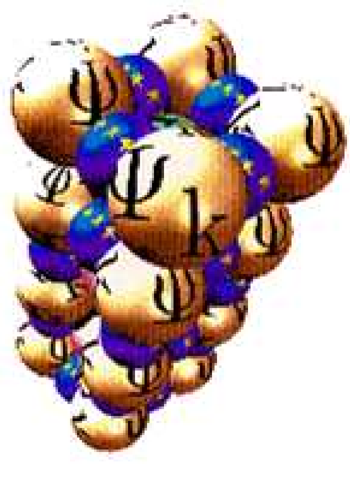
Ψ_k Newsletter

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

Number 85 February 2008



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

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and ESF Psi-k Programme

Contents

1 Editorial

As we are currently trying to change the format of the future Psi-k newsletters, the present newsletter in a way already reflects this transition period. It still contains some core information like workshop and position announcements, abstracts of recent or newly submitted papers, and a scientific highlight. However, in the future issues we would like to shift such contributions like workshop/meeting reports and the position and workshop announcements fully to the web, and in particular to the Psi-k Portal. The latter was already briefly described in the Psi-k Newsletter No 83, but we write about it again in this newsletter in the section following the editorial.

In this newsletter we also have a book announcement, just before the scientific highlight which is by James F Annett (Bristol, U. K.) Andrew I. Duff (Bristol, U. K., and Delft, The Netherlands), Balazs L. Gyorffy (Bristol, U. K.), Walter M. Temmerman (Daresbury, U. K.), Zdzislawa Szotek (Daresbury, U. K.) and Martin Lüders (Daresbury, U. K.). The title of the highlight is "Local Self-Interaction Correction of a Scattering Resonance: The Atom in Jellium Model". Please check the table of contents for details.

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

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

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 and Psi-k Mailing List

The Psi-k Portal, as already explained in the Psi-k Newsletter No 83, is a new interactive facility available on the Psi-k web pages (http://www.psi-k.org). From the portal it is possible to send e-mails to all the members of the portal, and to the original Psi-k mailing list which is also a member. One can create and join discussion forums, and upload files for a distribution across the portal member list and most importantly for an easy access to all members of the portal at all times. Thus, we would like to **encourage all our readers to join the portal**, if you have not done it yet, and to upload any announcements you may want to share with the Psi-k community, into the portal, and thus have them automatically distributed via e-mail. At the moment all the announcements appear also in the newsletters, but in future we would like to have them exclusively available only on the portal.

Similarly, in future we would also like everybody to upload their complete workshop/meeting reports, i. e. containing also a programme of the meeting, list of participants, and abstracts of presented papers, in addition to a one page summarizing report. The latter, namely the short report, we also want to include into the future newsletters, but not the former items. Thus, we would like to request that a separate file, in a latex format, containing a short report is also submitted to psik-coord@dl.ac.uk. In case of any problems with the uploads of reports, job/workshop announcements, etc., please do not hesitate to contact us and ask for help.

A useful calendar tool on the portal shows the dates of upcoming workshops and conferences. Users of the portal can enter their own workshops directly into the calendar.

The usual Psi-k mailing list is also a member of the portal, and the announcements uploaded to the portal go also to the mailing list. However, as the list is moderated, the e-mail containing the announcement first bounces to the psik-coord@dl.ac.uk for approval to avoid SPAM distribution. Unlike in the case of the portal, where only the members of the portal can distribute information, anybody can send an e-mail to the Psi-k mailing list and this is why it is moderated. So, if you are not a member of the portal a certain e-mail announcement may reach you with delay, caused by the fact that a human intervention is needed to approve that e-mail. There are times, unfortunately, when all the psik-coord members are away and therefore such delays are unavoidable. At present we are trying to arrange that the messages of the portal members to the Psi-k mailing list be also unmoderated, but not for the people who are only members of the Psi-k mailing list. **The intention is that in due course everything is distributed exclusively via the portal.** However, in this transition period, when some people only send their announcements directly to the Psi-k mailing list and not via the portal, then the people who are members of the portal, but not of the Psi-k mailing list, will not receive such e-mail messages. So, in the transition period to the portal **it is advisable to be a member of both**.

3 Psi-k School/Workshop/Conference Announcements

3.1 THIRD Psi-k/NANOQUANTA SCHOOL & WORKSHOP

Time-Dependent Density-Functional Theory: Prospects and Applications

August 31st to September 14th 2008

Benasque Center for Physics, Spain

http://benasque.ecm.ub.es/2008tddft/2008tddft.htm

Organizers:

E. K. U. Gross
Institut fuer Theoretische Physik
Freie Universitaet Berlin
Arnimallee 14, D-14195 Berlin, Germany
Phone: +49-30-838-54784
Fax: +49-30-838-55258
Mail: hardy@physik.fu-berlin.de
`http://www.physik.fu-berlin.de/~ag-gross/`

Miguel A. L. Marques
Laboratoire de Physique de la Matière Condensée et des Nanostructures (LPMCN)
Université Lyon I, UMR CNRS 5586, Bâtiment Brillouin
Domaine scientifique de la DOUA, Villeurbanne F-69622, France
Mail: marques@tddft.org

Fernando Nogueira
Dep. de Física, Faculdade de Ciências e Tecnologia
Universidade de Coimbra and
Centro de Física Computacional
Rua Larga, 3004-516 Coimbra, Portugal
Phone: +351-239410114
Fax: +351-239829158
Mail: fnog@teor.fis.uc.pt
`http://nautilus.fis.uc.pt/~fnog/`

Angel Rubio
Dpto. Fisica de Materiales, Facultad de Quimicas U. Pais Vasco,
Centro Mixto CSIC-UPV/EHU and
Donostia International Physics Center (DIPC)
Apdo. 1072, 20018 San Sebastian/Donostia, Spain
Phone: +34-943018292

Fax: +34-943015600
Mail: arubio@sc.ehu.es
http://dipc.ehu.es/arubio/

History:

The "School and Workshop on Time-Dependent Density Functional Theory" was first hosted by the Benasque Center for Science, Spain from August 28th to September 12th, 2004. The aim of the school was to introduce theoretical, practical, and numerical aspects of time-dependent density-functional theory (TDDFT) to young graduate students, post-docs and even older scientists that were envisaging a project for which TDDFT would be the tool of choice. The outstanding success of this school led to the organization of a second event, held once more in Benasque, from August 27th to September 11th, 2006.

This school is also part of a more general training effort conducted at the European level through the Psi-k Marie Curie Series of Events (Psi-k Training in Computational Nanoscience) and the NANOQUANTA network of Excellence.

The school will be followed by an international workshop, where the new developments of TDDFT and Many-Body Techniques for the calculation of excitations will be discussed. Students attending the school will be encouraged to attend the workshop, so they can get in contact with state of the art research in the field. The purpose of the workshop is to bring together leading experts in all these fields with different backgrounds, like density functional, many-body, nuclear physics, quantum chemists, and biophysicists. This will allow the exchange of ideas between the different fields and the creation of links between the traditionally separated communities. We believe that the intense and informal discussion which is possible in this kind of workshops can contribute to the formation of a strong community in the field of TDDFT.

Tentative program for the school:

The school will be attended by a maximum of around 40 students, and will last 9 days, with theoretical sessions (mostly) in the mornings and practical (tutorial) sessions in the afternoons. The theoretical sessions will consist of four lectures lasting for 45m each (including discussions). The practical sessions will last for 3 hours and a computer will be allocated for every two students. This will allow the students to have some time every day for studying and talking to the teachers. The program of the school starts with basic TDDFT, then continues with more complex theoretical and numerical aspects of TDDFT, and will end with an outline of some of its many applications. Basic knowledge on ground state DFT calculations is required. Also during the school we will address other approaches to describe excite state properties based on either many-body perturbation theory or quantum-chemistry schemes.

The preliminary program is:

Sunday, 31/08, afternoon: Registration

Monday, 01/09, morning:

TDDFT (2 x 45m, T)
Overview of spectroscopies (45m, T)
Many-Body - GW (45m, T)

afternoon:

Introduction to the practical classes
Introduction to the codes

Tuesday, 02/09, morning:

Overview of spectroscopies (45m, T)
TDDFT (45m, T)
Many-Body - GW (45m, T)
Many-Body - BSE (45m, T)

afternoon: Quantum Dots I (3h, P)

Wednesday, 03/09, morning:

TDDFT (45m, T)
Overview of spectroscopies (45m, T)
Propagation schemes (45m, T)
Many-Body - BSE (45m, T)

afternoon: Quantum Dots II (3h, P)

Thursday, 04/09, morning:

Advanced TDDFT (45m, T)
Models for time-dependent phenomena (45m, T)
Overview of spectroscopies (45m, T)
TDDFT as a tool in chemistry (45m, T)

afternoon: Quantum Dots III (3h, T)

Friday, 05/09: Free day

Saturday, 06/09, morning:

TDDFT as a tool in chemistry (45m, T)
Models for time-dependent phenomena (45m, T)
Advanced TDDFT (45m, T)
Current DFT (45m, T)

afternoon: OCTOPUS I (3h, P)

Sunday, 07/09, morning:

TDDFT as a tool in chemistry (45m, T)

Optimal control theory (45m, T)
Current DFT (45m, T)
Models for time-dependent phenomena (45m, T)

afternoon: OCTOPUS II (3h, P)

Monday, 08/09, morning:

TDDFT vs. Many-Body (45m, T)
TDDFT as a tool in chemistry (45m, T)
TDDFT as a tool in biophysics (45m, T)
Advanced TDDFT (45m, T)

afternoon: ABINIT+SELF I (3h, P)

Tuesday, 09/09, morning:

TDDFT vs. Many-Body (45m, T)
Models for time-dependent phenomena (45m, T)
TDDFT as a tool in biophysics (45m, T)
Current DFT (45m, T)

afternoon:

ABINIT+SELF II (3h, P)
Final Remarks

Wednesday, 10/09: Free day

During the school we will incentive a close and informal contact between the students and the teachers. Furthermore, the students will be stimulated to talk about their current research activities and future interests. We feel that this is an important point, since young scientists should be involved in the building up of a strong community.

The preliminary program of the workshop is:

The 4 day workshop will start September 10, 2008 in the afternoon and will end September 14 in the morning. It will include both invited talks on key aspects of TDDFT (45m each), contributed talks (30m) and a poster session. The tentative We plan an informal workshop with sufficient time for discussions. The informal character of the talks will be encouraged and presentations which are partly tutorial, given the mixed character of the audience, are most welcome. The time for each talk will be divided into 75

We will select some posters from the young researchers participating in the workshop to be presented as oral communications.

The update list of invited speakers and teachers can be found at

http://benasque.ecm.ub.es/2008tddft/2008tddft.htm

Location/Timing

We plan to organize this event at the “Benasque Center for Science”, Benasque, Spain, from August 31, 2008 to September 14, 2008. Benasque is a beautiful town in the heart of the Pyrenees. The school will take place from August 31 (Day 0 - arrival of students for the school) to September 10, and the workshop will start September 10 (arrival of participants to the workshop) and finish on September 14 (departure of all participants). See http://benasque.ecm.ub.es/.

Participants

The call for participation will be mainly directed to students and scientists specialized on computational physics, quantum chemistry and biophysics. We will limit the number of students to the school to 40 and participants to the workshop to less than 100, in order to ensure a maximum interaction between all the scientists participating. Attendance of graduate students and postdocs will be strongly encouraged through the inclusion of short contributed talks and a poster session. Furthermore, we will award to PhD students who present an outstanding poster short oral presentations.

3.2 Psi-k Training - Marie Curie Summer School

Modern Concepts for Creating and Analyzing Surface and Nanoscale Materials

12 - 16 May 2008

Hotel Eden Roc, Sant Feliu de Guíxols (Costa Brava), Spain

http://www.fhi-berlin.mpg.de/th/Meetings/MarieCuriePsik2008/

This Summer School seeks to foster discussion between leading and new practitioners in the science of surfaces, nanoscale materials, and heterogenous catalysis. Together, we will explore new experimental methods, new computational approaches, new model systems, and new applications of Surface and Nanoscale Materials Science through a series of plenary and invited lectures as well as lively poster sessions.

The School is suitable for advanced graduate students and post-docs, young faculty researchers, and industry professionals.

Space is limited; please follow the links below to submit an application as soon as possible.

