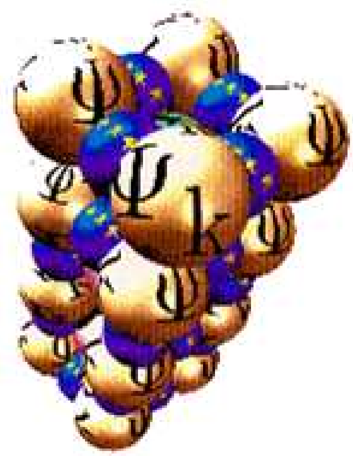
Ψ_k Newsletter

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

Number 83 October 2007



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Sponsored by: UK's CCP9
and ESF Psi-k Programme

Contents

1 Editorial

In this issue we would like to turn our readers' attention to the General News section where we write about the "Psi-k Portal" which is the web-interface which at the moment supplements our Psi-k services, but might gradually replace our conventional ways of distributing the Psi-k relevant information. In the same section we repeat the call for workshop proposals for 2008.

The scientific highlight of this issue is on "An extensible and portable file format for electronic structure and crystallographic data", which is different than our usual highlights, but we hope that you will find it equally useful and captivating. It has been written by Xavier Gonze (Louvain-la-Neuve, Belgium) and his collaborators.

Please see the table of content for further details.

The *Networks* have a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:

`http://psi-k.dl.ac.uk/`

The above contains information on the Psi-k 2007 workshops and hands-on courses (subject to funding).

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

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

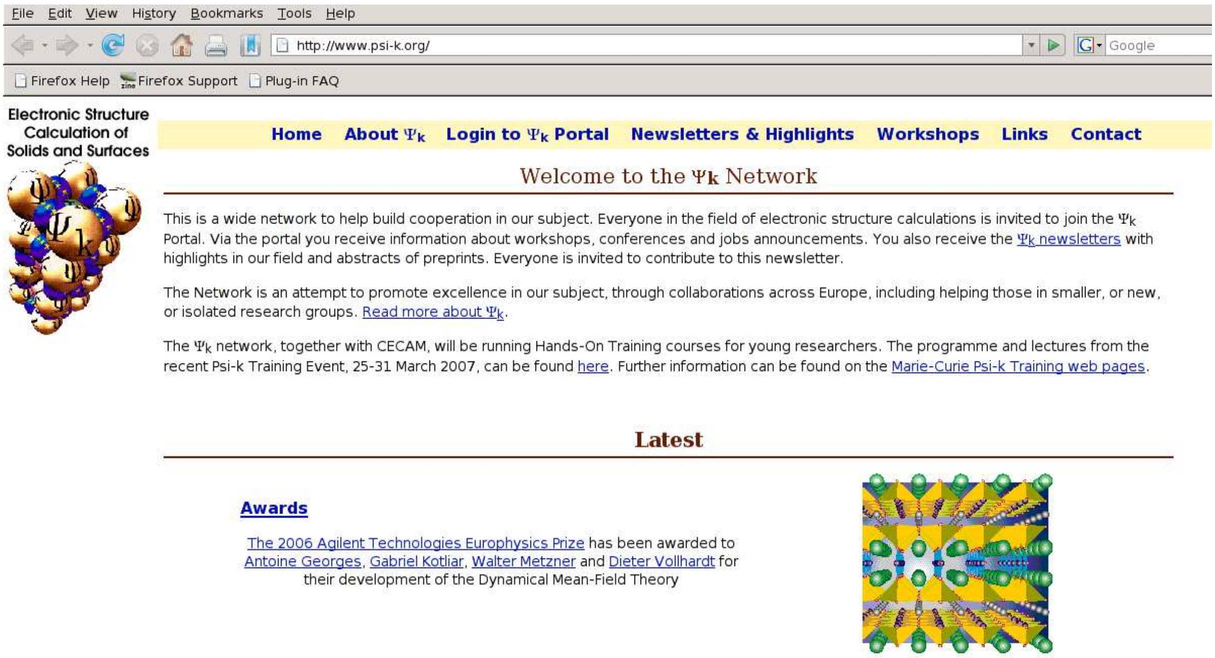
	function
psik-coord@dl.ac.uk	**messages to the coordinators, editor & newsletter**
psik-network@dl.ac.uk	**messages to the whole Ψ_k community**

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

2 General News

2.1 Psi-k Portal

In the past few months there have been major changes to the Psi-k website. We have now registered the domain name **www.psi-k.org** which will become the main Psi-k website. The old web address will continue to work, but the new one is preferred. The new address signifies the change to Psi-k becoming an independent non-profit organization. STFC Daresbury are happy to continue to host the website on behalf of Psi-k, but the new address emphasizes the new fully indepenent status of Psi-k.



Welcome to the Ψ_k Network

This is a wide network to help build cooperation in our subject. Everyone in the field of electronic structure calculations is invited to join the Ψ_k Portal. Via the portal you receive information about workshops, conferences and jobs announcements. You also receive the Ψ_k newsletters with highlights in our field and abstracts of preprints. Everyone is invited to contribute to this newsletter.

The Network is an attempt to promote excellence in our subject, through collaborations across Europe, including helping those in smaller, or new, or isolated research groups. Read more about Ψ_k.

The Ψ_k network, together with CECAM, will be running Hands-On Training courses for young researchers. The programme and lectures from the recent Psi-k Training Event, 25-31 March 2007, can be found here. Further information can be found on the Marie-Curie Psi-k Training web pages.

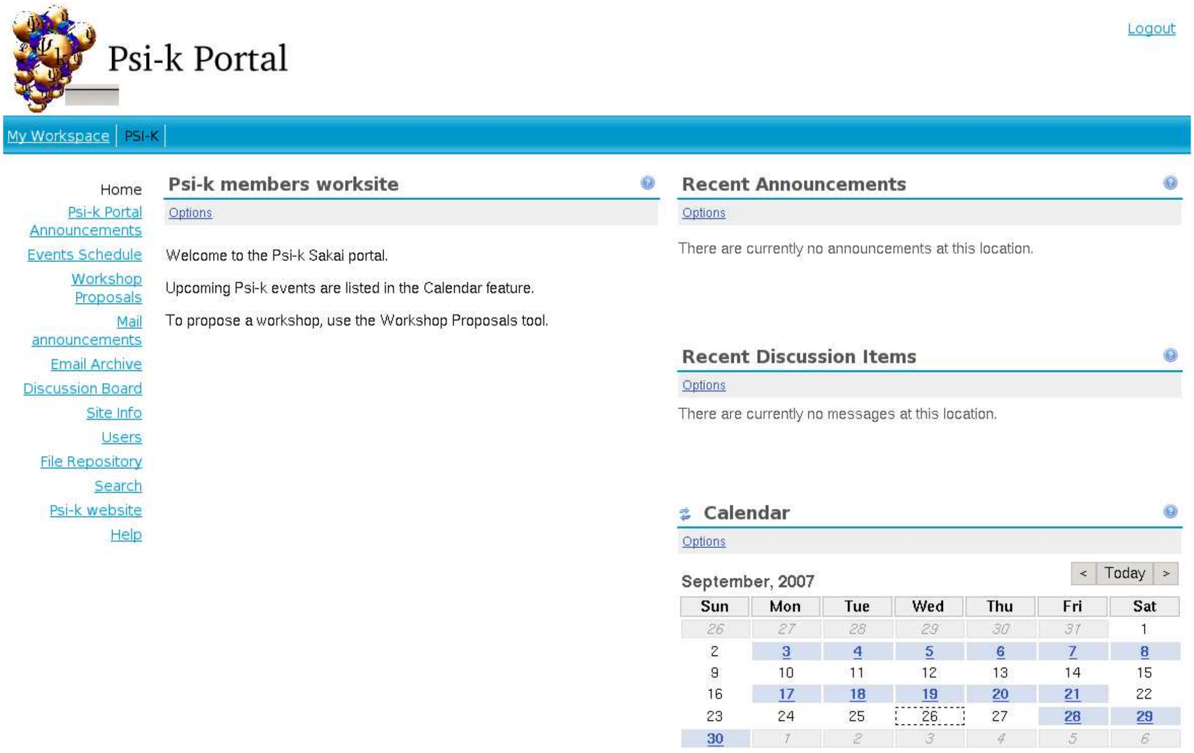
Latest

Awards

The 2006 Agilent Technologies Europhysics Prize has been awarded to Antoine Georges, Gabriel Kotliar, Walter Metzner and Dieter Vollhardt for their development of the Dynamical Mean-Field Theory

Within the website a major change has been the introduction of a new portal for Psi-k. The portal gives new interactive facilities to Psi-k members. From the portal it is possible to send emails to the Psi-k email list, or to specific groups of members such as the core management group. One can create and join discussion forums, and upload files. A special tool automates submission of proposals for Psi-k workshops, and in future new tools could be added for example to submit workshop final reports or scientific highlights. A useful calendar tool shows the dates of upcoming workshops and conferences. Users of the portal can enter their own workshops directly into the calendar.

In fact we plan to eventually switch much of what is currently in the Psi-k newsletters to web-page-only information and services accessed through the portal. The subscribers to the Psi-k Portal will be able to upload to the web all the information that they want to share with the Psi-k community. This will include workshop and available job announcements, workshop/conference reports, abstracts of newly submitted papers, etc. At present we already have a possibility of submitting proposals for workshops to be organized in 2008. Also emails sent from within the portal are automatically sent to the full Psi-k mailing list.



Welcome to the Psi-k Sakai portal.

Upcoming Psi-k events are listed in the Calendar feature.

To propose a workshop, use the Workshop Proposals tool.

There are currently no announcements at this location.

There are currently no messages at this location.

September, 2007

Sun	Mon	Tue	Wed	Thu	Fri	Sat
26	27	28	29	30	31	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	1	2	3	4	5	6

The Psi-k Portal is accessed from the new Psi-k web pages (new address: `http://www.psi-k.org`) by clicking on ”Login to Psi-k Portal”. You will first need to create an account before being able to upload any information yourself. For this please use your e-mail address as userid. After the successful creation of an account you will end up in your personal workspace. Please click Psi-k on the blue header banner to enter the Psi-k Portal.

Currently the main portal tools are accessed via the menu bar on the left side of the page:

- **Calendar tool**: lists upcoming workshops and conferences. potal users can add their own entries.
- **Workshop submission tool**: used to propose a future Psi-k workshop. See next page for detailed instructions.
- **Email tool**: used to send emails to all or groups of Psi-k users. Job announcements can be emailed directly to the Psi-k mailing list from here. Emails are automatically archived.
- **Groups** In future one can create groups of users, eg specialists in specific subjects or groups of common interests. Emails can just be sent to a specific group.
- **Upload tool**: share files with other portal users through this tool.
- **Discussion boards**: create new discussion threads, or join an existing discussion thread.

The Psi-k portal uses **Sakai** software, developed at Daresbury laboratory and elsewhere. A Bristol University undergraduate, Ruth Jackson, did much of the work of customization of the portal for Psi-k, with funding support from the UK’s CCP9 network. We are happy to receive comments and suggestions for improvements, but please be aware that there are no full time support staff for the Psi-k website or portal, and the Daresbury group are all full time scientists who have many other calls on their time.

