size a^2; color scales in arbitrary units). The Fe atoms are represented by spheres.

change of magnetization under switching.

While the magnetic moments do not change sign upon $\boldsymbol{P}$ reversal, we consider the possibility of a spin-reorientation transition as another type of magnetoelectric switching. To investigate this mechanism we were using the relativistic layer-KKR, the magnetic anisotropy for $(Fe_2)_1$/BTO(001) is computed within the framework of the magnetic force theorem [20]. For both P orientations perpendicular anisotropy is favored with respect to in-plane anisotropy, namely by 0.72 meV ($P_\downarrow$) and 0.54 meV ($P_\uparrow$) per Fe atom. It worth mentioning that the anisotropy energies are twice as large as in FePt [21,22]. In summary we find a change of the magnetization upon polarization reversal but no change of the magnetization direction.

2.2 Magnetic order

As previously mentioned, the magnetic order changes as a function of the Fe-layer thickness. In particular the magnetic order of two Fe layers becomes antiferrimagnetic (Fig. 4). For two layers the magnetic moments in the Fe interface layer are almost quenched while the sizable moments in the surface layer are ordered antiparallelly. This is due to the small distance of 1 Å between the iron layers. Since the two Fe sites in the top layer are inequivalent, e. g. Fe is on top of Ti (Ba) sites. They carry different magnetic moments; this reflects the environment of these atoms, in particular the atomic volumes and the hybridization. Polarization reversal affects mainly the positions of Ti atoms and consequently those of the Fe atoms atop. The small volume of interfacial Fe is reduced even further and leads to very small magnetic moments. The small size of Fe atoms in the interface layer explains as well the antiferromagnetic ordering of their local magnetic moments [23]. Adding a third Fe layer increases both the coordination numbers and the atomic volumes and consequently restores ferromagnetic order.

2.3 Oxygen coverage

So far, our *ab initio* studies of MF composites were focused on perfect interfaces without oxidants. However, the strength of the ME coupling may be sensitive to the degree of oxidation. The Fe oxidation is unavoidably motivated, firstly, by the growth process of the ferroelectric since oxygen will react with the iron during Fe growth. Secondly, for the uncovered Fe films further oxidation occurs when the sample is removed from the chamber. These two possible scenarios may result in some particular Fe-O compositions which vary from highly oxidized Fe to an almost clean surface. Thus, the *ab initio* based modeling would be extremely useful. In the following, we study from first principles the key electronic, magnetic and structure factors behind the oxidation process of the 1-ML Fe grown on $BaTiO_3(001)$ and $PbTiO_3(001)$. We demonstrate in which positions oxygen adatoms sit above the Fe layer and that the ME coupling in these composites is robust against the O composition.

The equilibrium bond length calculated for molecular O_2 is 1.23 Å. For $Fe_2/TiO_2/A TiO_3(001)$, the in-plane lattice parameter is about 3.9 Å, while the Fe-Fe separation is about 2.75 Å. The latter is two times larger than that of the O_2 dissociation. Therefore, to model the Fe oxidation of Fe/BTO and Fe/PTO we must consider O coverages, $c(O_x : Fe_2)$, ranging between $c = 1/2$ and two adsorbed O atoms per Fe atom ($c = 2$). There are twelve possible configurations for these coverages [Fig. 7(c)]. For $c = 0.5$, one oxygen adatom per unit cell can occupy the site either above A or above Ti or, alternatively atop Fe. For $c = 1$, the two O adatoms form four configurations marked in Fig. 7(c) as AT, AF, TF and FF. In the case of $c = 1.5$, we relax the ATF, TFF and AFF configurations. And, finally, for $c = 2$ there are two more possibilities to distribute four adatoms, such as ATFF (the case of full coverage) and 4H, which means that all four hollow sites are occupied by O. Using a $10 \times 10 \times 6$ Monkhorst-Pack [24] mesh for the Brillouin-zone integration, we relaxed the O adatoms and Fe atoms plus all atoms of the two top ABO_3 unit cells until the forces were less than $1.0 \cdot 10^{-2}$ eV/Å. After relaxation, oxygen forms an overlayer above the Fe layer, with the distance depending on coverage and direction of $\boldsymbol{P}$.