For details on the prominent invited speakers, the workshop program and the beautiful venue please visit the conference web site
`http://www.fhi-berlin.mpg.de/th/Meetings/MarieCuriePsik2008/startup.php?GOTO=invspeaker.html`

The conference fee is 550 Euro/person (double room) and 620 Euro/person (single room). This covers all the conference activities, as well as accommodation, meals, transfer from Barcelona, and the outing event (visit to the famous Salvatore Dalí museum)
(`http://www.salvador-dali.org/museus/figueres/en_index.html`).

Limited travel grants are available for qualified graduate students and post-docs, regardless of nationality. Please indicate your needs and reasoning when applying. Support comes from Marie Curie Training, Psi-k, CECAM, IDECAT, and the NSF. Please register soon!
(`http://www.fhi-berlin.mpg.de/th/Meetings/MarieCuriePsik2008/`)

Young colleagues are invited to take part in the "Young Investigator Competition". The winner will be awarded a diploma plus 500 Euro in cash. Details can be found here

`http://www.fhi-berlin.mpg.de/th/Meetings/MarieCuriePsik2008/startup.php?GOTO=researcher.html`.

The organizers

Kristen Fichthorn (fichthorn@psu.edu)
Matthias Scheffler (scheffler@fhi-berlin.mpg.de)

4 General School/Workshop/Conference Announcements

4.1 2nd International Workshop on "Ab initio Description of Iron and Steel (ADIS2008): Magnetism and Phase Diagrams"

Ringberg Castle (Tegernsee, Germany)

June 15 - 20, 2008

Organizers: Jörg Neugebauer, Martin Friák, Tilmann Hickel
(MPI für Eisenforschung GmbH, Düsseldorf, Germany)

This workshop is the second meeting in a series of workshops on "Ab initio description of Iron and Steel". The aim of this series is to form a platform for leading experts in ab initio simulation and metal research to discuss and exchange their recent results and scientific concepts. At the same time the workshops intend to provide young researchers a high-quality introduction into the field.

A major focus of the workshop in June 2008 will be on recent developments in simulating magnetic phases and excitations as well as the consequences for finite-temperature properties/processes and phase transitions. Key experts in the field will give tutorial-like lectures on fundamental material properties as well as details of code implementation and empirical potential developments. Beyond magnetism, the combination of ab intio approaches with various thermodynamic and kinetic concepts will be a central topic of the workshop.

All participants have the opportunity to present their results in poster sessions. A selected number of 30-minute oral contributions will also be possible. In order to provide ample time for discussion and exchange the workshop is restricted to 40 participants. In order to register, please send an e-mail to hickel@mpie.de. The selection will be on a "first come first served" basis. The final deadline of registration is April 1, 2008.

The conference fee of 700 EURO is intended to cover the full-board accommodation from 15th of June (dinner) until 20th of June (breakfast), the abstract booklet, social events and the conference dinner. The workshop is organized by the department of Computational Materials Design (http://cm.mpie.de) at the Max-Planck-Insitut für Eisenforschung GmbH and sponsored by Psi-k.

4.2 The CAMD Summer School

"Electronic Structure Theory and Materials Design"

August 18-29, 2008

Lyngby, Denmark

Purpose:

The primary purpose of this summer school is to provide an introduction to density functional theory with particular emphasis on practical methodology and implementation aspects. Extensions beyond the standard DFT formalism will also be discussed.

The summer school will be a combination of lectures given by leading experts in the field and a workshop with exercises on the methodology covered in the lectures and exercises giving hands-on- experience with the Atomic Simulation Environment (ASE) supervised by expert users. The ASE is a general purpose open source simulation environment that can be used to setup, control, and analyze simulations in a number of electronic structure codes, for example including GPAW, Dacapo, ASAP, and Siesta.

During the project part the students will work with the focus on learning to produce publication quality simulations in small groups. The choice of projects will be within the fields of e.g. Catalysis, Molecular electronics, Biophysics, Alloy theory, and Electrochemistry, etc.

Subjects covered in lectures:

- Density Functional Theory
- GPAW and Projector Augmented Waves
- The Siesta program
- Orbital dependent functionals (SIC, van der Waals interactions)
- Time-dependent DFT
- The GW approximation
- Quantum transport theory
- Excitations in nanotubes
- Energy Materials
- Materials Science
- Chemistry at surfaces/Heterogeneous Catalysis
- Electrochemistry
- Materials Informatics
- Coupled Cluster Theory
- Quantum Monte Carlo

Lecturers:

- Jerry Bernholc, North Carolina State University
- Kieron Burke, University of California Irvine
- Gerbrand Ceder, Massachusetts Institute of Technology
- Hardy Gross, Freie Universitt Berlin
- Bjrk Hammer, University of Aarhus
- Berit Hinnemann, Haldor Topse A/S
- Hannes Jonsson, University of Iceland
- Steven Louie, University of California Berkeley
- Bengt Lundqvist, Chalmers Technical University and Technical University of Denmark
- Jens Jrgen Mortensen, Technical University of Denmark
- Jeppe Olsen, University of Aarhus
- Pablo Ordejon, University of Barcelona
- Thomas Rod, Atomistix A/S
- Angel Rubio, Universidad del Pais Vasco
- Hans Skriver, Technical University of Denmark
- Cyrus Umrigar, Cornell University
- Tejs Vegge, Ris National Laboratory
- Thomas Bligaard, Technical University of Denmark
- Karsten W. Jacobsen, Technical University of Denmark
- Jens K. Nrskov, Technical University of Denmark
- Jan Rossmeisl, Technical University of Denmark
- Kristian S. Thygesen, Technical University of Denmark

Scientific Organizing Committee:

- Jens K. Nrskov, Technical University of Denmark
- Karsten W. Jacobsen, Technical University of Denmark
- Jan Rossmeisl, Technical University of Denmark
- Kristian S. Thygesen, Technical University of Denmark
- Thomas Bligaard, Technical University of Denmark

Venue:

The CAMD summer school is located at the Technical University of Denmark in the pleasant Lyngby area North of Copenhagen. The school is held here in proximity to the beach, forests, lakes, and the Royal Park 'Dyrehaven' with wild deer and 200-year old oak trees.

Registration:

The registration fee is 1000 euro, which covers lectures, materials, computer time, housing during the summer school, summer school dinner, summer school excursion, and lunch during the days with lectures.

A number of scholarships are available to cover the 70 % of the registration fee for participants. In special cases, we can even waive the entire fee. The number of students is limited to 60. To apply for the CAMD Summer School, please send a one-page application letter as a pdf-file to Assistant professor Thomas Bligaard: bligaard@fysik.dtu.dk including:

- Your contact details.
- Your educational background.
- The title of your Ph.D.-project or the focus area of your research.
- A short description of the methodology you plan to use (or already use) in your research project.
- The approximate date you expect handing in your Ph.D.-thesis or terminate your post doctoral contract.
- The contact details of your Ph.D.-supervisor or post doctoral advisor (incl. e-mail address).
- In case you apply for reduced registration fee, please indicate what level of reduction and why you need a reduced fee.

4.3 International Center for Materials Research (ICMR) Summer School on Multiferroic Materials and Beyond

July 20 - August 1 2008, Santa Barbara, USA

The NSF-sponsored International Center for Materials Research (ICMR) is pleased to announce a residential fortnight-long summer school on Multiferroic Materials and Beyond, focused on materials needs in selected energy conversion technologies. The school will be held July 20 - August 1 2008, at the campus of the University of California, Santa Barbara.

The format will be tutorial, with emphasis on fundamentals and examples from current research by the speakers. The tentative plan is to dedicate the mornings to lectures and the rest of the day to discussion groups, software and experimental demonstrations, and student posters.

The goal of the school will be to present a comprehensive picture of the state of the art in the field of multiferroic oxides with an emphasis on the theory of the coexistence and mutual interaction of different orders and fundamental aspects of the broken symmetries, the search for new compounds exhibiting magneto-electric coupling and multiferroicity, and the novel physical phenomena that result - for instance, extremely complex magnetic phase diagrams, ferroelectricity induced by magnetic order, the rotation or complete reversal of the ferroelectric polarization in magnetic field, ferromagnetic order induced by electric as well as magnetic fields, and the discovery of new elementary excitations. The summer school is designed to encourage cross-fertilization of ideas among the participants.

The organizing committee comprises Sang Cheong, Bernd Lorenz, Janice Musfeldt, Silvia Picozzi, and David Singh.

The ICMR summer schools are coordinated by Nicola Spaldin (ICMR Director) and Jennifer Ybarra (Program Coordinator).

We welcome applications for the Summer School from graduate (PhD) students, post doctoral fellow and early career faculty. Participants are expected to be actively involved in multiferroics research. Local hospitality, meals, and housing will be provided. Partial travel support may be available.

How to apply:

Applicants should follow application instructions presented on the ICMR website:

http://www.icmr.ucsb.edu/programs/multiferroics.html

For further details, please contact the ICMR Program Coordinator, Jennifer Ybarra, at Ybarra@icmr.ucsb.edu

The application deadline is April 1, 2008.

Lecturers

Sang Cheong (Rutgers)
Paul Chu (Houston)
Michael Kenzelmann (ETH, Hopkins, NIST)
Kee Hoon Kim (Seoul)
Bernd Lorenz (Houston)
Thomas Lottemoser (Bonn)
Maxim Mostovoy (Groningen)
Janice Musfeldt (Tennessee)
Yukio Noda (Tohoku)
Silvia Picozzi (L'Aquila)
Ramamoorthy Ramesh (Berkeley)
David Singh (ORNL)
Nicola Spaldin (UCSB)
Mas Subramanian (Oregon State)
Ichiro Takeuchi (Maryland)

4.4 15th WIEN2k hands-on workshop

Vienna University of Technology, Vienna, Austria

March, 26 - 29, 2008

K. Schwarz and P. Blaha

http://www.wien2k.at

The WIEN2k programme package is one of the most popular DFT codes in Computational Materials Science used by more than 1200 groups world wide. It allows calculations of the electronic structure of solids and surfaces with high precision. The WIEN2k workshop includes elementary and advanced tutorials on DFT, electronic structure calculations, magnetic, optical and spectroscopic properties. In hands-on exercises the participants will learn how to use the code and interprete the results. In addition, there will be oral and poster presentations given by invited speakers and participants.

Following a long tradition, the WIEN2k workshop provides an arena for new and experienced WIEN2k users to discuss both, elemental questions as well as the latest developments in the world of WIEN2k.

For more information go to http://www.wien2k.at

4.5 Meeting on Molecular Dynamics for Non-Adiabatic Processes

21-22 July, 2008, Institute of Physics, 76 Portland Place, London, UK

Nanoscale phenomena, spanning multiple disciplines, share a unifying core problem: excitations away from equilibrium that evolve through non-adiabatic processes. Numerous techniques for modelling these have been designed and are undergoing rapid further development, usually within individual disciplines. A meeting is to be held to survey the spectrum of molecular dynamics based methods in order to highlight their strengths and weaknesses and to establish fundamental connections between them. It will be held on 21-22 July, 2008, at the Institute of Physics, 76 Portland Place, London

The format will be of a discussion meeting with invited talks given by leaders in the field, followed by time for discussion. The speakers will include:

John Tully
Oleg Prezhdo
Todd Martinez
Arieh Warshel
Sebastian Westenhoff
Tchavdar Todorov
E K U Gross
Lev Kantorovitch
Mads Brandbyge
Jonathan Tennyson
Dorothy Duffy

There will also be a poster session which is open to anyone registered to attend the meeting. At registration please indicate if you will be presenting a poster. There will be a prize of £200 for the best student poster.

Online register for this meeting will be at:

`http://www.iop.org/Conferences/Forthcoming_Institute_Conferences/event_22243.html`

Andrew Horsfield
Department of Materials, Imperial College London
South Kensington Campus, London SW7 2AZ, U.K.
Phone: +44-(0)20-7594-6753
FAX: +44-(0)20-7594-6757
E-mail: a.horsfield@imperial.ac.uk
SKYPE: HorsfieldA
AIM: AndrewHorsfield

4.6 12th European Conference "Physics of Magnetism"

24-27 June, 2008, Poznan, Poland

This meeting is a continuation of the previous ones held every three years since 1975 in Poznan.