Finally note that currently the Psi-k portal is initially set for very highly open access. By default anyone can register as a user, and then send emails or upload files. Any user who abuses this trust will be removed immediately. If problems occur we may have to change to more strict vetting of posts and members. For increased security we will be asking users to provide a full name and insitution address, which can be entered in the **personal profile** section of the portal. In future we may restict access for this who do not provide this information.

2.2 Call for Psi-k Workshop Proposals for 2008

Here we repeat our call and ask for proposals for workshops, small conferences, hands-on tutorials and summer schools in the field of ab-initio calculations to be held in 2008 and to be partially funded by the new Psi-k network.

The deadline of proposals is 30. Sept. 2007.

The year 2008 is the first year of the new Psi-k Network, being funded by financial contributions of the large European research groups in the ab-initio field. We all aim at excellent workshop activities and therefore we ask you to write a detailed and well founded proposal. Training activities like computer tutorials and summer schools will be given some preference, but we hope for a similar workshop program as in the past.

Submission of Psi-k Proposals: Instructions for the submission of proposals are as follows:

The submission of Psi-k Workshop Proposals is to be done by logging into the Psi-k Portal of the Psi-k web pages (new address: `http://www.psi-k.org`).
You will first need to create an account before being able to submit. For this please use your e-mail address as userid. After the successful creation of an account you will end up in your personal workspace. Please click Psi-k on th e blue header banner to enter the Psi-k Portal. Click on the workshop proposal button, and then click on the number 1 (left col umn) of the call for proposals to view its details, including the option to submit a proposal. Then to submit a proposal for a workshop, click the Submit a Proposal button:

- Fill in all form fields correctly and you will be able to preview your proposal as a pdf. If the preview button does not prod uce a pdf please check carefully that all input fields have been filled in, valid dates are used (format dd/mm/2008-dd/mm/2008) 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 are able to view or modify your proposal, or download it as a pdf file.

Please note that the deadline for proposals is September 30. The full call can be read in the last Psi-k Newsletter.

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 latter ones funded partially by the EU contract of the Molecular Simulation Network and the EU-Psi-k Training contract. The collaboration with CECAM is working very well and has effectively increased our funding substantially.

The deadline for CECAM proposals is 1. October 2007.

As you know, CECAM likes very much discussion workshops on well focussed topics. Conferences will not be supported. Moreover, CECAM proposals have to be competitive. Thus, as for Psi-k, well founded proposals are required. The CECAM council has decided to upgrade CECAM and has published an open call for a (new) host institution. Thus in the planning of the proposals details about the future host are not yet known. However there will be a normal workshop program in 2008.

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. As pointed out by Christian Elsaesser, 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

3 News from the ESF Programme

"Towards Atomistic Materials Design"

3.1 ESF Psi-k Programme Workshop Announcements

3.1.1 International Workshop on "Non-Adiabatic Dynamics at Surfaces"

Schloss Reisensburg (close to Ulm, Germany)

22-25 October 2007

`http://www.fhi-berlin.mpg.de/~behler/Website/reisensburg.htm`

Objectives: Electronically non-adiabatic gas-surface interactions have been discussed in order to account for dissociation dynamics observed in molecular beam experiments, or in the context of electron or light emission during adsorption at metal surfaces. Intimately connected to this are mechanisms of energy dissipation to the bulk solid, which, if hindered, could give rise to controversially debated processes like abstraction or "hot" adatom diffusion. A full quantum-mechanical treatment of these phenomena is severely challenged by the lowered symmetry at the solid surface, by the sheer size and complexity of the systems when considering the extended surface, as well as by the time scales over which it is necessary to follow the coupled atomic and electronic motion. The aim of the workshop is to bring together scientists working on different approaches to dynamics on excited state potential energy surfaces, as well as distinguished experimentalists to discuss and promote advances in this field.

Confirmed Invited Speakers and Discussion Leaders: D. Bird, G. Darling, B. Gadzuk, A. Gross, E.K.U. Gross, E. Hasselbrink, S. Holloway, B. Kasemo, Th. Klner, A. Knorr, R. Kosloff, G.-J. Kroes, O. Kuehn, S. Louie, N. Marzari, E. Pehlke, M. Persico, M. Rohlfing, A. Rubio, T. Van Voorhis, A. Wodtke.

Format and Application: The number of participants is strictly limited to 50. Apart from the formal sessions of invited contributions, there will be a poster session allowing all participants to present their work. The conference fee is 450 Euro and includes full board and lodging.

Applications to participate in the workshop should be sent to Karsten Reuter (reuter@fhi-berlin.mpg.de).

Jörg Behler (ETH Zürich)
Patrick Rinke (FHI Berlin)
Karsten Reuter (FHI Berlin)
Matthias Scheffler (FHI Berlin)

3.2 Reports on ESF Programme Workshops/Meetings

3.2.1 REPORT on ESF Summer School on "Ab-initio many body theory"

July 22-28, 2007
San-Sebastian, Spain

Organizers:

A. Rubio
University of the Basque Country
A. Georges
Ecole Polytechnique, France
A. Lichtenstein
University of Hamburg, Germany
C. Filippi
University of Leiden, Netherlans
W.M. Temmerman
Daresbury, United Kingdom

Aims: The School on Ab-initio Many Body Theory is in response to very recent developments. The aim is here to understand electronic correlation effects on an ab-initio basis, by starting from realistic wave functions obtained from density functional calculations, leading to a material-specific description of many body effects. The School will reflect the strong progress in this field. The lectures review the whole field, as well as discuss latest results. The program consists of a good balance between theoretical and experimental lectures, as well as contributions from industry.

The list of topics include:

1. Basic density functional theory (DFT) and Time-dependent DFT.
2. New experimental techniques for excitation spectrum of materials Many-body theory
3. Physics of correlated materials - theory and experiments
4. Basic of Quantum Monte Carlo and Quantum chemical methods
5. Combining the best of different worlds: MBPT-GW-DMFT and TDDFT
6. Selected Applications.

The summer school will have a poster session where the young researchers will be able to present their work.

The aims are: - To review the present state of the art and understanding
- To give an overview on theoretical and experimental research methods
- To give a perspective of the future development of the field

- To discuss the possible technological applications

In collaboration with Marie Curie series of events programme ”Psi-k Training in Computational Nanoscience”, Nanoquanta Network of Excellence ”European Theoretical Spectroscopy Facility (ETSF)”, European Science Foundation (ESF) under Psik programme, Donostia International Physics Center (DIPC), Ministerio de Educación y Ciencia and National Science Foundation (NSF).

Summary

The School is a shared activity of the three PSI-K working groups, WG1 (GW method), WG2 (quantum Monte Carlo) and WG3 (dynamical mean field theory). It aims at giving a unified overview of the three many-body approaches.

The School is the first Summer School in the Psi-k Marie Curie Series of Events (Psi-k Training in Computational Nanoscience). These Schools are complementary to the Hands-on tutorials offered within the same Programme and aim at providing understanding of the physical phenomena and materials in addition to the computational techniques which are then covered in the hands-on tutorials.

The School is reach out to young researchers already working in the general field of many-body ab-initio theory, as well as researchers who are not yet practitioners but are interested in acquiring the necessary expertise. The School give a solid introduction to the description of electronic correlation effects on an ab-initio basis in both weakly and strongly correlated materials. The activity provided the necessary background and context, highlighting the most challenging problems, and the topics of current interest. Finally, the program achieved a good balance between theoretical and experimental lectures.

For further information, visit the website:

`http://www.mc-psi-k-training.cecam.org/index.php?content=activities/tutorial`

Description of the scientific content and discussion at the event

Despite the successes of density functional theory (DFT) in describing the electronic structure of complex molecules and solids, the treatment of electronic correlation within a local density approximation (LDA) to DFT is only approximate, often leading to incorrect results for both strongly and moderately correlated systems. An important area of research within electronic structure theory is therefore the development of alternatives to density functional methods. In particular, it is vital for researchers in electronic structure theory to be able to access a hierarchy of techniques that can describe electronic correlations at higher and higher levels of precision.

For the ground and excited properties of real materials in the weak correlation regime, Quantum Monte Carlo (QMC) methods are among the most successful of the post-DFT approaches. The required computing time in QMC scales algebraically as the cube (or better) of the system size, and it has yielded accurate results for the correlated properties of large molecules and solids where conventional quantum chemistry methods are extremely difficult to apply. QMC is establishing itself as a unique tool for exploring electronic correlation in systems of interestto materials science and for obtaining conclusive answers in cases where DFT is shown to be inadequate.

The QMC part of the school will focus on introducing the basics of the method as well as touching on current methodological developments, including efforts to incorporate molecular dynamics and improve geometry optimisation schemes, to find more efficient ways of optimising trial wave functions, and to develop new algorithms alternative to the fixed-node diffusion Monte Carlo method. Speakers involved in pushing the frontier of applications to ever more complex systems such as strongly correlated systems have been also invited.

While structural properties of materials are mainly determined by the static electronic ground state and can be treated within the QMC-scheme for correlated system, the response to external probes in modern non- destructive spectroscopies can only be explained in terms of dynamic excitations. Thus, the knowledge of excited states is essential not only for its fundamental importance in condensed matter physics, but also for the impact in practical applications like the design of new materials with technological or medical interest.

The theoretical foundations of this field are well established, and have been accompanied with physically well-motivated approximations suitable for ab-initio calculations in real materials. Namely, in the context of many-body perturbation theory (MBPT), Hedin's GW approximation has been highly successful in predicting single-particle spectra and quasiparticle lifetimes. It is also used as a first step in the theoretical many-body study of two-particle excitations within the Bethe-Salpeter equation (BSE), which is required to obtain a correct description of photoabsorption spectra. On the other hand, time- dependent density functional theory (TDDFT) is an alternative to calculate optical spectra with neutral excitations, with the important advantage of being more amenable for practical simplifications than MBPT-based schemes.

For strongly correlated systems such as transition metal or rare earth compounds, recent progress has been achieved with the development of a realistic dynamical mean field theory based on the LDA electronic structure (LDA+DMFT). New challenges here related with a basis- independent general implementation of the DMFT scheme based on the first-principle Wannier-function formalism and incorporation of efficient impurity solvers based on continuous-time quantum Monte Carlo approach starting on strong and weak coupling diagramatic expansion. Important development towards the first-principle description of strongly correlated systems connected with unification of the non-local GW approximation and local DMFT technique (GW+DMFT).

Modern electronic structure calculations for materials with strong electronic Coulomb correlations have thus developed into a new research field at the border between band structure theory and quantum many-body problems. Since this area of research requires knowledge of different electronic structure approaches and complicated field theoretical techniques, it is very hard starting problem for young PhD researches. The San-Sebastian summer school have been filled this gap and have allowed the graduate students to acquire simultaneously knowledge and understanding in different parts of the ab-initio many-body theory.

The school have started with the general discussion of the Density Functional Theory (DFT) and its Time Depemdent (TDDFT) generalization. This lecture have been given by Dr. Robert van Leeuwen from Groningen (The Netherlands) who is the active researcher in this field. Dr. van Leeuwen also discussed the connection of TDDFT scheme to standard many- body Green Function theory. At the same time perfect introduction to new experimental techniques for excitation spectrum of materials have been given by Prof. Franz Himpsel from Wisconsin (USA), who pioneered application of the Angle-Resolved Photoemission Spectroscopy (ARPES) to investigation of real correlated systems. Important basic of so-called GW-scheme in the context of the many body theory for electronic structure was introduced by Prof. Rex Godby from University of York (UK) who is one of the main practitioner of this methods and head of the ESF cluster of excellence. At the end of the fist day, Dr. Miguel Marques from University of Coimbra (Portugal) discussed the application of TDDFT for finite systems, which followed by general discussion on calculation of excited spectrum in molecules and solids by TDDFT scheme.