In the case $c = 0.5$, the most favorable configuration is A. However, the configurations A and T can coexist for this O coverage since the difference in energy between them is $E_T - E_A \sim 0.2$ eV. For the ABO_3 substrates, the energetics are almost the same while the $\boldsymbol{P}$ reversal yields the energy differences compatible with that of $E_T - E_A$. When the O atom relaxes above Fe this results in the highly unfavorable configuration F, with the energy of 2.1 eV larger than that of case A. This can be understood by inspecting the relaxed structures of the A and T configurations. These are very similar to that of a O/Fe(001), which were under debate in the literature [25]; the O adatom is relaxed at the hollow site by about 0.3 Å above the Fe ML. The configurations A and T do not differ significantly with respect to each other and with respect to the uncovered 1-ML Fe on ABO_3. In the case of configuration F, the coverage $c = 0.5$ makes the two Fe sites nonequivalent and, as a result, the Fe atom below oxygen moves outward the

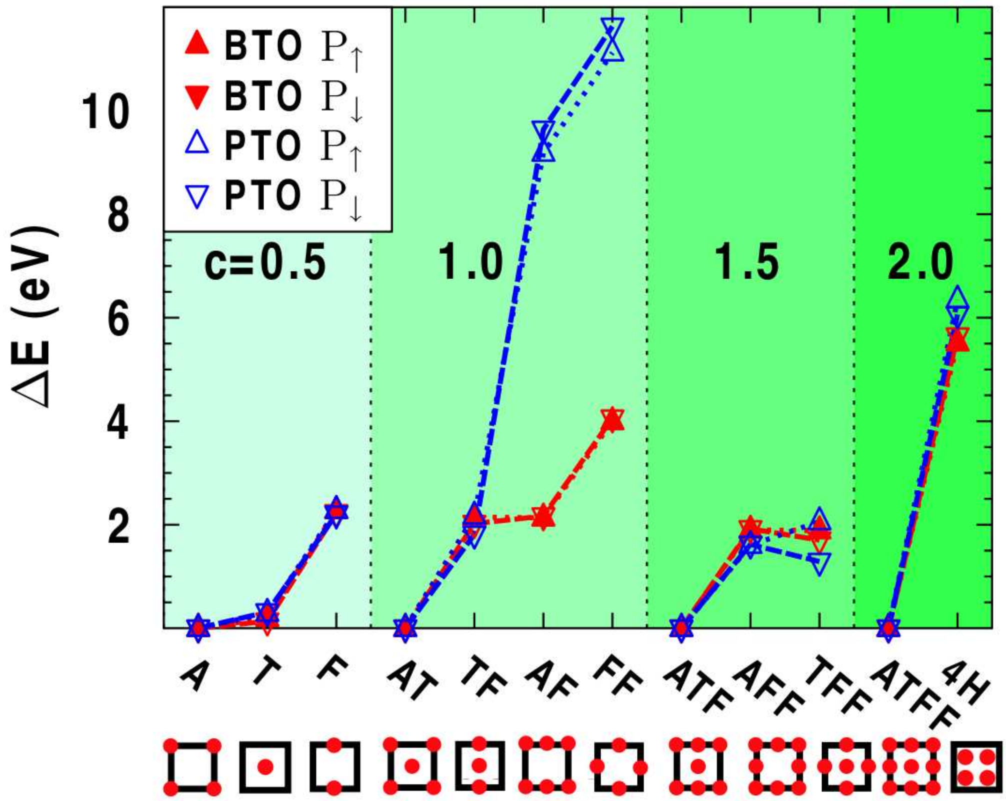

Figure 7: Relaxed total energy of $O_x/Fe_2/ATO(001)$ (A = Ba, Pb and $0 < x < 4$) is plotted for twelve simulated O configurations. The latter are given schematically below the labels. For each coverage c, the configuration with lowest energy pins the energy zero.