The Conference is meant as an international forum for the presentation and discussion of novel scientific ideas, in a field of broadly understood magnetic phenomena, experimental results and new magnetic materials.

A special emphasis will be focused on:

1. Strongly Correlated Electrons and High Temperature Superconductivity
2. Quantum and Classical Spin Systems
3. Magnetic Structure and Dynamics
4. Spin Electronics and Magneto-Transport
5. Nano-structure, Surfaces, and Interfaces
6. Soft and Hard Magnetic Materials
7. Applications

Details on the PM'08 can be found on the conference web page at

http://www.ifmpan.poznan.pl/zp2/pm08.html.

Please note that the deadline for abstracts submission is March 1, 2008.

Please feel free to advertise the PM'08 in your institution and distribute this email among colleagues that could be interested to attend our meeting.

Note that our Conference will start just after workshop "Entanglement in Spin & Orbital Systems", organized in Cracow (Poland).

Feliks Stobiecki and Roman Micnas
PM'08 Chairmen

4.7 Symposium G, EMRS Fall Meeting

”Morphology and dynamics of nanostructures and disordered materials via atomic-scale modelling”

Warsaw, September 15-19, 2008

This symposium will be a forum of interaction and exchanges among scientists involved in the atomic-scale, computer based modeling of nanostructures (encompassing clusters, isolated or supported on substrates, complex molecules and supramolecular structures adsorbed at surfaces, and bulk systems for which nanostructural units can be clearly identified) and disordered systems, in particular those based on collections of constitutive units (such as network-forming glasses and liquids). It appears that modern approaches of modeling are applied to these two classes of systems on the basis of identical methodological requirements. These are targeted to provide the most accurate characterization of structure and migration mechanism. Therefore, a scientific meeting rooted on the consideration of nanostructures and disordered systems on the same theoretical footing becomes fully legitimate. To ensure adequate exposure and interaction with the experimental counterpart, two leading scientists reporting on experimental open issues and recent achievements in the area of nanostructures and disordered materials will be involved (one for each class of systems).

INVITED SPEAKERS:

Hervé Bulou (Strasbourg) (nanostructures on surface)
Carme Rovira (Barcelona) (biological nanostructures)
Mark Wilson (Oxford) (disordered systems)
J. Y. Raty (Lige) (disordered systems)
C. Molteni (London) (nanosystems, liquids and biomolecules)
Alessandro Mattoni (Cagliari) (nanocrystals in amorphous systems)
C. Dellago (Wien) (methodology, transition path sampling approaches)
Annick P. Dejaegere (Strasbourg) (bio-computing)
Phil Salmon (exp glasses, Bath)
K. Morgenstern (exp nanostructures, Hannover)
S.Ispas (simulation of glasses, Montpellier)
D. Chrobak (simulation of nanophases, Katowice)

CONTRIBUTED TALKS WILL BE SELECTED AND ARE ENCOURAGED IN THE FIELDS COVERED BY THE MEETING

DEADLINE: May 12, 2008.

In order to plan your venue, please check the web site:

http://www.e-mrs.org/meetings/fall2008/

Deadlines:

- Abstract deadline: May 12, 2008 - Notification of acceptance and mode of presentation: June 23, 2008

Fees for the whole conference:

Early registration fees (before July 31):

- Regular fee: 395 Euro
- Student fee: 260 Euro

For further information, please contact:

Carlo Massobrio (Carlo.Massobrio@ipcms.u-strasbg.fr)
Fabrizio Cleri (fabrizio.cleri@isen.iemn.univ-lille1.fr)
Rafal Kozubski (rafal.kozubski@uj.edu.pl)

4.8 Summer School on Ab Initio Modelling in Solid State Chemistry - MSSC2008

September 15-19, 2008 - London

http://www.cse.scitech.ac.uk/events/MSSC2008/

Directors

N M Harrison - Imperial College London
F Cora - University College London

The Department of Chemistry of Imperial College London, the Computational Materials Science Group of the Science and Technology Facilities Council, and the Department of Chemistry of University College London is organizing the tenth MSSC Summer School on the ab initio modelling of crystalline and defective solids with the CRYSTAL code. The week long school is designed for PhD students, Post-Docs and researchers with interests in solid state chemistry, physics, materials science, surface science, catalysis, magnetism and nano-science. It will provide both an introduction to the capabilities of quantum mechanical simulation and to the practical use of CRYSTAL06 (http://www.crystal.unito.it).

Outline of the Subjects

- Basic ingredients in solid state calculations: space groups and point symmetry; reciprocal space and Bloch functions; Hamiltonians and basis sets.
- The structure of the CRYSTAL code: selection of the basis set and Hamiltonian; controlling accuracy and numerical precision.
- Total energy and related quantities: equations of state, solid state reactions, phase transitions.
- Geometry optimization: strategies and techniques.
- Vibrational frequencies in solids: lattice dynamics and thermodynamics.
- One electron properties: DOS, band structure, charge and spin density maps, electrostatic potential.
- Surface chemistry and heterogeneous catalysis: models, accuracy and limitations.
- Local defects in solids: the observables of interest; the possible strategies.
- Dielectric properties .
- Magnetism and properties associated with unpaired electrons.
- Localized crystalline orbitals - Wannier Functions.
- Explicit electron correlation: MP2 for crystals.

Program

The school will last five days (15-19 September 2008) and will be held at the Chemistry Department at Imperial College London. The course is self-contained with the morning lectures providing the theoretical and computational background required for the afternoon sessions involving practical tutorials. By the end of the week an attentive student will be able to perform reliable calculations of material properties. There will be the possibility to present posters that will be on display for the whole school and discussed during a special session. Participation is limited to 50 people with local accommodation available at Beit Hall in single rooms for £49 per night. The registration fee is £150, which does not include accommodation. A small number of bursaries will be available.

Lecturers

The local staff of the Computational Materials Science Group will be joined by international experts including: M Alfredsson - University of Kent (UK), S Casassa, R Dovesi, B Civalleri University of Torino (Italy), I Bush, B Searle, A Wander - STFC Daresbury (UK), F Cora - UCL (UK), K Doll - MPI Stuttgart (Germany), CM Zicovich Wilson - Cuernavaca (Mexico).

Deadlines and Contact Information

Registration will close on Friday 15 August 2008 - or before if the limit of 50 people is reached.

Poster abstracts must be submitted by Friday 15 August 2008.

E-mail : d.r.jones@dl.ac.uk Fax: +44 (0)1925 603634 Tel: +44 (0)1925 603805
Postal Address: Damian Jones, MSSC2008, Daresbury Laboratory, Warrington, WA4 4AD, UK

4.9 Computational Molecular Science 2008

The Royal Agricultural College, Cirencester, UK

22 - 25 June 2008

http://www.chm.bris.ac.uk/cms

This conference is to promote and explore the best of UK computational molecular science. It will have 5 plenary speakers (Martin Karplus, Martin Head-Gordon, Mike Robb, Jean-Pierre Hansen and Michael Klein) as well as a number of mostly UK invited speakers. The basic aim is to bring together the best practitioners in the field, with a broad and inclusive interpretation of 'computational molecular science'.

Registration is open at http://www.chm.bris.ac.uk/cms, and the deadline is 21st March 2008. Registrations after this date will attract a higher fee.

The Organizers

Fred Manby
Jeremy Harvey
Neil Allan
Gabriel Balint-Kurti
Adrian Mulholland

Centre for Computational Chemistry
School of Chemistry, University of Bristol
Bristol BS8 1TS, UK

5 General Job Announcements

Two Postdoctoral Fellowships in Condensed-Matter Atomistic Modeling

Commissariat à l'Energie Atomique, Bruyères-le-Châtel, France

Applications are invited for two post-doctoral positions based in Bruyères-le-Châtel, (35 km from Paris), within the atomistic simulation group of the Electronic and Optoelectronic Hardening Laboratory of Commissariat à l'Energie Atomique (CEA). Our lab consists of 15 researchers with national and international collaborations and conducts applied research in the fields of microelectronic and optoelectronic hardening.

This position is for a one-year term, extendable by one year. The appointments will be available from March 2007.

1. The research will focus on growth of HfO_2 on silicon surface; electronic structure calculations using ab initio methods will be used to investigate the reaction of molecules containing Hf on the silicon surface. Collaborations with national and international experimental labs will allow getting an experimental validation of calculations. A PhD in quantum chemistry or in condensed matter simulation and experience of ab initio (DFT) calculations are essential.

2. The research will focus on growth of SiO_2 on silicon surface; electronic structure calculations using ab initio methods will be used to investigate the reaction of O_2 molecules on the silicon surface. A Kinetic Monte Carlo Code will then be used starting from the ab initio results to reproduce industrial processes. Here again, collaborations with national and international experimental labs will allow getting an experimental validation of calculations. A PhD in quantum chemistry or in condensed matter simulation and an experience of ab initio (DFT) calculations or Kinetic Monte Carlo codes are essential.

Informal enquiries about the post and applications can be made directly to Dr N Richard by e-mail (nicolas.richard@cea.fr). Candidates should include a full CV and a list of publications.

POSTDOCTORAL OPENING

Theoretical Chemistry of Surfaces, Interfaces and Catalysis

Laboratory of Chemistry, C.N.R.S.,

Ecole Normale Supérieure de Lyon, France

"Theoretical Insight in Selective Hydrogenation of Unsaturated Aldehydes in a Realistic Catalytic Environment"

A postdoctoral position is open in the field of theoretical modeling of reactivity at catalytic surfaces at the Laboratory of Chemistry of Ecole Normale Supérieure de Lyon, starting from January 2008.

In the recent years, the modeling of reactivity of multifunctional molecules at catalytic surfaces has been essentially performed by neglecting the influence of the catalyst support and of the solvent [1,2]. However, it is well-known that the environment plays a critical role on the catalyst activity and selectivity. A probative example is the selective hydrogenation of unsaturated aldehydes (crotonaldehyde and prenal for citral fine chemistry) on platinum particles deposited on oxide supports (ceria, zirconia). Indeed, understanding the origin of the activity and selectivity requires a more realistic description of the metal/support interface, on one hand, and of the solvent/metal interaction, on the other hand.

In the Laboratory of Chemistry, the theory group has gained expertise throughout the years for adsorption properties and reactivity of organic molecules at metallic and oxide surfaces. In particular, the mechanism of a chemoregioselective reaction occuring at a metal surface has been recently elucidated by examining all the elementary steps at the atomistic level and by modeling kinetics [1,2]. It is worth mentioning that our theoretical group is involved in several european research networks such as IDECAT, MONET, EUROSYM.

Hence, the successful post-doctoral candidate will tackle these complex systems on the basis of density-functional theory calculations (VASP program). The applicant should have a PhD in theoretical chemistry and/or condensed matter theory from a reputable higher education institution. Experience with DFT electronic structure calculations of periodic systems would be very helpful.

The project is part of a National Research Agency contract (SIRE, "SImulation of chemical REactivity at interfaces", other annoucements can be found at http://perso.ens-lyon.fr/paul.fleurat-lessard/ANR) in collaboration with three other French institutions (ENPC, IFP in Paris and LSDSMS in Montpellier). So the candidate is also expected to interact with these theoretical groups. The position is funded with a net salary of 2039 Euros per month.

The Ecole Normale Supérieure de Lyon provides an outstanding environment for research and teaching with a permanent staff of experts in chemistry and physics, and a continuously renewed staff of young graduate and postdoc researchers who wish to launch a successful career in these fields (see http://www.ens-lyon.fr for more details). Living in Lyon is also very nice and pleasant. The city is famous for its gastronomy.

Please send a cover letter and professional CV to Dr Françoise Delbecq or Dr David Loffreda at francoise.delbecq@ens-lyon.fr or David.Loffreda@ens-lyon.fr. Recommendation letters will be requested after a preliminary selection.

Dr David Loffreda
University of Lyon, Institute of Chemistry of Lyon
Laboratoire de Chimie, UMR CNRS 5182
Ecole Normale Supérieure de Lyon,
46 Allée d'Italie, F-69364 Lyon Cedex 07, France
tel: (+33) 4 72 72 88 43
fax: (+33) 4 72 72 88 60
email:David.Loffreda@ens-lyon.fr
http://perso.ens-lyon.fr/david.loffreda

Dr Françoise Delbecq
University of Lyon, Institute of Chemistry of Lyon
Laboratoire de Chimie, UMR CNRS 5182
Ecole Normale Supérieure de Lyon,
46 Allée d'Italie, F-69364 Lyon Cedex 07, France
tel: (+33) 4 72 72 88 43
fax: (+33) 4 72 72 88 60
email:francoise.delbecq@ens-lyon.fr

References

[1] Loffreda, D.; Delbecq, F.; Vigné, F.; Sautet, P. *Angwandte Chemie International Edition* **2005,** *44,* 5279.