In the second day Prof. Mikhael Katsnelson from the Radbout University of Nijmegen (The Netherlands) gave complete introduction to advanced Many-body perturbation theory (MBPT) and general way to calculate excitation spectrum of solid including the spin-wave excitation and optical spectrum. Starting from this many-body background Prof. Steven Louie from University of Berkeley discussed the GW scheme and the Bethe- Salpeter equation to investigate spectroscopic properties of real correlated solids. The first basic lecture on continuum Quantum Monte Carlo methods was given by Prof. Matthew Foulkes from Imperial College London (United Kingdom) who is one of the most active researcher in this field. An important lecture on general introduction to the physics of correlated clectron materials have been presenter by Prof. Dieter Vollhardt from University of Augsburg (Germany) who recently was awarded the Europhysics prize for this research. At the end of the second day an introductory lecture on angle-resolved photoemission spectroscopy (ARPES) and its application to the experimental study of the electronic structure of solids was given by Prof. Andrs Felipe Santander-Syro from Universit Paris-Sud (France) followed by short discussion on the many body effects in solids.

The third day was devoted to introduction to Dynamical Mean-Field Theory (DMFT) by Prof. Dieter Vollhardt from University of Augsburg (Germany) who is one of the co-founders of this very important new developments. In the following the diagrammatic (continuous-time) quantum Monte Carlo Methods for classical and quantum spins was introduced by Prof. Matthias Troyer from ETH Zurich (Switzerland) with very interesting presentation of the origin of the so-called sign problem in fermionic QMC simulations. Prof. Ralph Claessen from University of Wuerzburg (Germany) give very useful overview of physics of correlated electron materials from the point of view of experiments with photoelectron spectroscopy. The second lecture on application of Time Dependent Density Functional Theory, in this case to extended systems was presented by Francesco Sottile from Ecole Polytechnique, Paris (France). The applications of Quantum Monte Carlo to Solids have been discussed by Prof. Matthew Foulkes. At the end of this day the prospects and details of the new technique for electronic structure calculation of correlated solids, so-called LDA+DMFT scheme was given by Prof. Silke Biermann Ecole Polytechnique, Paris (France) following be general discussion on the problem of first-principle calculations of effective electron-electron interactions in solids.

The third day was devoted to realistic QMC scheme and Prof. Lubos Mitas from North Carolina State University, (USA) gave the impressive example of practical implementation of Quantum Monte Carlo for nanosystems and materials resulting in accurate description of electronic structure and dynamics. In addition, a novel so-called Resonating Valence Bond (RVB) approach for QMC simulations was discussed by Prof. Sandro Sorella from SISSA, Trieste (Italy). The correlated effects in f-electron materials within the Self-Interaction Correction (SIC) Scheme have been introduce by Prof. Z. (Dzidka Szotek) from Daresbury Laboratory (United Kingdom). The second part of diagrammatic continuous-time quantum Monte Carlo Methods for fermions was given by Prof. Matthias Troyer. An important new development of Wannier functions in the context of the Dynamical Mean- Field Approach to strongly correlated materials presented by Prof. Frank Lechermann from University of Hamburg (Germany). An interesting cluster generalization of the DMFT methods was introduced by Dr. Olivier Parcollet from CEA-Saclay (France).

The last day of the school start from the discussion on topology of fermion nodes and pfaffian wavefunctions by Prof. Lubos Mitas. A new important development to go beyond simple DMFT approximention within so- called Dual-fermion Approach to Nonlocal Correlations was introduce by Prof. Aleksey Rubtsov from Moscow State University. And finally Prof. Liu Hao Tjeng from University of Cologne (Germany) presented the crucial experimental talk on the testing modern theories for correlated systems. The school was ended with general panel discussion on perspectives and practical importance of the new development in the field of correlated electron materials.

Assessment of the results and impact of the event on the future direction of the field:

The School on Ab-initio Many-Body Theory in San-Sebastian was very well presented by young researchers all over the Europe and considered to be a successful attempt to introduce a comprehensive scheme for practical investigation of correlation effects in electronic structure calculation of real materials. The students and postdocs from different fields of computational materials science and many-body scheme were discussed futures of the Ab-initio Many-Body Theory for real materials. The number of applications (above 250) surpassed all expectatives and, of course, the limit of 90 places that we had to satisfy in order for the students to get the maximum benefit from the school, and also due to space and computer resource limitations. The students (graduate and postgraduate) also did actively participate in the round-tables and discussions.

The impact of this school on the future direction of correlated electronic structure is clearly seen on the very active discussion on the final panel meeting concerning the predictive power of new many- body scheme for realistic materials. It is clear that all participants will be involved in the future in the developments on accurate scheme for complex structure of correlated materials and nanosystems. The important future development in the field will be related with unifications of efficient LDA+DMFT scheme with accurate GW or TDDFT methods in electronic structure calculations, which was discussed in the present summer School in San-Sebastian.

Final programme of the meeting:

All lectures can be found on the website:

`http://dipc.ehu.es/arubio/mbschool.php`

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    Monday, July 23rd
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8:45 Registration

9:00-10:30 Introduction to density functional theory (DFT) and time-dependent DFT
Dr. ROBERT van Leeuwen
Rijksuniversiteit Groningen, The Netherlands

10:30-11:30 New experimental techniques for excitation spectrum of materials
Prof. Franz Himpsel
University of Wisconsin, USA

Coffee Break

12:00-13:30 Many-body theory in a nutshell and Hedin equation (GW)
Prof. REX Godby
Univertity of York, United Kingdom

Lunch

16:00-17:30 Theoretical advances in time-dependent DFT
Dr. ROBERT van Leeuwen
Rijksuniversiteit Groningen, The Netherlands

17:30-18:30 Aplications of TDDFT to finite systems
Dr. MIGUEL MArques
University of Coimbra, Portugal

18:30 Discussion session: TDFT and excitation spectrum of materials

Tuesday, July 24th

9:00-10:00 Advanced Many-body perturbation theory (MBPT)
Prof. MIKHAIL Katsnelson
Radboud University of Nijmegen, The Netherlands

10:00-11:30 GW and Bethe-Salpeter Equation Approach to Spectroscopic Properties
Prof. Steven G. Louie
University of California at Berkeley, United States

Coffe Break

12:00-13:30 Introduction to continuum quantum Monte Carlo (QMC) methods
Prof. MATTHEW Foulkes
Imperial College London, United Kingdom

Lunch

16:00-17:00 Introduction to the physics of correlated materials
Prof. DIETER Vollhardt
University of Augsburg, Germany

17:00-18:00 Experimental techniques for correlated materials
Prof. Andres Santander-Syro
Universite Paris-Sud, France

18:00 Round table: Basics of ab-initio and MBPT techniques

Wednesday, July 25th

9:00-10:00 Introduction to dynamical mean field theory (DMFT)
Prof . DIETER Vollhardt
University of Augsburg, Germany

10:00-11:0 0 Introduction to Quantum impurity solvers
Prof. Mathias Troyer
ETH Zurich, Switzerland

Coffee Break

11:30-12:30	Physics of correlated materials: Experiments Prof. RALPH Claessen University of Wuerzburg, Germany
12:30-13:30	Applications of TDDFT to complex systems Dr. FRANCESCO SOTTILE Ecole Polytechnique, Paris, France

Lunch

16:00-17:00	Applications of quantum Monte Carlo to solids Prof. MATTHEW Foulkes Imperial College London, United Kingdom
17:00-18:30	Prospects of LDA+DMFT calculations Prof. Silke Biermann Ecole Polytechique Paris, France
18:30	Discussion session and Round table: Correlated materials and LDA+DMFT

Thursday, July 26th

9:00-10:00	Quantum Monte Carlo for nanosystems and materials: Electronic structure and Dynamics Prof. Lubos Mitas North Carolina State University, United States
10:0-11:00	A novel resonating valence bond approach for QMC simulations Prof. Sandro Sorella SISSA, Trieste, Italy

Coffee Break

11:30.12:30 Self-interaction correction (SIC) scheme and f-electrons materials
Prof. Z. (Dzidka) Szotek
Daresbury Laboratory, United Kingdom

12:30-13:30 Continuous time Quantum Monte Carlo method
Prof. Mathias Troyer
ETH Zurich, Switzerland

Lunch

16:00-17:00 General DMFT scheme in Wannier basis
Prof. Frank lechermann
University of Hamburg, Germany

17:00-18:30 Cluster extension of DMFT scheme
Dr. Olivier Parcollet
CEA-Saclay, France

18:30 Discussion session and Round table: Applications of DMFT and QMC

Friday, July 27th

9:00-10:15 QMC: the fixed-node problem and the topology of fermion nodes
Prof . Lubos Mitas
North Carolina State University, United States

10:15-11:15 Beyond DMFT: dual fermion approach for non-local correlations
Prof. Aleksey Rubtsov
Moscow State University, Russia

Coffee Break

12:00-13:00 Testing modern theories for correlated systems
Prof. Liu Hao Tjeng
University of Cologne, Germany

Lunch

16:00-18:00 Synthesis session, Concluding remarks and
Round table: frontiers in the field new challenges

4 General Workshop/Conference Announcements

4.1 ADVANCED SCHOOL ON QUANTUM MONTE CARLO METHODS IN PHYSICS AND CHEMISTRY

21 January - 2 February 2008

Abdus Salam ICTP, Miramare, Trieste, Italy

Organizers: C. Filippi, S. Moroni, S. Sorella, C. Umrigar, S. Zhang

with the co-sponsorship of the DEMOCRITOS National Simulation Center

This Advanced School follows the "School on Continuum Quantum Monte Carlo" held at the ICTP in January 2004. After introducing the basics of the methods and giving a broad overview of the field, the School will focus on new developments in methodology and applications.

TOPICS:

- Random walks, Variational Monte Carlo, Projection Monte Carlo, Path Integral Monte Carlo;
- Improved wave functions and wave function optimization techniques, computation of forces and observables;
- Lattice Regularized Diffusion Monte Carlo, Auxiliary-Field Monte Carlo for any single-particle basis set, Auxiliary-Field Monte Carlo for spin/isospin-dependent problems, Coupled Electron-Ion Monte Carlo, Worm Algorithm and Diagrammatic Monte Carlo.

LECTURERS:

D.M. Ceperley, C. Filippi, W.M.C. Foulkes, S. Moroni, N. Prokof'ev, K.E. Schmidt, S. Sorella, C.J. Umrigar, S. Zhang.

Further information and the Online Application Form can be found at:

`http://agenda.ictp.it/smr.php?1929`.

The deadline for application is 5 October 2007.

As a rule, travel and subsistence expenses of the participants are borne by their home institutions. Some ICTP funds are available for a limited number of applicants who are nationals of, and working in, developing countries. See the Application Form.

Additional funding for partial support of a limited number of participants is available from DEMOCRITOS and the Materials Computation Center of UIUC.

EU applicants should send an e-mail to ¡qmc2008@democritos.it¿.
US applicants should consult `http://www.mcc.uiuc.edu/travel`.

There is no registration fee to attend this activity.