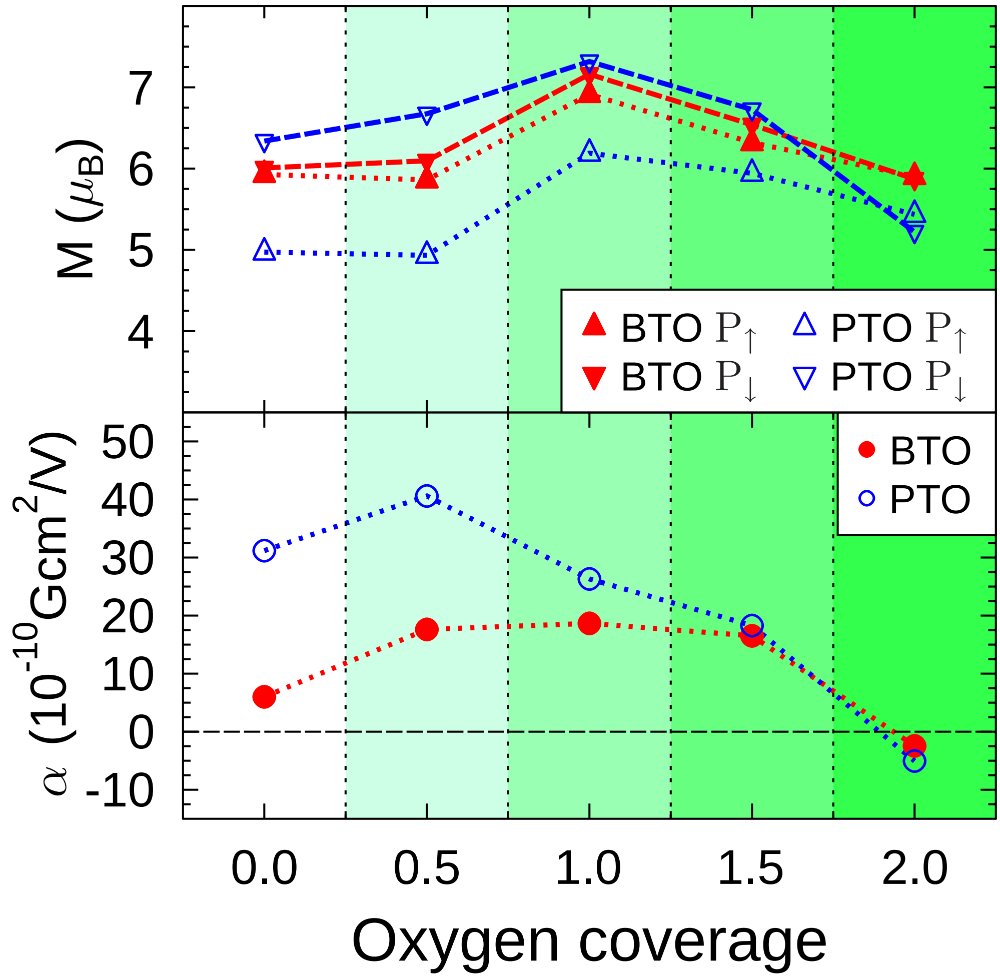

Figure 8: The total magnetization M of $O_x/Fe_2/ATO(001)$ (A = Ba, Pb and $0 < x < 4$) as a function of oxygen coverage is shown in the top panel. For each coverage the energetically favorable configuration was assumed. The magnetoelectric coupling coefficient α is shown in the lower panel.

Fe layer, displacing therefore the O atoms of the interface TiO_2 layer in the same way. The structural distortions make the configuration F energetically unfavorable.

The energetics which is calculated for the coverage $c = 1$ can be explained using our findings for $c = 0.5$. We expect the two O adatoms occupy the positions above A and Ti. Here, $\boldsymbol{P}$ reversal gives a change in energy of about 0.2 eV for both systems. Any of the three other configurations TF, AF or FF always includes at least one energetically unfavorable position atop Fe that drastically increases the associated surface energy. The configuration FF represents the most distorted system whose energy is larger by 12 eV (4 eV) compared to that of the AT configuration of PTO (BTO). For the same reason, the energetically favorable scenario of $c = 1.5$ is the configuration ATF when one site above Fe is empty. Regarding $c = 2$, we have inspected two configurations: ATFF and 4H (shown in Fig. 1). It turns out that the 4H configuration, with all four hollow sites occupied by O, is unfavorable.