[2] Loffreda, D.; Delbecq, F.; Vigné, F.; Sautet, P. *Journal of the American Chemical Society* **2006,** *128,* 1316.

Postdoctoral Position in Electronic Materials Theory
University of Nebraska-Lincoln, USA

A postdoctoral position in computational materials science is immediately available in the group of Prof. Kirill Belashchenko at the University of Nebraska-Lincoln. The research work will involve applications of electronic structure theory in materials and nanoscience. Powerful computing resources are available. The initial appointment will be for one year, with a possible extension upon mutual agreement and availability of funding. Candidates must have a doctoral degree in physics and experience in electronic structure calculations. Interested candidates should send an application letter, CV, list of publications, and contact information for at least two references to Kirill Belashchenko (preferably by email in PDF format).

Review of applications will begin immediately and continue until the position is filled. UNL is committed to a pluralistic campus community through EEO/AA. We assure reasonable accommodation under ADA/504; contact Beth Farleigh at (402)472-2770 for assistance.

Kirill Belashchenko
Assistant Professor
Department of Physics and Astronomy
University of Nebraska-Lincoln
Lincoln, NE 68588-011
Phone: (402)472-2396
Fax: (402)472-2879
Email: kdbel@unlserve.unl.edu

PhD Student Position at the EPF-Lausanne, Switzerland

The Institute for Numerical Research in the Physics of Materials (IRRMA) at the EPFL in Lausanne is seeking an outstanding PhD student to perform research in the domain of defects at semiconductor-oxide interfaces. Typical methods involve first-principles electronic structure calculations and ab initio molecular dynamics simulations. The position shall become available at the earliest on 1st April 2008 and requires a universitary degree in physics or physical chemistry (or equivalent), which should have been obtained by the starting date. The candidate will have teaching duties and shall prepare a doctoral thesis at EPFL. The hiring of the candidate is subject to admission to a doctoral programme at EPFL (on-line application is possible at

http://phd.epfl.ch/application).

A good background in quantum mechanics and previous experience in FORTRAN programming are required. The interested candidates should as soon as possible send their (1) curriculum vitae, (2) the list of passed examinations and relative marks, and make sure that (3) confidential letters of recommendation are sent to

Prof. Alfredo Pasquarello
EPFL-SB-ITP-CSEA, Station 13 / PPH-340
CH-1015 Lausanne, Switzerland
Tel. +41/21/6934416
email: Alfredo.Pasquarello@epfl.ch

More information on

http://irrmawww.epfl.ch/

and

http://itp.epfl.ch/page13360.html

Ph. D. and Postdoctoral Positions

”Electronic ground state and exited state properties of complex oxidic structures”

Max Planck Institute of Microstructure Physics Halle

and University of Halle, Germany

(with Dr. A. Ernst/Prof. W. Hergert)

Main topic of the project is the investigation of electronic and magnetic properties of complex oxides by means of ab initio methods. We will investigate ground state and exited state properties of strongly correlated oxidic systems. Magnetic properties of defects and impurities in layered oxidic systems are of special interest.

The project is part of the research initative (SFB762) ”Functionality of oxidic interfaces”.

The two positions will become available in January 2008.

A good background in quantum mechanics and solid state theory will be necessary. For a postdoc position experience with first-principles electronic structure calculations and high perfomance computing is expected.

The interested candidates should send their application (CV, list of passed examinations, confindetial letters of recommendation) as soon as possible to:

Prof. W. Hergert
MLU Halle-Wittenberg
Institut of Physics
Von-Seckendorff-Platz
1 D-06120 Halle

For more information email:

wolfram.hergert@physik.uni-halle.de or aernst@mpi-halle.de.

Postdoctoral Position at the Universite de Poitiers, France

Postdoc position in Condensed Matter/Atomistic Modelling at the Laboratoire de Mtallurgie Physique, University of Poitiers, France.

Applications are invited for a post-doctoral position in the ”Physics of defects and plasticity” group, based in the Laboratoire de Mtallurgie Physique of the University of Poitiers (France). The focus of the research will concern dislocation cores, and in particular the study of core stability and mobility in relation with the presence of impurities. The materials of interest are silicon and silicon carbide. Numerical simulations will be mainly performed with first principles methods.

The position is part of a large project ”Atomic Scale Simulation of Dislocations in Materials: ab initio and semi-empirical calculations”, gathering research groups in four laboratories, and is funded by the French National Agency for Research. Interactions with groups involved in the project are possible.

The group ”Physics of defects and plasticity” is constituted by 13 researchers, with a strong expertise in the study of defects in materials using theoretical and experimental methods, and with national and international collaborations. 4 researchers are theoreticians, all active in performing various kinds of numerical simulations (DFT, ab initio and classical molecular dynamics) with different standard tools, and are strongly involved in the project. Calculations are performed using local PC clusters, as well as with access to National Computing Centers. There is also a large experimental component in the group, with expertise in the structural and electrical characterization of defects (DLTS, TEM, RX,...), working in close collaboration with theoreticians.

The ideal candidate should have a deep background in solid state physics or materials science, and be very familiar with electronic structure calculations, in particular Density Functional Theory. In addition, he should have an experience in defect investigations, especially dislocations. The position is for a one year term. The appointments will be available from April 2008. For further information or submission of your complete application (CV, list of publications, references, letters of recommendation) please contact

Dr. Laurent Pizzagalli
Laboratoire de Mtallurgie Physique
UMR CNRS 6630 - Universit de Poitiers
SP2MI, BP 30179
F-86962 Futuroscope Chasseneuil Cedex
France

Laurent.Pizzagalli@univ-poitiers.fr
Phone +33 (0) 549497499
Fax +33 (0) 549496692

Postdoctoral Position

National Renewable Energy Laboratory, Golden, USA

Postdoctoral Research Positions in Computational Materials Physics/Chemistry

National Renewable Energy Laboratory (http://www.nrel.gov/cms/) invites applications for a theoretical postdoctoral position, available immediately. Initial assignment is for one year, but renewable upon funding availability, performance, and mutual agreement up to a total of three years. Research direction will be one of the followings: (1) Development and application of first-principles computational methods for weak interactions including van der Waals, Kubas, and hydrogen. (2) Computational materials design and characterization for high-density energy storage in forms of hydrogen and electrochemical energies. A recent Ph.D. (less than three years) in physics, chemistry, and/or materials science with significant experience and ability to use state-of-the-art electronic structure analysis softwares is preferred. The starting salary is US$45-55K per year depending on qualification and experience. Candidates should send electronically curriculum vitae including research interest and publication list, and two or three electronic files of their selected publications to

`Yong_Hyun_Kim@nrel.gov`, and arrange two or three reference letters upon request.

NREL, 14 miles away from downtown Denver, is one of US Department of Energy's prestige National Laboratories, a gate to the beautiful Rocky Mountains and ski resorts, and an equal opportunity/affirmative action employer.

Yong-Hyun Kim
National Renewable Energy Laboratory
1617 Cole Blvd.
Golden, CO 80401, USA

Postdoctoral Position at Molnac

http://www.molnac.unisa.it

An exceptional Post Doc candidate is required to carry out a collaborative research project between the group of Dr. Giuseppe Milano and an a well known industrial partner ('ST Microelectronics').

The project involves the development and application of new molecular simulation methods at atomistic and coarse-grained level to polymeric materials relevant in Nanoelectronics. Experience in modifying and writing Molecular Dynamics and/or Monte Carlo codes (not simply using packages) is required.

The appointment is for one year with the possibility of a yearly renewal thereafter. The research group has good computational facilities, and friendly atmosphere. Computational facilities at Molnac include local workstations, two beowulf cluster, and access to large computer resources via membership at the main supercomputer centres in Europe.

Please send a CV and names of 3 references to Dr. Giuseppe Milano (gmilano@unisa.it)

Postdoctoral Position

Nanoscience Center, Copenhagen University, Denmark

THEORY OF TRANSPORT IN NANOCONDUCTORS: ENERGY-DISSIPATION AND INDUCED ATOMIC DYNAMICS

A postdoctoral position (2 years) is available within theory/simulation of electron transport in nano-scale conductors. The position is with Mads Brandbyge at MIC, DTU in close collaboration with Per Hedegrd, Nanoscience center, Copenhagen University. The preferred starting date is early 2008.

The aim is to develop theory and methodology, and undertake numerical simulations of vibrational excitation and atomic dynamics in nanoconductors under non-equilibrium conditions, e.g. in the presence of electronic current. The applicant should have a strong background in condensed-matter theory, preferably experienced in electronic transport and programming/numerical calculations. We offer a stimulating environment encompassing theoretical groups both at DTU (www.mic.dtu.dk, www.nano.dtu.dk) and Nanoscience Center (Copenhagen University, www.nano.ku.dk), as well as good contact to experimental groups in Denmark and abroad. The salary and appointment terms are negotiated in accordance with the current collective agreement for Danish University faculty members.

Applications (marked ”nano-transport post doc.”) should be send to HR@mic.dtu.dk and must be received no later than March 1, 2007. Applications should include a CV, a list of publications, and the names of at least two references.

Postdoctoral Position

Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, France

A postdoctoral position is available in the condensed matter theory group of the Centre de Physique Theorique of Ecole Polytechnique, Palaiseau, France:

http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm

The purpose is the further development and application of the GW+DMFT approach which combines Hedin's GW approximation and dynamical mean field theory. This approach aims at a description of the electronic structure of correlated materials from first principles.

The starting date of the position is fall 2008 or earlier.

Candidates should be familiar with first principles electronic structure calculations. Previous experience with GW calculations will be a very positive point.

Please send your CV, a brief description of your research interests, and the names of at least two referees to: silke.biermann@polytechnique.edu

Additional postdoctoral positions are also available in the group, see:

http://www.cpht.polytechnique.fr/cpht/correl/jobs/jobs.htm

Two PhD studentships in Computational Materials Theory
School of Physics, Trinity College Dublin, Ireland

Two PhD studentships in the field of electronic structure calculations for strongly correlated oxides, ferroelectrics, and magnetic materials are available within the School of Physics at Trinity College Dublin. Possible starting dates for both positions are April 2008 or October 2008. All tuition and fees as well as an annual stipend of 16,000 euro are covered. The successful candidates will perform research in one of the following areas:

1. First principles modeling of functional complex oxide heterostructures, in particular combinations of magnetic and ferroelectric materials.

2. Combining density functional theory with many-body approaches such as dynamical mean field theory (DMFT), and application to functional transition metal oxides.

A strong overall motivation and a keen interest in theory and computation, as well as in addressing specific materials science problems and in working interdisciplinary between physics, materials science, and chemistry is required. Experience in working with UNIX/Linux environments and programming in either Fortran or C/C++ is beneficial.

Founded in 1592, Trinity College Dublin is Ireland's oldest university and was recently ranked 53rd of the top world universities in the Times Higher Education Supplement (1st within Ireland and 13th within Europe). Trinity's campus is located in the heart of Dublin, one of Europe's most vibrant capital cities. The School of Physics at Trinity College has a very strong research program in computational materials science and maintains close links with several on-campus interdisciplinary research centers, such as CRANN (Center for Research on Adaptive Nanostructures and Nanodevices) or TCHPC (Trinity Center for High Performance Computing), and also with many research groups abroad. Typically, to obtain a PhD degree from the School of Physics takes about three to four years.

Applications including cover letter, CV, references, and a short statement of research interests (pdf format preferred) should be sent to:

Dr. Claude Ederer
School of Physics
Trinity College
Dublin 2
Ireland
email: edererc@tcd.ie

Please feel free to contact Dr. Ederer directly for more information (see also: www.tcd.ie/Physics/People/Clau

Postdoctoral Opportunities in Copenhagen

Electronic Structure Theory and Simulation

The Center for Atomic-scale Materials Design (CAMD)
Technical University of Denmark

The Center for Atomic-scale Materials Design (CAMD) invites applications for two postdoctoral positions in the field of electronic structure theory and simulations. Applicants should have a background in theoretical physics or quantum chemistry at the PhD level. Basic knowledge of Density Functional Theory (DFT) as well as some programming experience is preferred.