Secretariat:

SMR.1929 - Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry
c/o Ms. N. Ivanissevich the Abdus Salam International Centre for Theoretical Physics (ICTP)
Strada Costiera 11 I-34014 Trieste, Italy

Telephone: +39-040-2240383
Telefax: +39-040-224163
E-mail smr1929@ictp.trieste.it

ICTP Home Page: `http://www.ictp.trieste.it/`

4.2 2nd Workshop on "Ab Initio Phonon Calculations"

Cracow, 6-8 December, 2007

http://wolf.ifj.edu.pl/workshop/

The second workshop on Ab Initio Phonon Calculations" will take place in Cracow in December. The Workshop is devoted to discuss the results of application of ab initio approach to calculate finite temperature properties of materials via analysis of the phonons. Results of property modification by phonons in crystals with defects, disorder, grain boundaries, then specific phonon behaviour on surfaces, decorated surfaces, interfaces and amorphous systems will be disscussed.

Contributions dealing with strong electron-phonon and/or magnetic- phonon couplings are very welcome. Phonon measurements obtained by a number of sophisticated techniques like inelestic coherent and incoherent neutron scattering, coherent x-ray scattering, nuclear inelastic scattering, infrared absorption, and raman scattering, etc., are expected.

Participants from physics, chemistry, materials engineering, mineralogy, geophysics, etc., are very welcome, even if the ab initio approach plus phonon computations are not yet a routine practice for them.

We expect the participants to arrive on Wensday, December 5-th, and stay till Saturday afternoon, December 8-th, or longer to visit the Cracow old city.

The talks and oral presentations will be selected from the submitted abstracts.

Deadlines:

- registration: October 28, 2007.
- Abstract submission: October 28, 2007.

For more details look at: http://wolf.ifj.edu.pl/workshop/

Correspondence: workshop@wolf.ifj.edu.pl

Looking forward to hearing from you and seeing you at the Workshop.

Krzysztof Parlinski

4.3 DPG Symposium on Ferroic Materials and Novel Functionalities

Berlin, February 26, 2008

We are pleased to inform you about the upcoming DPG symposium on

”Ferroic materials and novel functionalities”

held in Berlin February 26, 2008 during the the next Spring Meeting (or the annual meeting) of the German Physical Society: Berlin, 25-29 February 2008 (Monday 8:30 am to Friday 4:00 p.m.).

For the detailed announcement and program please visit the web site of the workshop at:

http://nanoscience.physik.uni-halle.de/dpg/

or contact one of the organizers.

We hope that you or members of your group will participate.

Looking forward to see you in Berlin.

Ingrid Mertig

(on behalf of the organizers)

4.4 Forum on "Exact-exchange and hybrid functionals meet quasiparticle energy calculations"

at the Spring Meeting of the German Physical Society

Berlin, 25-29 February, 2008

Dear colleagues,

we would like to draw your attention to a forum on

"Exact-exchange and hybrid functionals meet quasiparticle energy calculations"

embedded into the upcoming Spring Meeting of the German Physical Society (25-29 February 2008). The Spring Meeting will take place in Berlin and has become the second largest conference (after the APS) covering all aspects of condensed matter and chemical physics, material science, surface science, as well as polymer and biophysics, etc. For 2008 more than 5000 participants are expected. The conference language has been English for a few years now.

The forum combines an invited symposium with contributed oral and poster sessions in a mini-workshop-like environment. For more information please visit the forum's web site at:

`http://www.fhi-berlin.mpg.de/th/Meetings/hybrid2008/`

or contact one of the organizers.

We are looking forward to welcoming you and/or members of your group at this event and invite you to participate directly by submitting an abstract for one of the contributed sessions.

Patrick Rinke and Matthias Scheffler

4.5 3rd Annual CNF Fall Workshop: *Defining the Interface Between Nanoscience and Geology*

Cornell Nanoscale Science and Technology Facility, Ithaca, NY

November 12th-13th, 2007

Organized by the NNIN/C (`http://www.nnin.org/nnin_compsim.html`)

Sponsored by the National Science Foundation

Workshop Coordinator: Derek Stewart (stewart@cnf.cornell.edu)

`http://www.cnf.cornell.edu/cnf_fallworkshop2007.html`

Overview: While nanoscale research and geology at first glance deal with vastly different time and length scales, several areas exist where nanoscale research can have profound impacts on geologic questions. Density functional approaches provide crucial tools for predicting high pressure crystal structures beneath the Earth's crust. Calculated phonon dispersions can also be linked to seismology research. Fluid transport through porous rocks can also benefit from tools used in microfluidics. While biomineralization creates macroscale structures like shells and coral, the nanoscale process that organisms use to create large inorganic structures is still largely unknown.

Format: This workshop will provide morning lectures on the theory behind different approaches followed by *hands-on* sessions on each code. In some cases, the participants will be able to learn directly from the code's creator. Graduate students and young researchers with theory or experimental backgrounds are encouraged to attend. In addition, complementary presentations on current experimental efforts will also help define high-impact areas for future simulation efforts.

Focus: Current computational needs in geology, first principles modeling of materials in the Earth, fluid flow through porous media, biomineralization

- Current Needs for Modeling at Small Scales for Geology
  - Linking predicted physical properties to large scale models (Jason Phipps-Morgan)
  - MEMs options for diamond anvil experiments (William Bassett)
- First principles modeling of materials in the Earth's core
  - Determining high pressure crystal structures (Richard Hennig)
  - Calculating phonon dispersions and links to seismology (Derek Stewart)
- Biomineralization

  - Molecular dynamics for biomineralization (John Harding)
  - An experimental perspective on biomineralization (Lara Estroff)
- Fluid flow through porous rocks
  - Modeling water and petroleum flow through materials with micro and nanoscale pores (TBD)

Tentative Code List: Quantum Espresso Package (plane wave density functional approach), DL POLY (Molecular Dynamics), Elmer (microfluidics)

Important Dates:
Registration deadline: **October 31st, 2007**
Financial aid may be available for graduate students
Seating is limited to 40 participants. Please register early!

5 General Job Announcements

Ph. D. Position in Materials Science and Physics

Department of Materials, Imperial College London, UK

A PhD position in Materials Science and Physics is available in the Materials Department at Imperial College starting in October 2007. The pro ject is to use density functional theory to model novel carbon nanotube based electronic devices. Funding is available for UK students, and possibly for EU and overseas students (for more information please contact Andrew Horsfield at a.horsfield@imperial.ac.uk)

Carbon nanotubes have extraordinary properties on account of their one dimensional structure (http://en.wikipedia.org/wiki/Carbon nanotube). From the point of view of electronic devices, they are attractive because of their high conductance, physical robustness and chemical inertness. Field effect transistors that operate at room temperature were constructed from nanotubes in 1998. Recently a new device that uses a nanotube for the gate as well as for the source and drain has been demonstrated (Park, J.-Y., Nanotechnology 18 (2007) 095202 (http://stacks.iop.org/Nano/18/095202)). Other three terminal devices have been constructed and modeled that are based on a Y shaped nanotube (Bandaru, P. R., et al, Nature Materials 4 (2005) 663 (http://dx.doi.org/10.1038/nmat1450)).

The first part of this project will be to use a novel density functional theory open boundary scheme ('hairy probes') to understand the electrical characteristics of known multi-terminal nanotube devices. We will then proceed to investigate a completely novel nanotube device which is anticipated to operate as an electronic nose able to detect a wide range of small molecules. Electronic noses are important in many areas including: detecting explosives, identifying diseases, and recognising gas leaks. The calculations will be performed with a view to motivating experimentalists to make the new device into a reality.

This project will require some code development using the C programming language, and the application of quantum mechanics to electrons and phonons. It will be supervised by Andrew Horsfield at Imperial College, but will be carried out in collaboration with Tchavdar Todorov at Queens University Belfast and David John at the University of Wales in Bangor.

Interested candidates should send an electronic copy of their CV to Andrew Horsfield
at a.horsfield@imperial.ac.uk .

Andrew Horsfield
Department of Materials, Imperial College London
South Kensington Campus, London SW7 2AZ, U.K.

a.horsfield@imperial.ac.uk
Phone:+44-(0)20-7594-6753; FAX:+44-(0)20-7594-6757

POSTDOCTORAL OR RESEARCH ASSOCIATE POSITION IN NREL'S SOLID STATE THEORY GROUP

THEORY OF NANOSTRUCTURES AND ALLOY THEORY

National Renewable Energy Laboratory (NREL), Golden, Colorado, USA

`http://www.sst.nrel.gov`

NREL's Solid State Theory Group is looking to fill a Postdoctoral or Research Associate position (depending on qualifications). The research areas include theory of nanostructures, alloy theory, and defect physics in solids. The positions are for up to 3 years, depending on mutual consent. The salary range is \$48,000 - \$65,000 per year, depending on seniority, qualifications, and experience. Applicants are expected to have a strong background in solid-state theory.

The position is with Alex Zunger, Solid State Theory Group Leader. The position is available for a start date between now and fall 2007. Applications are being considered now. For more details about ongoing work, see

`http://www.sst.nrel.gov`.

The Solid State Theory Group currently consists of ten Ph.D.s in condensed matter theory and interacts with a broad range of experimentalists. The group has outstanding computational facilities, an excellent basic-research atmosphere, and is located in the beautiful Rocky Mountains. Consult our web page for additional information on the group, its history, research subjects, publications, current and past personnel, and facilities.

Interested candidates should immediately send (electronic or paper) curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two to three references addressed to:

Alex Zunger
Solid State Theory Group
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401
USA

Post-doctoral Research Opening

Computational Materials Research Group

University of Tennessee in Knoxville, TN, USA

The Computational Materials Research Group at the University of Tennessee in Knoxville, TN is looking for a post-doctoral researcher to conduct molecular-level simulations of complex molecules in Metal- Organic-Frameworks (MOFs) as part of a larger multiscale materials modeling effort. Specifically, the researcher will be expected to use Monte Carlo and Molecular Dynamics simulations to generate adsorption isotherms and diffusivities of organic explosive molecules in MOFs.

The post-doc will have the opportunity to work in the dynamic research environment of the UT Computational Materials Research Group

(http://clausius.engr.utk.edu/cmrg/index.html)

which currently includes five UT professors, several post-docs, eight graduate students and numerous undergraduate researchers, all working on a variety of multiscale materials modeling projects from the quantum to the macroscopic scale. Furthermore, with near proximity to Oak Ridge National Laboratory (ORNL), the post-doc will interact closely with staff scientists in the UT/ORNL Joint Institute of Computational Science. Through the UT Computational Science Initiative, the post-doc will have access to the massively parallel machines at ORNL. Knoxville is a city of 175,000 situated in a beautiful and mild part of the country near the Smoky Mountains.

Researchers with PhDs in chemical engineering, physics, chemistry or a related field, with significant molecular modeling experience are encouraged to apply. The position starts no earlier than October 1, 2007 and, based upon satisfactory work in the first year, can be extended to two years. The salary is $40,000 per year. This project is sponsored by the National Science Foundation.

Interested individuals should send a CV and a list of references to Dr. David Keffer at dkeffer@utk.edu.

Ph.D. Position in Multiscale Computational Material Science University of Salerno (MolNaC Research Group), Italy

One Ph.D. position is available within the MolNaC Research Group

(`http://www.chem.unisa.it/groups/molnac`),

which is in the Department of Chemistry of University of Salerno (Italy)

The position is funded by a University grant. The succesful candidate will be part of a team working on multiscale modelling of polymers.