In the top panel of Fig. 8 we show the total M, calculated for the lowest energy configuration of $O_x/Fe_2/ATiO_3$ for each O coverage. These are the configurations A, T, AT, ATF and ATFF obtained for $c = 0.5, 1, 1.5$ and 2, respectively. For $c = 0.5$ we used the average between the A and the T configuration since they can coexist. The magnetization of uncovered Fe/PTO and Fe/BTO is also shown as well. The increase of M seen for $c = 0.5$ and $c = 1$, as compared to that of $c = 0$, is due to a induced magnetic moment at the O adatom which is aligned parallel to the Fe magnetic moment. In the case of low coverage, namely for $c = 0.5$ and $c = 1$, the Fe moment is not affected by the presence of adatoms. Contrarily, when the O adatom relaxes above Fe in the configurations ATF and ATFF, the Fe magnetic moment is decreased by about $1\,\mu_B$. This is mostly due to a relatively small distance between the O adatom and Fe along [001]. As a result, M gradually decreases with increasing $c > 1$.

In summary we demonstrate here that in the case of O/Fe/BTO the magnitude of ΔM remains rather stable for O coverages $c < 1.5$. With further increase of c, $\Delta M \to 0$ at $c = 2$. For the PTO substrate, the trends of ΔM computed for $c > 1.5$ are similar to those of BTO. It should be kept in mind that the dense coverage of $c = 2$ is unrealistic since the highest oxidation state of iron seen in Fe_2O_3 mimics the coverage $c = 1.5$.

The lower panel of Fig. 8 shows the change of the interface ME coupling coefficient, α, which can be evaluated as the ratio of the surface magnetization change $\mu_0 \Delta \boldsymbol{M}/S$ and the coercive field E_c, where S is the interface area. The experimental $E_c = 10\,\text{kV/cm}$ and $E_c = 33\,\text{kV/cm}$ were used for Fe/BTO and Fe/PTO, respectively. In general, the variation of α as a function of c follows the trends of ΔM. However, for $1 < c < 1.5$ we find that the two systems obey almost the same strength of α and, hence, there would be no advantage to use a highly polar PTO substrate for the dense O coverage.

3 Summary

In summary, the magnetism of two-phase multiferroics, realized by ultrathin Fe films on $ATiO_3$ perovskites (A = Ba, Pb, Sr), is found to exhibit a rich and peculiar structure, as is predicted from first-principles computational materials science. A ferromagnetic-to-ferrimagnetic transition which is accompanied by a strong reduction of the Fe magnetic moments could be used in device applications to tailor the properties of the magnetic subsystem. Significant magnetoelectric coupling via the Fe/$ATiO_3$ interface is predicted, a spin-reorientation transition under switching is not found. In view of device applications it appears highly desirable to investigate theoretically and experimentally the thickness-dependent magnetic properties of Fe films sandwiched between ferroelectric perovskites.

Furthermore we discussed the effect of oxidation on the strength of magnetoelectric coupling seen at the biferroic interface in epitaxial ferromagnetic/ferroelectric nanocomposites. The oxygen coverage, ranging between $c = 0.5$ and two adsorbed O per Fe atom were simulated for $O_x/Fe_2/BaTiO_3(001)$ and $O_x/Fe_2/PbTiO_3(001)$ multiferroics. We suggest that oxygen adatoms may find their relaxed positions atop the Ba (Pb) and/or Ti sites. For $c > 1$, the magnetic properties computed for the Fe layer gradually degrade with increasing O coverage. However, when $c < 1.5$ the change in magnetization induced by polarization reversal is robust for all energetically preferable compositions. On the basis of our calculations we, therefore, suggest that intrinsic oxidation of biferroics may not destroy their magnetoelectricity significantly. In the case of realistic oxygen coverage ($c = 1$), we expect that the strength of magnetoelectric coupling is similar for both biferroic systems under consideration.

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