CAMD is a theoretical physics and chemistry research center located at the Technical University of Denmark north of Copenhagen. We offer a dynamic and international working environment with research activities within several areas of theoretical and computational solid state physics including surface science, catalysis, biophysics, and molecular electronics. The center consists of five professors, and presently twelve postdocs, and seventeen PhD students. We have extensive experience in electronic structure theory and its applications, and maintain and develop our own real space DFT code 'GPAW'. Our own Linux supercomputer cluster, Niflheim, containing 1400+ CPUs provides optimum conditions for large-scale computer simulations.

Self-interaction corrections in electron transport: Avoiding self-interactions is important for a proper description of electronic transport through molecules and other nanosystems. The successful applicant will work on the development and implementation of self-interaction correction schemes in the GPAW DFT code and applying the method to quantum transport simulations. During the implementation the applicant is expected to work independently on the project, but will interact with and profit from the rest of the GPAW code development team.

Simulations of metallic gold nanoparticles: The applicant will work on quantum simulations of gold nanoparticles with special emphasis on the electronic and chemical properties close to the transition point from molecular to metallic behavior. The simulation of gold clusters containing ¿100 atoms will take advantage of the unique scalability of the GPAW code to large numbers of processors.

The monthly salary will be approximately 27.500 DKK (3670 Euro).

For both positions funding is available for two years.

Applications including CV and list of publications should be sent to Professor Karsten W. Jacobsen (kwj@fysik.dtu.dk) or Assistant Professor Kristian S. Thygesen (thygesen@fysik.dtu.dk) before February 15, 2007.

Postdoctoral Position(s) opened at Duke University

Posdoctoral position(s) opened at the Department of Mechanical Engineering and Materials Science, Duke University. We are looking for highly qualified candidates from theoretical materials science and/or applied computational physics.

Type of appointment: postdoctoral associate(s)

The work to be done by the postdoc(s) will be related to the one (or more) of the following topics:

- phase stability of titanium superalloys - high-throughput investigation of novel superconductors - non proportionality of ceramics for nuclear detection (Research supported by ONR, NSF and NSF-DNDO).

Candidates must have deep knowledge of thermodynamics of materials, solid state theory, kinetics of materials, surface science and ab initio calculations and programming (there is a lot of C/C++ coding involved on UNIX servers).

Further information on the research of our group as well as a publication list can be found in the group web page: http://materials.pratt.duke.edu

We consider applications until the positions are filled.

Candidates should send (in PDF)

1) short cover letter
2) curriculum vitae (including list of publications)
3) description of their research activity and interests (1-2 pages)
4) list of 2-3 names (emails/phones) of potential references

to stefano.curtarolo@duke.edu

NOTES

- Please send only PDF materials.
- Do not send pdf reprint of important papers, instead add the proper "DOI" or "ARXIV" links to the cover letter.
- Positions are for 1 year (renewable every year).

Prof. Stefano Curtarolo
Assistant Professor of Materials Science
Duke University, Dept. Mechanical Engineering and Materials Science
144 Hudson Hall, Box 90300, Durham, NC 27708-0300
Phone: 919-660-5506
E-mail: stefano@duke.edu
http://materials.pratt.duke.edu

PhD Position
Lund University, Sweden

Lund university announces a PhD position within the area

"Ab Initio Theory of Time-Dependent Phenomena at the Nanoscale".

For full detail see

http://www.teorfys.lu.se/phd08/phdeng08a.html

Deadline for applications: 13 February 2008.

A fundamental, and yet largelyunexplored aspect of condensed matter physics is time dependentphenomena. While being a challengingtask to accomplish, a detailed understanding of time-dependent phenomena has far reaching implications (often involving new physical concepts) and high potential pay-off, especially at the nano scale: virtually all future nano-technologies will use devices interacting in some way with an environment which rapidly changes in time. In the last decade, time-dependent density functional theory, TDDFT, has emerged as a most effective way of treating such non-equilibrium phenomena.

Research Project

We are looking for a PhD student to work at a TDDFT description of non-equilibrium, time dependent phenomena with strong electron-electron (and possibly electron-phonon) interactions. The student will have the chance to learn about theoretical solid state and nano scale physics and ab-initio many-body theory. Starting from an available density functional theory (DFT) computer program, he/she will develop a TDDFT code for timedependent phenomena. This will require the study of novel exchange-correlation potentials, a key ingredient to DFT and TDDFT. He/she will apply the new TDDFT code in the areas of quantum transport, laser induced material phase changes, quantum entanglement, dynamical response to high pressure and high magnetic fields. These topics deal with some of the most active and exciting fields in theoretical and experimental physics, and are of direct relevance to nano-electronics, quantum information, geo- and bio-physics, catalysis, etc. The theoretical research in Lund will be done in collaboration with US Air Force Research Laboratories and Sandia National Laboratories in Albuquerque, New Mexico, USA.

Carl-Olof Almbladh
Dept of Mathematical Physics
Lund University
E-mail: coa@teorfys.lu.se

Postdoctoral Researcher in Quantum Chemical Simulation of Materials Deposition

Theory, Modelling and Design centre, Tyndall National Institute, Cork, Ireland

http://www.tyndall.ie/

Applications are invited for a postdoctoral research fellowship at Tyndall National Institute applying quantum chemical simulation techniques to the deposition of high-permittivity materials. This is part of an EU-funded project to develop new flash memory devices and the research will be carried out in collaboration with experimental groups across Europe.

Job Title: Researcher
Location: Theory, Modelling and Design centre, Tyndall National Institute
http://www.tyndall.ie/
Reports to: Dr Simon Elliott
Reference No.: SE-07

1. Principal Accountabilities

To model the atomic layer deposition of dielectric layers needed for high-density flash memory, in particular the top dielectric, and for the transistor gate stack in CMOS technology. The modelling results will be used to guide precursor selection, optimise growth conditions and minimise impurities. First principles (ab initio) calculations will be used to investigate the key chemical reactions in the atomic layer deposition process. Dependence on process conditions will be examined via kinetic Monte Carlo simulations. In both cases, new models will be developed using existing simulation software.

To report and disseminate the results. To survey the literature and assess emerging alternatives for precursor chemistries, deposition technologies and novel materials in high-density flash memories.

To promote the use of materials simulation in high-tech industry, via publications, conferences and training events, as well as fostering bilateral partnerships.

To pursue research in associated areas of materials science.

2. Vision/Context/Nature

This is part of an EU-funded project to develop new flash memories and the research will be carried out in collaboration with experimental groups in academia and industry across Europe.

It is also expected that the research will feed into related activities (both experimental and theoretical) in Tyndall and around Ireland, including interaction with partners in the semiconductor industry. It is expected that the research will enhance the status of Tyndall within the relevant research communities and strengthen our ties with industry.

3. Knowledge and Experience/Personal Attributes

Applicants should hold a doctoral degree (or equivalent) in chemistry, physics, computational or materials science, or a related discipline, and must have experience in first principles or quantum chemical methods, such as density functional theory. A background in stochastic methods for modelling kinetic processes would be beneficial. Alternatively, experience in the processing and characterisation of nanostructured oxide materials would be advantageous. The ideal candidate will have a good publication record, be self-motivated and show enthusiasm for research.

4. Nature of position

Fixed term contract for two years, to start as soon as possible. Renumeration based on level of experience and on the Irish postdoctoral salary scale
(http://www.iua.ie/iua-activities/documents/07scalesdefinitions.pdf).

5. Contacts

Please send your CV, a cover letter, contact info for referees and copies of relevant publications to simon.elliott@tyndall.ie

This advertisement is also available at

`http://www.tyndall.ie/control/include_database.html?TC=65&DB=~/jobs.dbf&OL`

or via ”careers” - ”research” - ”SE-07” at http://www.tyndall.ie

Postdoctoral Position for Atomistic Study of Metastable Phases

Nanostructured Materials Group
Department of Physical Metallurgy and Materials Testing
University of Leoben, Austria

The research will focus on first-principles calculations for ternary transition metal nitrides and the effect of alloying elements (group III, V, and VI transition elements) on structure, elastic properties, phase stabilities, and electronic configuration. Nitrides in various fields for mechanical as well as functional uses are increasingly important for tools, components in automotive and aerospace application, as well as for the always growing field of microelectronics like diffusion barriers, gate-electrodes, heat-sinks and light-emitting diodes. The aim of the project is the development of a state-of-the-art understanding of metastable phases in nitrides and their decomposition processes to reach equilibrium. For this, high-quality density-functional theory (DFT) calculations will have to be combined with concepts from statistical mechanics, thermodynamics, and kinetics.

Applicants should have a PhD in physics, chemistry, or materials science, and have experience with atomic-scale simulations and electronic-structure theory. The candidate should enjoy working in an open and dynamic environment, and actively interact with the other groups in the department as well as with the experimental co-workers.

The research is part of a START Program funded by the FWF (the Austrian Science Found) with partners from other departments, research institutes, and universities. The salary will be according to the rules of the University of Leoben and the Austrian Science Found. The position is limited to two years, with the possibility of extension.

The University of Leoben is an equal opportunities employer. Women are encouraged to apply.

Interested candidates should send an application letter, CV, and list of publications, preferably by email or fax, to:

Doz. Dr. Paul Mayrhofer
Associate Professor for Nanostructured Materials
Department of Physical Metallurgy and Materials Testing
Montanuniversität Leoben
Franz-Josef-Strasse 18, A-8700 Leoben
Tel.: +43 3842 402-4211
Fax-DW: 4202
E-mail: paul.mayrhofer@unileoben.ac.at

PhD Position for Atomistic Study of Metastable Phases

Nanostructured Materials Group
Department of Physical Metallurgy and Materials Testing
University of Leoben, Austria

The research will focus on first-principles calculations for ternary transition metal nitrides and the effect of alloying elements (group III, V, and VI transition elements) on structure, elastic properties, phase stabilities, and electronic configuration. Nitrides in various fields for mechanical as well as functional uses are increasingly important for tools, components in automotive and aerospace application, as well as for the always growing field of microelectronics like diffusion barriers, gate-electrodes, heat-sinks and light-emitting diodes. The aim of the project is the development of a state-of-the-art understanding of metastable phases in nitrides and their decomposition processes to reach equilibrium. For this, high-quality density-functional theory (DFT) calculations will have to be combined with concepts from statistical mechanics, thermodynamics, and kinetics.

Applicants should have a master in physics, chemistry, or materials science, and have experience with atomic-scale simulations and electronic-structure theory. The candidate should enjoy working in an open and dynamic environment, and actively interact with the other groups in the department as well as with the experimental co-workers.

The research is part of a START Program funded by the FWF (the Austrian Science Found) with partners from other departments, research institutes, and universities. The salary will be according to the rules of the University of Leoben and the Austrian Science Found. The position is limited to two years, with the possibility of extension.

The University of Leoben is an equal opportunities employer. Women are encouraged to apply.

Interested candidates should send an application letter, CV, and list of publications, preferably by email or fax, to:

Doz. Dr. Paul Mayrhofer
Associate Professor for Nanostructured Materials
Department of Physical Metallurgy and Materials Testing
Montanuniversität Leoben
Franz-Josef-Strasse 18, A-8700 Leoben
Tel.: +43 3842 402-4211
Fax-DW: 4202
E-mail: paul.mayrhofer@unileoben.ac.at

Postdoctoral Fellowship: History of Computational Quantum Physics

Max Planck Institute for the History of Science

and the Fritz Haber Institute of the Max Planck Society Berlin, Germany

A postdoctoral research fellowship in the History and Foundations of Quantum Physics is available at the Max Planck Institute for the History of Science and the Fritz Haber Institute of the Max Planck Society in Berlin. The position is part of a joint research project between the two institutes,

http://quantum-history.mpiwg-berlin.mpg.de,

and is embedded into a vibrant international community of scholars based both in Berlin and elsewhere.

We are looking for a motivated researcher with a strong background in quantum mechanics and a PhD or equivalent in physics, chemistry, or history of science. In line with the current research strengths at the Fritz Haber Institute, the intended project focuses on the history of quantum mechanical concepts, methods, and computational techniques in solid state physics and materials research. A keen interest in the study of the historical sources is essential, together with the ability to place these sources in their historical context, up to the central role of quantum mechanical methods in materials research today. Candidates with prior experience in computational condensed matter research and materials science are particularly encouraged to apply.