Requirements:

We are looking for candidates with a Master's degree in Chemistry, Physics or Chemical Engineering, and a background in physical chemistry or chemical physics. Actual experience with computational modeling is highly appreciated. We expect the candidate to have a clear affinity with computer programming and molecular simulations. Candidates should speak English fluently.

Application and information:

Suitable candidates are invited to send their Curriculum Vitae with motivation (half A4), a list of followed courses including grades, at least three references, and a list of publications to the following address, who is also available for further information:

Dr. Giuseppe Milano, Assistant Professor
University of Salerno
Department of Chemistry
Mailing Adress:
via Ponte don Melillo -I-84084 - Fisciano (SA)
Tel: +39 089 96 9567
Fax: +39 089 96 9603
E-mail: gmilano@unisa.it

webpage: `http://www.chem.unisa.it/groups/molnac`

Postdoctoral Positions
Rutgers University, New Jersey, USA

Up to three postdoctoral positions may be available in the groups of Prof. David Langreth, Prof. Karin Rabe, and Prof. David Vanderbilt in the Department of Physics and Astronomy at Rutgers University, to begin as early as January 1 2008. The target areas are: (1) application of van der Waals density functionals to the study of hydrogen storage materials; (2) multifunctional oxides and intermetallics with highly-reversible first-order structural phase transitions; and (3) fundamentals of domain retention and reversal in ferroelectric thin films.

Experience with first-principles density-functional methods is essential. Interested applicants should apply by email, attaching a CV (PDF preferred) and listing names and contact information of 2-3 references. Consideration of candidates will begin immediately and will continue until the positions are filled. Please send applications to the following address, using "Computational Electronic Structure Search" as the subject line:

Ms. Fran DeLucia
Department of Physics and Astronomy
Rutgers University

fran@physics.rutgers.edu

Postdoctoral Position

”Surface Reactivity: beyond Born-Oppenheimer approximation”

Surface Science Research Centre/Department of Chemistry,
The University of Liverpool, Liverpool, UK

A postdoctoral position is available to work on the EPSRC-funded project ”Surface Reactivity: beyond Born-Oppenheimer ”. The main objective is to go beyond the Born-Oppenheimer approximation and develop a theoretical and computational framework based on density functional theory for understanding the role of electronic non-adiabatic effects in surface dynamics and reactions.

The project will be supervised by Prof. Mats Persson (`http://www.liv.ac.uk/~mpersson`) and Prof. Stephen Holloway (`http://www.liv.ac.uk/chemistry`, `http://www/Staff/holloway.html`) and will also involve close collaborations with the project partner Prof. David Bird, Dept of Physics, Univ. of Bath (people.bath.ac.uk/pysdb/). You will be placed in the theory constellation at the Surface Science Research Centre (`http://www.ssci.liv.ac.uk`), comprising Prof. W. Hofer and Dr G. Darling and many international postdoctoral and PhD students. This centre also includes experimental activities in the field of surface science with a high international profile.

You should have (or be about to obtain) a PhD degree in theoretical/computational chemistry or physics. Good communication skills, experience of software and method development and density functional calculations are essential. Earliest starting date is 1 October 2007 and deadline for application is 7 september.

Please, contact Prof. M. Persson (e-mail: mpersson@liv.ac.uk) for informal enquires about the post.

For further details about the post and how to apply please consult

`http://www.liv.ac.uk/working/job_vacancies/research/R-563366.htm`

This post is funded from an EPSRC grant for nineteen months with possible extension.

Contact: Mats Persson
E-mail: mpersson@liv.ac.uk
Phone: +44-151-794 3518
Fax: +44-151-794 3870

Professorship of Materials Modelling - University of Oxford, UK

The University of Oxford has created a new professorship in Materials Modelling in the Department of Materials. This is an important post which complements the statutory chairs in Materials Processing and Materials Characterisation. The Professor of Materials Modelling would be expected to become the Director of the Materials Modelling Laboratory, a position currently held by Professor David Pettifor CBE FRS, the Isaac Wolfson Professor of Metallurgy. The University seeks to appoint a person with a record of outstanding international excellence in research within the field of materials modelling who, through leadership and the distinction of his or her contribution to the field, will ensure the pursuit of the highest standards in research and teaching in materials modelling at Oxford, and its wide recognition outside. The holder of the chair will be elected to a professorial fellowship at St Anne's College.

Applications are invited for the above post, tenable from 1 January 2008, or such later date as may be arranged. Further particulars, including details of how to apply, are available from

`http://www.admin.ox.ac.uk/fp/`

or from the Registrar, University Offices, Wellington Square, Oxford OX1 2JD (tel: 01865 270200).

The closing date for applications is Monday 1 October 2007.

Professor David Pettifor CBE FRS
Isaac Wolfson Professor of Metallurgy
Department of Materials
University of Oxford
Parks Road
Oxford OX1 3PH
UK

Tel.: +44 1865 273751
Fax: +44 1865 273783

Postdoctoral Position (m/f) in "Theory of Semiconductor Nanostructures"

Max Planck Institut for Solid State Research, Stuttgart, Germany

A Postdoctoral position (m/f) is available starting October at the Max-Planck-Institut for Solid State Research in Stuttgart, Germany. The research will be performed within a newly created Independent Junior Research Group (Nachwuchsgruppe). We wil building a vigorous and highly motivated group and will tackle a variety of problems related to electronic and optical properties of nanostructures. We will follow a bilateral approach with, on one hand, focused and short/medium-term projects on actual topics of interests that can be addressed with existing state-of-the-art theoretical methodologies, mostly in collaboration with experimentalists. On the other hand we will engage in medium/long-term method development projects.

Applicants should have a PhD in physics, chemistry, or materials science. The skills required from the candidate could originate from different (or a combination of different) research fields, such as atomic-scale simulations and electronic-structure theory at the LDA level (ABINIT, VASP, WIEN, etc...); beyond LDA calculations such as GW (+ Bethe Salpeter), time-dependent DFT, CI or DMFT; effective mass or k.p theory. It would be advantageous for the applicant to have applied the method(s) to nanostructures and to have a good knowledge of semiconductors, and some programming experience. The candidate should enjoy working in an open and dynamic environment where the exchange of ideas is an important component of day-to-day work. The salary will be according to general tariff regulations for employees in public service (TVOED-Bund). The position will be initially for 1 year with possible extension up to 3 years, upon mutual agreement. The selection process will start now and continue until the position is filled.

Interested candidates should send an application letter, CV, list of publications and the name of two referees, preferably by email to:

Dr. Gabriel Bester (Head of Group)
Max Planck Institute for Solid State Research
Heisenbergstr. 1
D-70569 Stuttgart
e-mail: G.Bester@fkf.mpg.de
`http://www:http://www.fkf.mpg.de/bester`

The Max Planck Society is committed to employing more handicapped individuals and especially encourages them to apply. The Max Planck Society seeks to increase the number of women in those areas, where they are underrepresented and therefore explicitly encourages women to apply.

Postdoctoral Position

Institute for Research and Development of Photovoltaic Energy (IRDEP), Paris, France

Ab initio simulation of materials for photovoltaic application

The purpose of the work is to model lattice vibration in semiconductors. These have an impact on the way photogenerated carriers loose energy in photovotaic cells and it is expected that by a better understanding of existing phonon modes losses experienced in existing semiconductors can be overcome.

This will be done using molecular dynamics after interatomic forces have been computed by ab initio models.

The work will be carried out at the Institute for Research and Development of Photovoltaic Energy, a joint CNRS-EDF laboratory, in the framework of a french consortium research effort.

Excellent references required.

Type of funding: Public sector funding (Grant)
Wage: 35000 euros/year (including benefits)

To be started a soon as possible.

HOW TO PUT FORWARD MY CANDIDATURE

Contact:

Jean-Francois Guillemoles

email: jf-guillemoles@enscp.fr

Institut de Recherche et Développement sur l'Energie Photovoltaïque (IRDEP),
UMR 7174 - CNRS-EDF-ENSCP

EDF R&D, 6 quai Watier, 78401 Chatou Cedex
fax: 33-1 30 87 85 65

Postdoctoral Position at Stanford/UC Davis in Quantum Simulations

A joint postdoctoral position is available immediately in the area of quantum simulations. The successful candidate will work with the Micro and Nano Mechanics group led by Prof. Wei Cai in the Mechanical Engineering Department at Stanford University (`http://www.stanford.edu/~caiwei`) and the Angstrom group led by Prof. Giulia Galli in the Chemistry Department at University of California, Davis (http://angstrom.ucdavis.edu). This position is sponsored by a 5-year US/DOE SciDAC project on quantum simulations of materials. The base of this postdoctoral position will be at Stanford.

The main purpose of this project is to develop efficient computational methods for quantum simulations of condensed matter under magnetic fields. The successful candidate is expected to implement new methods to large-scale quantum simulation codes and to perform massively parallel simulations to investigate the electronic structures of materials under magnetic fields. The electronic and structural property of nano-structures is also an important aspect of this project.

Postdoctoral candidates should have earned a PhD in Physics, Chemistry, Chemical Engineering or Materials Science. A strong computational background in the quantum modeling of materials properties is preferred while some experience with scientific software development and massively parallel computing would be a definite plus. Interested candidates should send their curriculum vitae and a list of references to:

Prof. Wei Cai (caiwei@stanford.edu)

and

Prof. Giulia Galli (gagalli@ucdavis.edu)

Please mark your message on the subject line: application for the postdoctoral position.

This job posting is also on line at

`http://www.stanford.edu/~caiwei/JobOpening`

Two year Postdoc Position

"Exploration of the self-healing potential of ionic liquids for solid materials"

Department of Materials Science, Delft University of Technology, The Netherlands

Applications are invited for a two-year post-doctoral position that is available immediately. The ideal candidate has experience in computational materials science. A PhD in materials science, physics, theoretical chemistry, or related field is required.

The objective is to explore computationally the utility of ionic liquids in materials systems, in particular with regard to creating self-healing materials. Therefore it is envisaged that it will be necessary to perform computer simulations on ionic liquids and their interaction with solids involving the development of effective potentials, molecular dynamics simulations, and quantum chemical calculations.

You will be interacting with a group of PhD students, postdocs, and staff so that good verbal communication skills in English are essential. The department of Materials Science at Delft University of Technology offers an exciting research environment with excellent facilities and working conditions. Candidates should have a detailed resume including an outline of their research achievements and interests as well as contact information for academic references to

Marcel Sluiter (M.H.F.Sluiter@tudelft.nl)
Virtual Materials Lab (M.H.F.Sluiter@tudelft.nl)
Department of Materials Science
Delft University of Technology
Mekelweg 2, 2628 CD Delft
The Netherlands

Email:M.H.F.Sluiter@tudelft.nl

Consideration of candidates will begin immediately and continue until the position is filled.

Postdoctoral Position

THEORY & MODELLING of CHARGE TRANSPORT in SEMICONDUCTING NANOWIREBASED DEVICES

CEA/DRFMC, Grenoble, France

A postdoctoral position (2 years) is opened at CEA/DRFMC (Grenoble, France) starting from January 2008 to work on the theory and simulation of charge transport in semiconducting nanowires(SCNWs) basedmaterialsanddevices(fieldeffecttransistors).