The candidate will be based at the Max Planck Institute for the History of Science, supported by a strong collaboration with the nearby Fritz Haber Institute. The initial appointment is for two years; an extension by one year is possible upon mutual agreement.

Applications including a current CV, list of publications, statement of research interests, and two letters of reference should be sent by electronic mail to Dr. Volker Blum (blum@fhi-berlin.mpg.de) or by conventional mail to

Dr. Volker Blum
Abteilung Theorie
Fritz-Haber-Institut der Max-Planck-Gesellschaft
Faradayweg 4-6
D-14195 Berlin
Germany

Applications should be submitted by February 29, 2008.

The Max Planck Society is an equal opportunity employer.

Postdoctoral Research Associate

”First principles simulation of mineral surface chemistry”

Nanochemistry Research Institute, Curtin University of Technology, Perth, Western Australia

A postdoctoral position exists within the Computational Chemistry Group of the Nanochemistry Research Institute to work in the area of first principles simulation of mineral-aqueous interfaces and the reactions of small molecules within this environment. This position is funded by the Australian Research Council and is to work with Professors Julian Gale and Kate Wright at Curtin University in collaboration with Drs Stefano Piana and Alessandro Laio (SISSA, Italy).

Duration: 3 years; position available now.

The Nanochemistry Research Institute is a Tier 1 Research Institute of Curtin University of Technology and is part of the new Resources and Chemistry Precinct (http://rcp.curtin.edu.au).

Qualifications: Candidates should possess a PhD in either physics, chemistry, mineralogy or materials science. Previous experience of first principles simulation is essential.

Any interested candidates should contact either

Prof. Julian Gale or Prof. Kate Wright who will be happy to provide further information.

Nanochemistry Research Institute,
Curtin University of Technology,
P.O. Box U1987,
Perth 6845,
Western Australia
Phone: +61 8 9266 3838
Email: julian@ivec.org/kate@ivec.org

Web: http://nanochemistry.curtin.edu.au/

PhD Studentships

Tyndall National Institute, Cork, Ireland

Several PhD studentships are on offer at the Tyndall National Institute http://www.tyndall.ie at University College Cork. Group details may be found at

http://www.tyndall.ie/research/computational-modelling-group

We seek students with strong interest in electronic structure theory and with a background in quantum physics or quantum chemistry. Background or familiarity with scientific computing is an advantage.

Research topics include:

Application of many-electron methods to molecular electronics
Contact: Dr. Jim Greer (Jim.Greer@tyndall.ie)

Simulating quantum transport in semiconductor nanowires
Contact: Dr. Giorgos Fagas (Georgios.Fagas@tyndall.ie)

Density functional theory studies of atomic layer deposition of oxide materials
Contact: Dr. Simon Elliott (Simon.Elliott@tyndall.ie)

Positions are available immediately through funding provided by Science Foundation Ireland (SFI). Additional opportunities exist through the Irish Research Council for Science, Engineering and Technology's PhD scholarship programme:

http:
www.ircset.ie

These studentships are open to all nationalities.

To obtain further details on the application procedure or to discuss project details, please write the relevant contact person including a copy of a recent CV or transcript.

Postdoctoral Position at NREL

Computational Physics/Chemistry of Hydrogen Storage Materials

NREL, Golden, Colorado, USA

The National Renewable Energy Laboratory (NREL) invites applications for a theoretical postdoctoral position, available immediately. The successful individual will be a member of the Computational Materials Science group, and work closely with experimental and theoretical scientists in DOE's Hydrogen Sorption Center of Excellence. Activities include conducting computational materials design and characterization of nanoscale hydrogen storage materials using quantum mechanical electronic structure and molecular dynamics simulation techniques. The materials systems of interest include porous crystalline, molecular, or amorphous materials. NREL has excellent computational facilities and a stimulating, collegial working environment. The Initial assignment is for a year, but renewable upon funding availability, performance, and mutual agreement for up to a total of three years. A recent Ph.D. (less than three years) in physics, chemistry, and/or materials science with significant experience and familiarity with state-of-the-art electronic structure analysis software, is preferred. The starting salary is competitive with similar position elsewhere.

NREL is the nation's primary laboratory for research, development and deployment of renewable energy and energy efficiency technologies. NREL is currently leading the DOE Hydrogen Sorption Center of Excellence (HSCoE), one of the three centers for frontier research on hydrogen storage under the US Department of Energy. As part of the HSCoE mission, theory and computational efforts play important roles in initiating new ideas, design of novel materials, property characterization, and simulation of synthesis pathways. The team, consisting of leading scientists and talented postdoctoral researchers, offers great resources and collaboration environment in both theory and experimentation. Located at the foothills of the Rocky Mountains in Golden, Colorado, 14 miles away from downtown Denver, NREL is a gate to the beautiful Rocky Mountains and ski resorts.

Candidates should send a curriculum vitae including research interest, publication list, two or three electronic files (PDF) of their selected publications to `yufeng_zhao@nrel.gov`, and arrange two or three reference letters upon request.

NREL is an equal opportunity/affirmative action employer.

Postdoctoral Positions in First-Principles Based Modeling of Oxides for Energy and Environmental Applications

Stony Brook University, Prof. Clare Grey

http://www.sunysb.edu/chemistry/faculty/cgrey.htm/

We invite applications for multiple postdoctoral positions in the Materials Chemistry Research Group of Prof. Clare Grey in the Department of Chemistry at Stony Brook University (http://www.sunysb.edu/chemistry/faculty/cgrey.htm). The NSF, DOE and NY State -supported research will use state-of-the-art first-principles methods for studying complex oxides, with applications in solid oxide fuel cells, lithium-ion rechargeable batteries, and sorption properties of iron oxyhydroxides. The focus will be on developing thermodynamic and kinetic models of atomic scale processes and assisting in interpretation of NMR and PDF data. The work will be done in parallel with extensive ongoing experimental characterization, allowing opportunities for collaborations with a wide range of experimentalists. The work will also involve close collaboration with Prof. Dane Morgan and the Computational Materials Group at University of Wisconsin. Interested candidates could spend time at both universities, providing opportunity to work with a range of modelers. Candidates would be able to make use of the recently installed IBM Blue Gene computer (http://www.newyorkccs.org/). A PhD in chemistry, materials science, or related discipline is required. Familiarity with first-principles methods is essential

The appointment is initially for one year with possible extension. Candidates should send a detailed CV (preferably in pdf format) and contact information for 3 references to Clare Grey (cgrey@notes.cc.sunysb.edu). Review of applicants will begin immediately and will continue until the position is filled.

Solid State Chemistry Research Group (http://www.sunysb.edu/chemistry/faculty/cgrey.htm):

Clare Grey's Solid-State Chemistry Research Group at Stony Brook comprises 16 members and focuses on the development and application of novel NMR, PDF, and other characterization methods to study energy and environmental issues. She is the Associate Director of the NSF Center for Environmental Molecular Sciences and the P.I. of a Collaborative Grant in Chemistry 'Structure and Properties of Disordered Iron-Oxyhydroxides', involving co-PIs at Stony Brook University, Penn. State, U. Wisconsin and Temple University.

Computational Materials Group (CMG) (http://matmodel.engr.wisc.edu/):

CMG is a joint effort of Izabela Szlufarska and Dane Morgan in the Department of Materials Science and Engineering at UW Madison. The group has 16 members and DOE and NSF funded work in areas including nanomechanics, nano-bio interfaces, energy materials, iron oxyhydroxides, and lower mantle geophysics.

Dane Morgan, Assistant Professor, 244 Materials Science & Engineering, 1509 University Avenue, Madison, WI 53706-1595, Phone: 608-265-5879, Fax (department): 608-262-8353, Email: ddmorgan@wisc.edu.
Web: `http://www.engr.wisc.edu/mse/faculty/morgan_dane.html`

Open Position for a Post-doctoral Researcher at EPF-Lausanne (date of announcement: 01/02/2008)

A post-doctoral position is available for a talented and motivated individual to work jointly at the Ceramics Laboratory (http://lc.epfl.ch) (Tagantsev, Setter) and the Institute for Numerical Research in the Physics of Materials (IRRMA) (irrmawww.epfl.ch) (Pasquarello) of the EPFL in Lausanne, Switzerland. The individual will join a research project on ferroelectric-semiconductors in which the origin of ferroelectricity in this group of materials and the interplay between ferroelectricity and semiconduction are studied theoretically and experimentally. The focus of the work described here is to bring the potential of first-principles simulation to the study of atomic scale phenomena in these materials.

The position is for one year and may be extended on a yearly basis up to a maximum of four years. Previous experience with computational techniques based on density functional theory is highly desirable. The interested candidates should send their (1) curriculum vitae, (2) publication list, (3) one or two reprints representative of previous research to Nava.Setter@epfl.ch and cc to Alfredo.Pasquarello@epfl.ch and to Alexander.Tagantsev@epfl.ch.

(see also: `http://irrmawww.epfl.ch/~pasquarello/post-doc-ferro.html`)

Post-doctoral Position in Electronic Structure Algorithms
University of California Davis, USA

A post-doctoral position is available immediately in the area of numerical algorithms and software development for first-principles simulations. The successful candidate will work in the group of Prof. Francois Gygi at the Department of Applied Science of the University of California Davis (http://eslab.ucdavis.edu). Research on first-principles algorithms and software is supported by a 4-year NSF project on petascale first-principles simulations. The main goal of this project is to develop new scalable electronic structure numerical algorithms and implement them on petascale computers. Candidates should have a PhD in Physics, Applied Mathematics, Computer Science or equivalent discipline. Proficiency in scientific computing and programming is required. Familiarity with electronic structure methods and/or previous experience with MPI parallel programming, object-oriented programming, C++, and XML are strong advantages.

Interested candidates should send a curriculum vitae with a list of references to Prof. Francois Gygi (fgygi at ucdavis dot edu).

Francois Gygi
Professor
Department of Applied Science
University of California, Davis
One Shields Avenue
Davis, CA 95616-8254

phone: 530-752-4042
http://eslab.ucdavis.edu

Research Fellow Position in Catalysis and Density Functional Theory

http://www.topsoe.com

Haldor Topsoe A/S, Denmark

We are looking for a Research Fellow for our Characterization Department, part of the Research & Development division. The department combines state-of-the-art experimental and theoretical techniques and competences in the area of catalyst characterization to meet our customers' needs.

The successful candidate will undertake a wide variety of tasks within the field of computational methods, such as density functional theory (DFT) and microkinetic modelling, working in close collaboration with dedicated staff on R&D projects.

The position is limited to one year, but may become permanent.

Further information can be obtained from the Head of Department Alfons Molenbroek (tel. +45 4527 2483).

PhD Studentship in Spin Transport/Spin-injection in Semiconductors

Department of Physics, University of York, UK

Supervisor: Dr Irene D'Amico

`http://www-users.york.ac.uk/~ida500/`

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

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

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

This is an Engineering and Physical Sciences Research Council (EPSRC)-funded studentship, with a stipend in line with EPSRC directions. Note for non-EU candidates: this studentship does not cover overseas tuition fees for non-EU students.

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

For more details please contact Dr Irene D'Amico, ida500@york.ac.uk.

To apply please go to the University of York Application Procedure page

`http://www.york.ac.uk/depts/phys/gsp/app_proc.htm`

or email phys-grad-admin@york.ac.uk for an application pack. If applying please inform either Dr D'Amico (ida500@york.ac.uk) or Ms Miller (sm530@york.ac.uk)

Research Assistant in Theoretical Condensed Matter Physics/Nanomagnetism

Department of Mathematics, City University London and Open University Milton Keynes, UK

£28,289 - £30,012 pa

Based in London and Milton Keynes

Fixed-term for 3 years

Applications are invited for the post of Postdoctoral Research Assistant in theoretical physics, to work on a project carried out jointly between City University London and the Open University Milton Keynes under the leadership of Professor J. Mathon and Dr A. Umerski. You will undertake research into the theory of quantum transport of charge and spin across a ferromagnet-semiconductor interface. This is one of the fundamental problems in the exciting emergent field of spintronics, the area for which the physics Nobel Prize was awarded this year. Relevant information about our research in spintronics can be found at

http://mcs.open.ac.uk/au73/index1.htm.

The proposed research is part of a collaborative EPSRC funded project involving Cambridge University where a parallel experimental investigation will be carried out. You will also interact with a PDRA and a graduate student working on a closely related EPSRC funded project, Spin@RT, involving some forty researchers based in eight UK institutions. A PhD in a relevant area of theoretical physics or materials modelling is required and experience in using/modifying/developing electronic structure codes is highly desirable.

Informal enquires should be addressed to either Prof. J Mathon: j.mathon@city.ac.uk or Dr A Umerski: A.Umerski@open.ac.uk.

Application forms are available from the websites:

http://www.city.ac.uk/jobs and http://www3.open.ac.uk/employment/

Completed forms must be submitted to both City and Open Universities. They should be sent with a full curriculum vitae and list of publications to:

HR Department, City University, London EC1V 0HB and MCS-Recruitment, Open University, Milton Keynes, MK7 6AA, quoting reference numbers SW/11298 and 4195 respectively.

Closing date: 29th February 2008.

6 Abstracts

Orbital magnetism in transition-metal systems: The role of local correlation effects

S. Chadov[1], J. Minár[1], M. I. Katsnelson[2], H. Ebert[1], D. Ködderitzsch[1]
and A. I. Lichtenstein[3]
[1] *Dept. Chemie und Biochemie, Physikalische Chemie, Universität München,*
Butenandtstr. 5-13, D-81377 München, Germany
[2] *Institute for Molecules and Materials, Radboud University Nijmegen,*
NL-6525 ED Nijmegen, The Netherlands
[3] *Institute of Theoretical Physics, University of Hamburg, Germany*

Abstract

The influence of correlation effects on the orbital moments for transition metals and their alloys is studied by first-principle relativistic Density Functional Theory in combination with the Dynamical Mean-Field Theory. In contrast to the previous studies based on the orbital polarization corrections we obtain an improved description of the orbital moments for wide range of studied systems as bulk Fe, Co and Ni, Fe-Co disordered alloys and $3d$ impurities in Au. The proposed scheme can give simultaneously a correct dynamical description of the spectral function as well as static magnetic properties of correlated disordered metals.

(Submitted to Europhysics Letters)

Contact person: jan.minar@cup.uni-muenchen.de

Ab initio calculations of free-energy reaction barriers

Tomáš Bučko
Fakultät für Physik and Center for Computational Materials Science,
Universität Wien, Sensengasse, Wien 1090 AUSTRIA

Abstract

The theoretical description of chemical reactions was until recently limited to a 'static' approach in which important parameters such as the rate constant are deduced from the local topology of the potential energy surface close to minima and saddle points. Such an approach has, however, serious limitations. The growing computational power allows now to use advanced simulation techniques to determine entropic effects accurately for medium-sized systems at ab-initio level. Recently, we have implemented free-energy simulation techniques based on molecular dynamics, in particular on the blue-moon ensemble technique and on metadynamics, into the popular DFT code VASP. In the thermodynamic integration (blue-moon ensemble) technique, the free-energy profile is calculated as the path integral over the restoring forces along a parametrized reaction coordinate. In metadynamics, an image of the free-energy surface is constructed on the fly during the simulation by adding small repulsive Gaussian-shaped hills to the Lagrangian driving the dynamics. The two methods are tested on a simple chemical reaction - the nucleophilic substitution of methyl-chloride by a chlorine anion.

Published in
J. Phys.: Condens. Matter 20 (2008) 064211.

Spin, charge, and orbital ordering in $R\mathrm{BaMn_2O_{5+\delta}}$ (R = Y, La; $0 \leq \delta \leq 1$) and their dependence on oxygen content and size of the R constituent

R. Vidya, P. Ravindran, A. Kjekshus, and H. Fjellvåg
Center for Materials Science and Nanotechnology,
Department of Chemistry, University of Oslo,
Box 1033 Blindern, N-0315 Oslo, Norway

Abstract

The effect of oxygen content on spin, charge, and orbital ordering in $R\mathrm{BaMn_2O_{5+\delta}}$ (R = Y, La; $0 \leq \delta \leq 1$) is studied by density-functional-theory-based calculations as implemented in the full-potential linearized-augmented plane-wave method. Structural optimizations using the projector augmented wave method have been performed for all the phases and the calculated structural parameters are found to be in good agreement with experimental values. Total energy calculations have systematically been performed including force as well as stress minimization for paramagnetic, ferromagnetic, and antiferromagnetic configurations. For $\delta = 0$ the ground state is found to be ferrimagnetic whereas the variants with oxygen contents $\delta = 1/2$ and 1 give rise to an antiferromagnetic ground state, all in perfect agreement with experimental findings. The electronic band characteristics are analyzed using total, site-, and orbital-projected density of states and the examination shows that the electronic structure undergoes a gradual change from semiconductor-to-metal behavior on going from $\delta = 0$ to 1. Even the GGA+U approach failed to reproduce the insulating state for the phases with $\delta = 1$, indicating that introduction of the experimental CE-type magnetic structure may be important. The charge and orbital ordering are analyzed with the help of the energy-projected-density matrices of the d electrons. Very different ordering patterns have emerged for the different phases under investigation indicating that both cation radii and oxygen stoichiometry play an important role in deciding spin-, charge-, and orbital-ordering.

DOI: 10.1103/PhysRevB.76.195114
Contact person: vidya.ravindran@kjemi.uio.no

Entanglement in spatially inhomogeneous many-fermion systems

V. V. França and K. Capelle
Departamento de Física e Informática, Instituto de Física de São Carlos,
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil

Abstract

We investigate entanglement of strongly interacting fermions in spatially inhomogeneous environments. To quantify entanglement in the presence of spatial inhomogeneity, we propose a local-density approximation (LDA) to the entanglement entropy, and a *nested LDA* scheme to evaluate the entanglement entropy on inhomogeneous density profiles. These ideas are applied to models of electrons in superlattice structures with different modulation patterns, electrons in a metallic wire in the presence of impurities, and phase-separated states in harmonically confined many-fermion systems, such as electrons in quantum dots and atoms in optical traps. We find that the entanglement entropy of inhomogeneous systems is strikingly different from that of homogeneous systems.

(Phys. Rev. Lett. (2008), accepted, arXiv:0710.2095)
Contact person: Klaus Capelle (capelle@ifsc.usp.br)

How tight is the Lieb-Oxford bound?

Mariana M. Odashima and K. Capelle
Departamento de Física e Informática, Instituto de Física de São Carlos,
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil

Abstract

Density-functional theory requires ever better exchange-correlation (xc) functionals for the ever more precise description of many-body effects on electronic structure. Universal constraints on the xc energy are important ingredients in the construction of improved functionals. Here we investigate one such universal property of xc functionals: the Lieb-Oxford lower bound on the exchange-correlation energy, $E_{xc}[n] \geq -C \int d^3r\, n^{4/3}$, where $C \leq C_{LO} = 1.68$. To this end, we perform a survey of available exact or near-exact data on xc energies of atoms, ions, molecules, solids, and some model Hamiltonians (the electron liquid, Hooke's atom and the Hubbard model). All physically realistic density distributions investigated are consistent with the tighter limit $C \leq 1$. For large classes of systems one can obtain class-specific (but not fully universal) similar bounds. The Lieb-Oxford bound with $C_{LO} = 1.68$ is a key ingredient in the construction of modern xc functionals, and a substantial change in the prefactor C will have consequences for the performance of these functionals.

(J. Chem. Phys. 127, p. 054106 (2007))
Contact person: Klaus Capelle (capelle@ifsc.usp.br)

Quantitative determination of the Hubbard model phase diagram from optical lattice experiments by two-parameter scaling

V.L. Campo, Jr.[1], K. Capelle,[2], J. Quintanilla[3] and C. Hooley [4]
[1] *Centro Internacional de Física da Matéria Condensada,*
Universidade de Brasília, Brazil
[2] *Departamento de Física e Informática, Instituto de Física de São Carlos,*
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil
[3] *ISIS Facility, STFC Rutherford Appleton Laboratory*
Harwell Science and Innovation Campus, Didcot OX11 0QX, United Kingdom
[4] *School of Physics and Astronomy, University of St Andrews, North Haugh,*
St Andrews, Fife KY16 9SS, United Kingdom

Abstract

We propose an experiment to obtain the phase diagram of the fermionic Hubbard model, for any dimensionality, using cold atoms in optical lattices. It is based on measuring the total energy for a sequence of trap profiles. It combines finite-size scaling with an additional finite-curvature scaling necessary to reach the homogeneous limit. We illustrate its viability in the 1D case, simulating experimental data in the Bethe-ansatz local-density approximation. Including experimental errors, the filling corresponding to the Mott transition can be determined with better than 3% accuracy.

(Phys. Rev. Lett. 99, p. 240403 (2007))

Contact person: Klaus Capelle (capelle@ifsc.usp.br)

The generator coordinate method in time-dependent density-functional theory: memory made simple

E. Orestes[1,2], K. Capelle[1], A. B. F. da Silva[2] and C. A. Ullrich [3]
[1] *Departamento de Física e Informática, Instituto de Física de São Carlos,*
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil
[2] *Departamento de Química e Física Molecular,*
Instituto de Química de São Carlos,
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil
[3] *Department of Physics and Astronomy, University of Missouri*
Columbia, Missouri 65211, USA

Abstract

The generator coordinate (GC) method is a variational approach to the quantum many-body problem in which interacting many-body wave functions are constructed as superpositions of (generally nonorthogonal) eigenstates of auxiliary Hamiltonians containing a deformation parameter. This paper presents a time-dependent extension of the GC method as a new approach to improve existing approximations of the exchange-correlation (XC) potential in time-dependent density-functional theory (TDDFT). The time-dependent GC method is shown to be a conceptually and computationally simple tool to build memory effects into any existing adiabatic XC potential. As an illustration, the method is applied to driven parametric oscillations of two interacting electrons in a harmonic potential (Hooke's atom). It is demonstrated that a proper choice of time-dependent generator coordinates in conjunction with the adiabatic local-density approximation reproduces the exact linear and nonlinear two-electron dynamics quite accurately, including features associated with double excitations that cannot be captured by TDDFT in the adiabatic approximation.

(J. Chem. Phys. 127, p. 124101 (2007))

Contact person: Klaus Capelle (capelle@ifsc.usp.br)

Degenerate ground states and nonunique potentials: breakdown and restoration of density functionals

K. Capelle[1], C. A. Ullrich[2] and G. Vignale[2]

[1] *Departamento de Física e Informática, Instituto de Física de São Carlos,*
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil

[2] *Department of Physics and Astronomy, University of Missouri*
Columbia, Missouri 65211, USA

Abstract

The Hohenberg-Kohn (HK) theorem is one of the most fundamental theorems of quantum mechanics, and constitutes the basis for the very successful density-functional approach to inhomogeneous interacting many-particle systems. Here we show that in formulations of density-functional theory (DFT) that employ more than one density variable, applied to systems with a degenerate ground state, there is a subtle loophole in the HK theorem, as all mappings between densities, wave functions, and potentials can break down. Two weaker theorems which we prove here, the joint-degeneracy theorem and the internal-energy theorem, restore the internal, total, and exchange-correlation energy functionals to the extent needed in applications of DFT to atoms, molecules, and solids. The joint-degeneracy theorem constrains the nature of possible degeneracies in general many-body systems.

(Phys. Rev. A 76, p. 012508 (2007))

Contact person: Klaus Capelle (capelle@ifsc.usp.br)

Density-functional formulations for quantum chains

F. C. Alcaraz and K. Capelle

Departamento de Física e Informática, Instituto de Física de São Carlos,
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil

Abstract

We show that a lattice formulation of density functional theory (DFT), guided by renormalization-group concepts, can be used to obtain numerical predictions of energy gaps, spin-density profiles, critical exponents, sound velocities, surface energies, and conformal anomalies of spatially inhomogeneous quantum-spin chains. To this end, we (i) cast the formalism of DFT in the notation of quantum-spin chains to make the powerful methods and concepts developed in ab initio DFT available to workers in this field, (ii) explore to what extent simple local approximations in the spirit of the local-density approximation (LDA) can be used to predict critical exponents and conformal anomalies of quantum-spin models, and (iii) propose and explore various nonlocal approximations depending on the size of the system or on its average density in addition to the local density. These nonlocal functionals turn out to be superior to LDA functionals.