Chemically grown semiconducting nanowires are showing unprecedented structural quality which make them ideal systems to explore transport physics in low dimensionality, as well as to engineer novel nanodevices and architectures for nanoelectronics and optoelectronics applications. In this context, theoretical modeling and computational simulations are needed todeepentheunderstandingofthefundamentaltransportmechanismsinthesesystems.

The theory group of the CEA is presently developing several computational approaches to tackle the problem of charge transport in realistic models of SCNWs, including device (field effect transistors) simulation. Sophisticated tightbinding order N methods have been developed to investigate charge transport in different frameworks (Kubo, LandauerBüttiker, and Non Equilibrium Green's Function formalism (NEGF), selfconsistent Poisson SchrödingerSolvers).Abinitioapproaches are alsousedfordetailedunderstandingofatomicscale features (doping, defects, interfaces, etc.). These methodologies enable to address the intrinsic (quantum)transport properties of ideal and doped/disordered nanowires, as well as SCNWsbaseddevicecharacteristics.

This work will be performed within the context of the European Integrated Project "NODE" (NanowirebasedOneDimensionalElectronics). Thecandidatewillbeinchargetoinvestigate the transport properties of various semiconducting nanowire systems, in conjunction with transport experiments performed within the consortium. This will include exploration of quantumtransportphenomenainlowdimensionalsystems,aswellasdeviceorientedissues.

The candidate should have demonstrated some experience in state of the art semiempirical or/and abinitio methods, and preference will be given to people already familiar with transport physics, and/or electronic structure of semiconducting materials in confined geometries.

The candidate should send her/his CV to YannMichel Niquet (yniquet@cea.fr) and Stephan Roche (stephan.roche@cea.fr), with a list of publications, and contact details of two personsforreference

ThedeadlineforsubmittingapplicationsisOctober1.

AdditionalinformationsabouttheTheorygroup:

`http://wwwdrfmc.cea.fr/SP2M/L_Sim/QUI/YMNiquet`
`http://wwwdrfmc.cea.fr/Pisp/22/stephan.roche.html`

MoreaboutGrenobleanditssurroundings:

`http://www.iseretourisme.com/pages/index/id/1356`

Postdoctoral and Graduate Student Positions in the Angstrom Group at UC Davis

A postdoctoral and a graduate student positions are available immediately in the Angstrom group led by Prof. Giulia Galli in the Chemistry Department at University of California, Davis (http://angstrom.ucdavis.edu).

The postdoctoral position is to conduct classical and quantum simulations of oxide surfaces and interfaces under pressure, in collaboration with Shell Corporation. Candidates should have earned a PhD in Physics, Chemistry, Chemical Engineering or Materials Science. A strong computational background in the quantum modeling of materials properties is preferred, and experience with software development for large scale classical and quantum simulations would be a definite plus.

The graduate student position is to develop and implement methodologies beyond semi-local Density Functional Theory in large scale ab-initio simulation codes. Candidates are expected to have a strong interest in electronic structure calculations and software development for large scale quantum simulations.

Please send applications to Prof. Giulia Galli: gagalli@ucdavis.edu.

Giulia Galli
Professor of Chemistry
University of California, Davis
Phone: 530 754 9554
Fax: 530 752 8995
e-mail: gagalli@ucdavis.edu
http://angstrom.ucdavis.edu/

Administrative Assistant
Ms.Ibra Henley
Phone: 530-752-9744
e-mail: idhenley@ucdavis.edu

Postdoctoral Position at UC Davis/LLNL in Quantum Simulations

A joint postdoctoral position is available immediately in the area of quantum simulations. The successful candidate will work with the Angstrom group led by Prof. Giulia Galli in the Chemistry Department at University of California, Davis (http://angstrom.ucdavis.edu) and with the Quantum Simulations group led by Dr. Eric Schwegler (`http://www.llnl.gov/qsg`) at Lawrence Livermore National Laboratory. This position is sponsored by a 5-year US/DOE SciDAC project on quantum simulations of materials. The base of this postdoctoral position will be at UC, Davis.

The main purpose of this project is to develop and apply efficient computational methods for the study of the structural and electronic properties of condensed and nanostructured materials, both at ambient conditions and under pressure.

Postdoctoral candidates should have earned a PhD in Physics, Chemistry, Chemical Engineering or Materials Science. A strong computational background in the quantum modeling of materials properties is preferred, and experience with software development for electronic structure and ab-initio molecular dynamics calculations would be a definite plus. Interested candidates should send their curriculum vitae and a list of references to Dr. Eric Schwegler (schwegler1@llnl.gov) and Prof. Giulia Galli (gagalli@ucdavis.edu).

Four Professorship Openings in Mainz

At the University of Mainz there are four openings for professor positions (associate and full) in computational science. The aim is to strengthen the link between natural sciences and computer science. We would be very happy, if you could distribute this information and show it also to interested candidates.

For further information please contact

Kurt Kremer (kremer@mpip-mainz.mpg.de)

or anybody else you might know in Mainz.

6 Abstracts

Emergence of Strong Exchange Interaction in the Actinide Series: The Driving Force for Magnetic Stabilization of Curium

K.T. Moore
Lawrence Livermore National Laboratory, Livermore, California 94550, USA
G. van der Laan
Magnetic Spectroscopy Group, Daresbury Laboratory, Warrington WA4 4AD, UK
R.G. Haire
Oak Ridge National Laboratory, MS-6375, Oak Ridge, Tennessee 37831, USA
M.A. Wall, A.J. Schwartz,and P. Söderlind
Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Abstract

Using electron energy-loss spectroscopy in a transmission electron microscope, many-electron atomic spectral calculations and density functional theory, we examine the electronic and magnetic structure of Cm metal. We provide experimental evidence that angular momentum coupling in the $5f$ states plays a decisive role in the formation of the magnetic moment. The $5f$ states of Cm in intermediate coupling are strongly shifted towards the LS coupling limit due to exchange interaction, unlike most actinide elements where the effective spin-orbit interaction prevails. It is this Hunds rule coupling that is the key to producing the large spin polarization, which in turn dictates the newly found crystal structure of Cm under pressure. Our results are also in agreement with very recent dynamical mean field theory (DMFT) calculations for the actinide metals, which show the large change in spin-orbit expectation value between Am and Cm.

Published in Physical Review Letters **98**, 236402 (2007)
Manuscript available from g.vanderlaan@dl.ac.uk.

Electronic structure, chemical bonding, and magnetic properties in the intermetallic series $\mathbf{Sc_2Fe(Ru_{1-x}Rh_x)_5B_2}$ from first principles

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Abstract

First-principles, density-functional studies of the electronic structure, chemical bonding, ground-state magnetic ordering, and exchange-interaction parameters have been performed for the entire $Sc_2Fe(Ru_{1-x}Rh_x)_5B_2$ series of magnetic compounds. The results indicate that their magnetic properties depend in an extremely sensitive way on the degree of band filling and bandwidth. Continuous substitution of Ru by Rh changes the ground state from an antiferromagnet to a ferromagnet, as well as increases the effective spin moment caused by filling the bands with five additional electrons per formula unit together with a narrowing of the 4*d* band. The correlations between the character of the chemical bonding and the resulting exchange couplings are discussed. The enhancement of Fe–Fe exchange coupling caused by Rh/Ru atoms is estimated. Trends for the macroscopic ordering temperatures are correctly reproduced.

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Spin-mixing conductances of thin magnetic films from first principles

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Abstract

We present a first-principles theory of the spin-mixing conductance for a thin ferromagnetic film embedded epitaxially between two non-magnetic metallic electrodes. The complex spin-mixing conductance is formulated as a linear response of the spin torque experienced by the film due to the spin accumulation in one of the electrodes. The derivation is based on non-equilibrium Green's functions; the obtained result for the torque response is in agreement with the response of spin fluxes on both sides of the ferromagnet as well as with expressions derived within the Landauer-Büttiker scattering theory. Numerical implementation of the developed formalism employs the tight-binding linear muffin-tin orbital method and calculations are performed for selected metallic and half-metallic ferromagnetic films relevant for spintronics applications. The spin-mixing conductance of the Cu/Ni/Cu(100) system is found to exhibit pronounced oscillations as a function of Ni thickness; their period is explained by spin-resolved Fermi-surface properties of nickel. Investigated half-metallic films include the full-Heusler Co_2MnSi compound and the diluted (Ga,Mn)As magnetic semiconductors attached to non-magnetic Cr(100) leads; the imaginary part of their spin-mixing conductance has a magnitude comparable to the real part. This unusual feature has been qualitatively explained in terms of a free-electron model.

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Relation of Curie temperature and conductivity: (Ga,Mn)As alloy as a case study

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Abstract

Experimental investigations of diluted magnetic semiconductors indicate a strong relation between Curie temperature and conductivity. Both quantities depend nontrivially on the concentration of magnetic impurities, the carrier density, and the presence of compensating defects. We calculate both Curie temperature and conductivity of (Ga,Mn)As alloys in a self-consistent manner based on the same first-principles Hamiltonian in which the presence of compensating defects is taken into account. The effect of As antisites and Mn interstitials is determined separately, and a good agreement between theory and experiment exists only in the case where the dominating mechanism is due to the Mn interstitials.

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Magnetic Phase Control in Monolayer Films by Substrate Tuning

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Abstract

We propose to tailor exchange interactions in magnetic monolayer films by tuning the adjacent non-magnetic substrate. As an example, we demonstrate a ferromagnetic-antiferromagnetic phase transition for one monolayer Fe on a $\mathrm{Ta}_x\mathrm{W}_{1-x}(001)$ surface as a function of the Ta concentration. At the critical Ta concentration, the nearest-neighbor exchange interaction is small and the magnetic phase space is dramatically broadened. Complex magnetic order such as spin-spirals, multiple-Q, or even disordered local moment states can occur, offering the possibility to store information in terms of ferromagnetic dots in an otherwise zero-magnetization state matrix.

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Tuning LDA+U for electron localization and structure at oxygen vacancies in ceria.

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Abstract

We examine the real space structure and the electronic structure (particularly Ce*4f*electron localization) of oxygen vacancies in CeO_2 (ceria) as a function of U in Density Functional Theory studies with the rotationally invariant forms of the LDA+U and GGA+U functionals. The four nearest neighbour Ce ions always relax outwards, with those not carrying localized Ce*4f*charge moving furthest. Several quantification schemes show that the charge starts to become localized at $U \approx 3$ eV and that the degree of localization reaches a maximum at ∼6 eV for LDA+U or at ∼5.5 eV for GGA+U. For higher U it decreases rapidly as charge is transferred onto second neighbour O ions and beyond. The localization is never into atomic core-like states; at maximum localization about 80-90% of the Ce*4f*charge is located on the two nearest neighbouring Ce ions. However, if we look at the *total* atomic charge we find that the two ions only make a net gain of 0.2-0.4 e, so localization is actually very incomplete, with localization of Ce*4f*electrons coming at the expense of moving other electrons *off* the Ce ions.

We have also revisited some properties of defect-free ceria and find that with LDA+U the crystal structure is actually best described with U = 3-4 eV while the experimental band structure is obtained with U = 7-8 eV. (For GGA+U the lattice parameters worsen for $U > 0$ eV, but band structure is as for LDA+U.) The best overall choice is $U \approx 6$ eV with LDA+U and ≈ 5.5 eV for GGA+U since the localization is most important, but a consistent choice for both CeO_2 and Ce_2O_3, with and without vacancies, is hard to find.

(submitted to J. Chem. Phys.)
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Variational QMC study of a hydrogen atom in jellium with comparison to LSDA and self-interaction corrected LSDA solutions

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Abstract

A hydrogen atom immersed in a finite jellium sphere is solved using variational quantum Monte Carlo VQMC. The same system is also solved using density functional theory DFT, in both the local spin density LSDA and self-interaction correction SIC approximations. The immersion energies calculated using these methods, as functions of the background density of the jellium, are found to lie within 1 eV of each other with minima in approximately the same positions. The DFT results show overbinding relative to the VQMC result. The immersion energies also suggest an improved performance of the SIC over the LSDA relative to the VQMC results. The atom-induced density is also calculated and shows a difference between the methods, with a more extended Friedel oscillation in the case of the VQMC result.

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Bulk and surface electronic structure of alkaline-earth metal oxides: Bound surface and image-potential states from first principles

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Abstract

We present the results of a comparative *ab initio* study of the atomic and electronic structure of MgO, CaO, SrO and BaO and their relaxed (001) surfaces. Based on density functional theory (DFT), we use self-interaction-corrected (SIC) pseudopotentials which permit a reliable description of electronic properties, in particular. For the bulk crystals, we arrive at well established structural data and obtain valence as well as conduction bands which are in very good agreement with the results of quasiparticle calculations and experiment. The calculated geometric structure of the relaxed (001) surfaces is consistent with the literature data. Concerning electronic properties, the calculations reveal that MgO(001), CaO(001) and SrO(001) exhibit negative electron affinity allowing for the formation of image-potential states while BaO(001) does not. As a consequence, not only bound states which are localized at the surface occur in the former three cases but also a salient band of image states residing in vacuum in front of the surface appears in sections of the surface Brillouin zone. Such an image state band does not arise at the BaO(001) surface. Our results are in satisfying agreement with literature data from *GW* quasiparticle calculations and electron energy loss spectroscopy measurements which are only available for MgO(001), to date.

(submitted to Physical Review B)
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First-Principles Investigation of an Epitaxial Silicon Oxynitride Layer on a 6*H*-SiC(0001) Surface

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Abstract

In a recent Letter, Shirasawa *et al.* [Phys. Rev. Lett. **98**, 136105 (2007)] have experimentally shown that incorporation of nitrogen at the interface of a silicate adlayer on 6*H*-SiC(0001) leads to the formation of a well ordered, highly stable epitaxial silicon oxynitride (SiON) layer without dangling bond states. We investigate the structural and electronic properties of this intriguing novel system by employing density functional theory with self-interaction-corrected pseudopotentials. Our results corroborate the structural model infered from low-energy electron diffraction (LEED). In addition, our calculated filled- and empty-state scanning tunneling microscopy (STM) images are in excellent agreement with the experimental data clearly revealing that O and Si surface states of the silicate double-layer on top of the system, respectively, give rise to the observed images. The calculated surface band structure exhibits a surface band gap of 9 eV in agreement with the scanning tunneling spectrocopy (STS) data. The physical origin of this amazingly large gap is clarified.

(submitted for publication)
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Energy barriers for dissociative adsorption of H_2 molecules on Si, SiC, and diamond (001) surfaces: A comparison

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Abstract

We report first-principles investigations of the reaction of molecular hydrogen with the Si(001)-(2×1) and C(001)-(2×1) surfaces and discuss the results in light of our previous studies of H_2 reaction with two different SiC(001) surfaces, one of which is highly reactive to H_2 uptake. The calculations reveal that the reaction of H_2 with all above surfaces depends crucially on intricate combined effects of the substrate lattice constant, the arrangement of the surface dimers as well as the orientation and spatial extent of their dangling bond orbitals. In agreement with experiment, our results confirm that Si(001) and C(001) are inert to H_2 adsorption at room temperature because the adsorption pathways considered exhibit substantial energy barriers. They are in satisfying agreement with previous density functional and quantum Monte Carlo calculations which have been carried out for two specific reaction pathways only. Guided by our earlier studies on H_2 reaction with SiC(001) surfaces, we have considered a third reaction pathway which actually turns out to have the lowest energy barrier on C(001). A comparison of the energy barriers and reaction energies for the different surfaces addressed turns out to be particularly revealing.

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7 SCIENTIFIC HIGHLIGHT OF THE MONTH: An extensible and portable file format for electronic structure and crystallographic data

An extensible and portable file format for electronic structure and crystallographic data

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In order to allow software applications to interact and exchange data, file format specifications are mandatory. Widely agreed file format specifications are still lacking in the field of first-principles calculations of material properties. One of the (numerous) objectives of the European Network of Excellence “NANOQUANTA” (that is about to launch the “European Theoretical Spectroscopy Facility”) is precisely to specify file formats, for the contents that are relevant to the scientific activity of its constituent nodes. The present article gives an overview of the agreed specifications, relevant for selected content (crystallographic/density/potential/wavefunctions). The specification relies on the NetCDF library, widely used in many different scientific communities. It is a binary format, that provides complete portability of the files accross languages (C/C++/Fortran/...) and platforms (big/little-endian is irrelevant). The files are addressed by content, bringing in the additional advantages of extensibility and automatic backward compatibility. Different software applications already implement this specification, for which a specific I/O library has been developed. It is hoped that it will be implemented in other software projects, or (at least) will be the basis of even better file format specifications.

1 Introduction

In a domain of application where different software projects coexist, user's demand often drives file standardization. Different standards might be used concurrently, as, for example, JPEG, PNG, GIF, EPS, ... , that encode 2D images. The development of associated conversion software quickly follows the definition of the specification.

However, in a field which is in constant mutation, such as first-principles calculations of materials properties (electronic-structure based), every software project usually develops its own type of files, matching its capabilities at one moment in time, without paying much attention to file standardization. For reasons of ease of development and economical use of storage space, the large files are naturally based on the binary representation provided by the native programming language (e.g. F77/90, C/ C++). This has several drawbacks: (i) the produced files might not be portable between a big-endian platform to a little-endian platform (and vice-versa), or between a 32 bit and a 64 bit platform; (ii) files written in F77/90 cannot be easily read by C/C++ codes (and vice-versa); (iii) these files are not extensible, and one file produced for one particular version of the software might not be readable by a past/forthcoming version.

These problems were addressed by software scientists and several other scientific communities already a long time ago. In particular, the meteorology/climatology community developed a library, called NetCDF [1, 2], that provides tools for generating/reading files that are portable accross platforms (independent of the native binary encoding -big/little endian- but also of some platform specificity, like the 8-byte encoding of single precision on Cray machines, instead of the usual 4 bytes), independent of the programming language (C/C++, F77/90, Java, Perl, Python, ...), and addressed by content (usually solving the problem of backward compatibility). This appears in retrospect as a crucial step in the cross-validation of simulations performed by different groups, working with different platforms and codes.

The idea of standardization of file formats is not new in the electronic-structure community [3]. However, it proved difficult to achieve without a formal organization, gathering code developers with a sufficient incentive to realize effective file exchange between software. In the EU Nanoquanta Network of Excellence (see Appendix 1, where the connection with the future "European Theoretical Spectroscopy Facility" -ETSF- is outlined), the standardization of file formats appears as an explicit goal of the project. For the sake of brevity, we will refer to this project as NQ/ETSF. After several preliminary steps needed to achieve this goal, involving discussions on coding rules, selection of contact persons for the different NQ/ETSF software, and an agreement to use NetCDF for large files (instead of native binary files), a specification for NQ/ETSF file formats was gradually written, by way of "mini-workshops" and e-mail exchange.

The outcome of this procedure is a document available on the NQ/ETSF site [4], whose main ideas will be presented here, together with several detailed excerpts. This specification has already been implemented in different software, either on the basis of a full-fledged library, ETSF_IO [5, 6] or using an early exploratory interface [7] . Additional information can be found in Refs. [8, 9].

Actually, NetCDF is not the only possible standard in the above-mentioned context. HDF [10] also implements a software solution that addresses the portability and extensibility problems.

NetCDF being already used by several NQ/ETSF software projects at the start of our work, without major drawbacks (considering our target use), we simply stuck to this choice. As a matter of fact, NetCDF and HDF have now announced that they would merge within a few years.

Section II presents a brief account of the major characteristics of NetCDF, then outlines our generic design decisions for the NQ/ETSF file format specification, and lists the few global attributes of NQ/ETSF NetCDF files. The reader will not find there a full description of the use of NetCDF, but only sufficient NetCDF background to understand our design decisions and the NQ/ETSF specifications themselves. Then we present (Section III) the specification for files that contain (at least) a charge density, represented on a regular grid in real space. This is the simplest part of the NQ/ETSF specification, thus providing an excellent example of our methodology. In section IV, we briefly describe the specification for the potentials, crystallographic data and wavefunction parts of the NQ/ETSF files. Section V summarizes the present status of the specification, and planned improvements.

2 Generic design considerations

In a NetCDF (Network Common Data Form) file, a series of numerical arrays can be stored, each under the name of a variable, that might possess one or several attributes and possibly one or several dimensions. One finds also the global attributes of the file (not associated to one particular variable).

The NetCDF library provides functions to initialize a NetCDF file, to create variable names and their dimensions in this file, to associate attributes to them, to define their dimensions, and to store the associated numerical data. It provides also functions to inquire about the content of a file (names of variables, associated dimensions and attributes), to access the information associated to a variable name (in full or by segments), to copy it, to rename attributes or variables, or to delete some of its content. Thanks to the powerful inquiry functions, it is possible to get full information from a NetCDF file without *a priori* knowledge of its content. In most cases, however, the user knows the name of the variables, the content he/she would like to retrieve, and the associated dimensions.

The ability of NetCDF to retrieve the information, irrespective of the actual physical layout of the file, is a key characteristic allowing exchange of data between different software (and also different versions of the same software), that contrasts with the rigidity of the usual binary representations.

The first step in the NQ/ETSF specification consists in the definition of variable names, associated dimensions and attributes, and accurate definition of the corresponding physical quantities.

Our first design decision, following from the flexibility of NetCDF, dealt with the different types of variables/attributes and associated numerical information that might be stored in a NQ/ETSF NetCDF file. We distinguished four different types of variables:

(A) The actual numerical data (which defines whether a file contains wavefunctions, a density, etc), for which a name must have been agreed in the specification document [4] (and properly described in this specification document).

(B) The auxiliary data that is mandatory to make proper usage of the actual numerical data of A-type. The name and description of this auxiliary information is also agreed in the specification document [4].

(C) The auxiliary data that is not mandatory to make proper usage of the A-type numerical data, but for which a name and description has been agreed in the specification document [4].

(D) Other data, typically code-dependent, whose availability might help the use of the file for a specific code. The name of these variables should be different from the names chosen for agreed variables of A-C types. Such other data might even be redundant with them.

The four types are compatible with a file being sufficiently complete for use by many different codes, though adapted to the specific usage by each. The NQ/ETSF file descriptions to be provided below (and fully in the specification document [4]) are based on this generic classification: for three sets of numerical data (A-type : density/potential ; crystallographic ; wavefunctions), we define the auxiliary data that is mandatory to make proper usage of it (B-type variables). In addition, we provide names for variables that can be either mandatory or not (in the context of a file containing a density/potential, or a wavefunction, or crystallographic data, or other large numerical data not yet taken into account), but for which a NetCDF description has been agreed.

Some technical details concerning the use of NetCDF files will apply to all specifications in the NQ/ETSF framework:

(1) Concerning the names of variables, attributes, and dimensions, long names have been chosen, as close as possible to natural language (so inherently self-descriptive, e.g. "number_of_atoms").

(2) All names are lower case, except the global attribute "Conventions" - a name agreed by the NetCDF community.

(3) Underscores are used to replace blanks separating words in names.

(4) In the specification of the dimensions of the variables, the slow indices are left-most, and the fast indices are right-most, like in C, so that the order of indices has to be reversed in FORTRAN.

We come now to the description of global attributes, and of two attributes used for many different variables.

Global attributes are used for the general description of the file (mainly the file format convention). Important data is not contained in attributes, but rather in variables. There are five global attributes in NQ/ETSF files: "file_format", "file_format_version", "Conventions", "history", and "title". The first three are mandatory, while the fourth and fifth are optional. "file_format" is a character string, always equal to "ETSF Nanoquanta" . The real number "file_format_version" gives the version of the specification (2.1 at present). "Convention" is a NetCDF recommended attribute specifying where the conventions for the file can be found on the Internet, in our case "`http://www.etsf.eu/fileformats`". The string "history" is a NetCDF-recommended attribute: each code modifying/writing this file is encouraged to add a line about itself in the history attribute. The string "title" is a short description of the content of the file.

The problems associated with the definition of units have also been addressed in a global way, although the corresponding attributes will all be associated to a particular variable. “units” is one of the NetCDF recommended attributes. It applies to several variables in our case, although many of them (e.g. integer type variables) do not have a physical dimension (for variables with a physical dimension, this attribute is required). The use of atomic units (aka Hartree, the “units” variable attribute having the string value “atomic units”) is advised throughout for portability. If other units are used, the definition of an appropriate scaling factor to atomic units (“scale_to_atomic_units” attribute) is mandatory. Actually, the definition of the name “units” in the NQ/ETSF files is only informative: the “scale_to_atomic_units” attribute should be the only one used for machine reading of the file. Indeed, if “units” is something other than the character string “atomic units” (based on Hartree for energies, Bohr for lengths) we request the definition of an appropriate scaling factor. The appropriate value in atomic units is obtained by multiplying the number found in the variable by the scaling factor. Examples:

units=“eV” → scale_to_atomic_units = 0.036749326

units=“angstrom” → scale_to_atomic_units = 1.8897261

units=“parsec” → scale_to_atomic_units = 5.8310856e+26

This can be used to deal with unknown units. Note that the recommended values for the fundamental constants can be found in Ref. [11].

Dimensions (in the C/C++/Fortran sense) are used for one- or multi-dimensional variables. It is very important to remember that the NetCDF interface adapts the dimension ordering to the programming language used. The notation presented in the next sections is C-like, i.e. the last index varies fastest. In Fortran, the order is reversed. When implementing new reading interfaces, the dimension names can be used to check the dimension ordering. The dimension names also help to identify the meaning of certain dimensions in cases where the number alone is not sufficient.

NetCDF files that respect the NQ/ETSF specifications should be easily recognized, irrespective of whether they contain a density, wavefunctions, or crystallographic data. We suggest to append the string “-etsf.nc” to their names. The “.nc” extension is a standard convention for naming NetCDF files [12]. Some filesystems are case-insensitive, and this motivates the lower-case choice. Finally, a dash is to be preferred to an underscore to allow the files to be referenced by a Web search engine.

3 Specifying a density

We now specify the content needed for a file to be declared a NQ/ETSF density file (the density is represented on a real space grid). Of course, it should follow the general rules indicated above.

Such a file should contain (at least) three global attributes, two variables, and seven dimensions. The three global attributes (“file_format”, “file_format_version” and “Conventions”) have been mentioned in Section II.

The most important variable is “density”. It is a type-A variable for a file to be declared NQ/ETSF density file (and the only type-A variable needed for a file to be declared a density file). Its structure is the following (under C/C++ convention for ordering – Fortran is just the reverse):

double [number_of_components] [number_of_grid_points_vector3] [number_of_grid_points_vector2] [number_of_grid_points_vector1] [real_or_complex_density]

In the present status of the specification, such a "density" is suitable to represent densities obtained on a homogeneous 3D grid, typical of norm-conserving pseudopotential calculations, i.e. pseudodensities. In case of ultrasoft pseudopotentials, or Projector-Augmented Waves, the augmentation contribution is missing. Similarly, a specific treatment to represent the density inside an atomic sphere (as in Augmented Wave formalisms) is not yet defined. Later work will include the extension of the specification to such other basis methodologies.

The "units" attribute is mandatory. By default, the density is given in atomic units, that is, number of electrons per cubic Bohr. If another unit is used, the attribute "scale_to_atomic_units" is mandatory.

Eight other type-B variables or dimensions must also be specified in a NQ/ETSF density file, for the purpose of being able to interpret correctly the information contained in the "density" variable : "number_of_components", "number_of_grid_points_vector1", "number_of_grid_points_vector2", "number_of_grid_points_vector3", "real_or_complex_density", "primitive_vectors", "number_of_vectors", and "number_of_cartesian_directions". All of them, except "primitive_vectors", are NetCDF dimensions.

"number_of_components" is a dimension, with value 1, 2 or 4, related to the spin characteristics of the density: 1 if the density is a spin-scalar, 2 if the density is spin-collinear (spin up and spin down), 4 if the density is spin-non-collinear (average density, then magnetization vector in cartesian coordinates x, y and z).

"number_of_grid_points_vector1" gives the number of grid points along direction 1 in the unit cell in real space. A similar meaning applies to "number_of_grid_points_vector2" and "number_of_grid_points_vector3". The real space grid starts at the origin in real space, with coordinates (0 0 0).

"real_or_complex_density" is a dimension, with value 1 or 2, respectively, depending whether the density is real or complex, respectively. Complex densities in real space might happen in the framework of responses in perturbation theory.

The primitive vectors are now defined thanks to the variable "primitive_vectors", with structure (under C/C++ convention for ordering – Fortran is just the reverse):

double [number_of_vectors] [number_of_cartesian_directions]

The primitive vectors are specified in cartesian coordinates. The two additional dimensons "number_of_vectors" and "number_of_cartesian_directions" are always equal to 3. Despite the fixed value ("3") attributed to both of these dimensions, we choose to define them, in order to waive any ambiguity in the ordering of the dimensions for the "primitive_vectors" variable.

4 Outline of the full specification

The full specification document [4] proceeds from the simplest concepts to the most complex ones, at variance to the order by which we presented the specification of the density in Section III. After global attributes and the other widely used attributes, dimensions are defined, then several optional (typically type-C) variables, then finally the type-A and type-B variables.

Some of the dimensions have already been described in Section III : “number_of_vectors”, “number_of_cartesian_directions”, “number_of_components”, “number_of_grid_points_vector1”, “number_of_grid_points_vector2”, “number_of_grid_points_vector3”, “real_or_complex_density”.

Additional dimensions include (the list below is not exhaustive): “character_string_length”, “real_or_complex_wavefunctions”, “number_of_symmetry_operations”, “number_of_atoms”, “number_of_atom_species”, “number_of_kpoints”, “number_of_spins”, “number_of_spinor_components”, etc.

We decided to address from the very start the possibility to distribute the data on different processors, each accessing one of a series of files, which together contain the full information. In this context, we have associated to some of the dimension variables an additional pair of variables describing the distribution (or splitting) of data.

As an example, suppose that one deals with seven wavevectors (nicknamed kpoints) in the Brillouin Zone, with a wavefunction file to be distributed on two processors (hence two wavefunction files, one containing e.g. information related to wavevectors number 1, 3, 5 and 7, and the other containing information related to wavevectors number 2, 4 and 6). The value of the variable “number_of_kpoints” will be 7 in both files (as if the file had not been split), the value of the variable dimension “my_number_of_kpoints” (not defined if the file were not split), will be four for the first processor file and three for the second processor file. The value of the variable “my_kpoints” (not defined if the file were not split) will be (1,3,5,7) for the first processor, and (2,4,6) for the second processor.

In the category of optional variables (type-C), whose names were agreed upon in order to avoid divergence of the format for the additional data, one finds (the list below is not exhaustive): “valence_charges”, “number_of_electrons”, “kpoint_grid_vectors”, “exchange_functional”, etc.

At this stage, the specification document [4] presents the type-A and type-B variables for a file with crystallographic information. Such a file should contain (at least) three global attributes, seven variables and five dimensions. The type-A variables are “primitive_vectors”, “reduced_symmetry_matrices”, “reduced_symmetry_translations”, “space_group”, “atom_species”,“reduced_ato
and one among “atomic_numbers”, “atom_species_names”, “chemical_symbols”

After presenting the case of files with crystallographic information, the specification goes on with density and/or potential information. The density specification was fully described in Section III of the present article. The specification for different types of potentials (Hartree, Kohn-Sham, exchange-correlation) is very similar.

The last type of content of a NQ/ETSF NetCDF file concerns wavefunctions. The specification considers that such a file should contain enough information for one to be able to construct a density from it. Also, since the eigenvalues are intimately linked to eigenfunctions, it is expected that such a file contains eigenvalues. Of course, files might contain less information than that required above but still follow the naming conventions of NQ/ETSF. At least the above-mentioned considerations lead to a consistent choice of mandatory (type-A) variables. Such a file should contain at least three global attributes, twelve variables, and eleven dimensions. We will not describe in detail this last type of file in this overview.

5 Summary and discussion

A full specification for files with selected content related to electronic structure and crystallographic data has been defined, that relies on the NetCDF library. This specification inherits naturally of all the interesting properties of NetCDF-based files, in particular portability and extensibility. It is designed for both serial and parallel usage.

Several software in the Nanoquanta context can produce or read this file format. In order to further encourage its use, a library of Fortran routines [5] has been set up, and is available under the GNU LGPL licence. This library introduces an API with three levels of access. The lowest level is a wrapper around NetCDF calls to be able to call with one routine the commonly associated NetCDF calls (including dimension checks during read or write access). This level is independent of the NQ/ETSF specifications. Based on this low-level API, the group level is defined to give access to groups of variables matching the NQ/ETSF specifications. This group level gives an easy-to-use API to NQ/ETSF files with transparent handling of unit conversions... It is also designed to avoid as much memory copy as possible with a mapping between NQ/ETSF variable definitions and internal variables of user programs. Finally a third level API is available with incorporated routines such as validity checkers.

These API handle all the specifications (in their current version 2.1), including attributes and file splitting for parallel runs. An implementation in Fortran90 of these API has been done and is available on the Web [5]. A concurrent implementation in C is also scheduled.

Although the present version 2.1 of the specification allows already effective communication between different software, there is ample room for generalizations, along at least two different axes: (1) some other heavy numerical quantities might be specified, e.g. dielectric matrices that appear in the GW approximation, (2) basis sets beyond a regular 3D grid or a sphere of planewaves, naturally associated with norm-conserving pseudopotentials, might be supported. Concerning the latter axis, we are considering the definition of a support for wavelets in version 2.2 of the specification.

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7 Appendix

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[4] URL: `http://www.etsf.eu/fileformats`.

[5] URL : `http://www.etsf.eu/etsf\_io`.

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