(Phys. Rev. B 76, p. 035109 (2007))

Contact person: Klaus Capelle (capelle@ifsc.usp.br)

Competition between local potentials and attractive particle-particle interactions in superlattices

N. A. Lima[1], A. L. Malvezzi[2] and K. Capelle[3]
[1] *Fundação Universidade Federal do Vale do São Francisco*
Caixa Postal 252, 56306-410 Petrolina, PE, Brazil
[2] *Departamento de Física, Faculdade de Ciências, Universidade Estadual Paulista*
Caixa Postal 473, 17015-970 Bauru, SP, Brazil
[3] *Departamento de Física e Informática, Instituto de Física de São Carlos,*
Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil

Abstract

Naturally occuring, or man-made, systems displaying spatial modulations of their properties on a nanoscale — i.e., superlattices — are important both as paradigms of simple nanotechnological devices and as particular examples of emerging spatial inhomogeneity in interacting many-electron systems. Here we investigate the effect different types of modulation of the system parameters have on the ground-state energy, the charge-density distribution, and the local entanglement entropy of the system. The superlattices are described by the inhomogeneous Hubbard model, and the calculations are performed by density-functional and density-matrix renormalization group techniques. We find that modulations in local electric potentials are much more effective in shaping the system's properties than modulations in the effective on-site interaction, both for attractive and repulsive interactions.

(Sol. State Com. 144, p. 557 (2007) [special issue for SCENS conference])
Contact person: Klaus Capelle (capelle@ifsc.usp.br)

Global exploration of the energy landscape of solids on the *ab initio* level

K. Doll, J.C. Schön and M. Jansen
Max-Planck-Institute for Solid State Research,
Heisenbergstraße 1, D-70569 Stuttgart, Germany

Abstract

Predicting which crystalline modifications can be present in a chemical system requires the global exploration of its energy landscape. Due to the large computational effort involved, in the past this search for sufficiently stable minima has been performed employing a variety of empirical potentials and cost functions followed by a local optimization on the *ab initio* level. However, this entails the risk of overlooking important modifications that are not modeled accurately using empirical potentials. In order to overcome this critical limitation, we develop an approach to employ *ab initio* energy functions during the global optimization phase of the structure prediction. As an example, we perform a global exploration of the landscape of LiF on the *ab initio* level and show that the relevant crystalline modifications are found during the search.

Phys. Chem. Chem. Phys. **9**, 6128 (2007)

Electronic structure of GdN, and the influence of exact exchange

K. Doll
Max-Planck-Institute for Solid State Research,
Heisenbergstraße 1, D-70569 Stuttgart, Germany

Abstract

GdN bulk is studied with the local density approximation, on the Hartree-Fock level, and on the level of the hybrid functional B3LYP. A local basis set formalism is used, as implemented in the present CRYSTAL06 release. It is demonstrated that the code is technically capable of treating this system with its $4f$ electrons explicitly, i.e. out of the core. The band structure at the level of the local density approximation is in good agreement with earlier calculations and is found to be half-metallic. The Hartree-Fock band structure is insulating with a large gap. Interestingly, three solutions were found at the B3LYP level. The lowest of them is insulating for majority spin, and the Fermi surface for minority spin consists only of points, resulting in a very low density of states around the Fermi level.

Email: k.doll@fkf.mpg.de

J. Phys.: Condensed Matter, in press

A density-functional study of the structures, binding energies and magnetic moments of the clusters Mo_N (N= 2 - 13), $Mo_{12}Fe$, $Mo_{12}Co$, and $Mo_{12}Ni$

F. Aguilera-Granja
Instituto de Física, Universidad Autónoma de San Luis Potosí,
S.L.P. 78000, México
A. Vega
Departamento de Física Teórica, Atómica, y Óptica,
Universidad de Valladolid, E-47011 Valladolid, Spain
L. J. Gallego
Departamento de Física de la Materia Condensada,
Facultad de Física, Universidad de Santiago de Compostela,
E-15782 Santiago de Compostela, Spain

Abstract

We report the results of density-functional calculations of the structures, binding energies and magnetic moments of the clusters Mo_N (N= 2 - 13), $Mo_{12}Fe$, $Mo_{12}Co$, and $Mo_{12}Ni$ that were performed using the SIESTA method within the generalised gradient approximation to exchange and correlation. For pure Mo_N clusters, we obtain collinear magnetic structures in all cases, even when the self-consistent calculations were started from non-collinear inputs. Our results for these clusters show that both linear, planar and three-dimensional clusters have a strong tendency to form dimers. In general, even-numbered clusters are more stable than their neighboring odd-numbered clusters because they can accommodate an integer number of tightly bound dimers. As a consequence, the binding energies of pure Mo_N clusters, in their lowest-energy states, exhibit an odd-even effect in all dimensionalities. Odd-even effects are less noticeable in the magnetic moments than in the binding energies. When comparing our results for pure Mo clusters with those obtained recently by other authors, we observe similarities in some cases, but striking differences in others. In particular, the odd-even effect in three-dimensional Mo clusters was not observed before, and our results for some clusters (e.g., for planar Mo_3 and Mo_7 and for three-dimensional Mo_7 and Mo_{13}) differ from those reported by other authors. For $Mo_{12}Fe$ and $Mo_{12}Ni$, we obtain that the icosahedral configuration with the impurity atom at the cluster surface is more stable than the configuration with the impurity at the central site, while the opposite occurs in the case of $Mo_{12}Co$. In $Mo_{12}Co$ and $Mo_{12}Ni$, the impurities exhibit weak magnetic moment parallely coupled to the total magnetic moment of the Mo atoms, whereas in $Mo_{12}Fe$ the impurity shows high moment with antiparallel coupling.

Accepted in Nanotechnology
Contact author: F. Aguilera-Granja (faustino@dec1.ifisica.uaslp.mx)

Density Functional Characterization of the Multiferroicity in Spin Spiral Chain Cuprates

H. J. Xiang and M.-H. Whangbo
Department of Chemistry, North Carolina State University,
Raleigh, North Carolina 27695-8204

Abstract

The ferroelectricity of the spiral magnets $LiCu_2O_2$ and $LiCuVO_4$ was examined by calculating the electric polarizations of their spin spiral states on the basis of density functional theory with spin-orbit coupling. Our work unambiguously reveals that spin-orbit coupling is responsible for the ferroelectricity with the primary contribution from the spin-orbit coupling on the Cu sites, but the asymmetric density distribution responsible for the electric polarization occurs mainly around the O atoms. The electric polarization is calculated to be much greater for the *ab*- than for the *bc*-plane spin spiral. The observed spin-spiral plane is found to be consistent with the observed direction of the electric polarization for $LiCuVO_4$, but inconsistent for $LiCu_2O_2$.

(Phys. Rev. Lett. **99**, 257203 (2007))
Contact person: `hongjun_xiang@nrel.gov`

The morphology of mesoscopic Rh and Pd nanoparticles under oxidizing conditions

F. Mittendorfer, N. Seriani, O. Dubay, G. Kresse
Fakultät Physik, Universität Wien,
Sensengasse 8/12, A-1090 Vienna, Austria

Abstract

The thermodynamic equilibrium shape of rhodium and palladium crystals are predicted under conditions from ultrahigh vacuum (UHV) to high oxygen pressures using the Gibbs-Wulff construction. The analysis is based on data obtained from ab-initio calculations for the adsorption of oxygen on the low-index (111), (100) and (110) surfaces, and the stepped (311), (211) and (331) surfaces. While the close packed (111) facets dominate the shape in the low-coverage cases, the higher adsorption energies at the more open surfaces lead to a rounding of the crystallite. A linear correlation between the surface energies of the clean surfaces and the respective adsorption energies is found.

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Contact person: Florian Mittendorfer (florian.mittendorfer@univie.ac.at)

A DFT study of platinum oxides: from infinite crystals to nanoscopic particles

N. Seriani[1], Z. Jin[2], W. Pompe[3], L. Colombi Ciacchi[4,5]
[1] *Fakultät Physik, Universität Wien,*
Sensengasse 8, A-1090 Wien, Austria
[2] *Laboratory of Special Functional Materials, Henan University,*
Kaifeng 475001, China
[3] *Institut für Werkstoffwissenschaft, Technische Universität Dresden,*
Hallwachsstrasse 3, 01069 Dresden, Germany
[4] *Fraunhofer Institut für Werkstoffmechanik,*
Wöhlerstrasse 11, 79108 Freiburg, Germany
[5] *Institut für Zuverlässigkeit von Bauteilen und Systemen,*
Universität Karlsruhe, Kaiserstrasse 12, 76131 Karlsruhe, Germany

Abstract

Since over a century platinum oxides find technologically relevant applications in various fields ranging from catalysis to electrochemistry and nanoelectronics. We have performed a Density Functional Theory study of the PtO, Pt_3O_4 and PtO_2 bulk oxide phases. In our calculations PtO and Pt_3O_4 present metallic character at the simple GGA level. The application of Hubbard corrections to the Kohn-Sham Hamiltonian opens a small gap in the electronic band structure of PtO, but not of Pt_3O_4, in which metallic Pt-Pt bonds are revealed by a Bader Analysis of the calculated electronic structure. These results, together with the non-integer oxidation number of the Pt ions, are indicative of metallicity of the Pt_3O_4 phase which may be consistent with the known metallic character of platinum bronzes. Moreover, we have calculated the relative thermodynamic stabilities of platinum oxide Wulff's particles and discussed the results in the context of catalysis. Finally, we have predicted that the formation of α-PtO_2 nanotubes could be energetically feasible. This result is of potential interest both for nanotechnological and catalytic applications, and may explain the formation of curled α-PtO_2 sheets observed in high-resolution TEM images.

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Contact person: Nicola Seriani (nicola.seriani@univie.ac.at)

Stable liquid Hydrogen at high pressure by a novel *ab-initio* molecular dynamics

Claudio Attaccalite[1] and Sandro Sorella[2]
[1] *European Theoretical Spectroscopy Facility,*
Departamento de Fisica de Materiales, Universidad del Pais Vasco,
Centro Mixto CSIC-UPV, Edificio Korta, Av. Tolosa 72,
E-20018 San Sebastian, Spain
[2] *Democritos National Simulation Center, SISSA,*
Via Beirut n.2, Trieste, Italy

Abstract

We introduce an efficient scheme for the molecular dynamics of electronic systems by means of quantum Monte Carlo. The evaluation of the (Born-Oppenheimer) forces acting on the ionic positions is achieved by two main ingredients: i) the forces are computed with finite and small variance, which allows the simulation of a large number of atoms, ii) the statistical noise corresponding to the forces is used to drive the dynamics at finite temperature by means of an appropriate Langevin dynamics. A first application to the high-density phase of Hydrogen is given, supporting the stability of the liquid phase at $\simeq 300GPa$ and $\simeq 400K$.

In press on PRL

Contact person: claudio.attaccalite at gmail.com

Water on the hydroxylated (001) surface of kaolinite: From monomer adsorption to a flat 2D wetting layer

Xiao Liang Hu and Angelos Michaelides

Materials Simulation Laboratory, London Centre for Nanotechnology
and Department of Chemistry, University College London, London WC1E 6BT, U.K.

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

Abstract

In order to understand the role played by kaolinite in heterogeneous ice nucleation, an extensive density-functional theory study has been performed for water on its (001) basal plane. Water monomers at low coverage, water clusters, water bilayers and water multilayers have all been examined. The most important and interesting results from this study are: (i) Water monomers bind strongly to kaolinite compared to many other substrates. In the preferred adsorption structure water accepts two H bonds from and donates one H bond to the substrate, revealing that kaolinite, like water, is amphoteric with the the ability to accept and donate H bonds; (ii) Clustering of adsorbed water molecules is not significantly favored. All water clusters (dimers, tetramers, and hexamers) examined are, at best, equally stable to water monomers; (iii) A 2D ice-like bilayer, with a stability matching that of ice Ih has been identified implying that water can wet kaolinite; (iv) Multilayer ice growth is not favored, being considerably unstable compared to bulk ice, indicating that the water covered kaolinite surface is itself hydrophobic. Overall we see that amphoterism of the hydroxylated surface is key to many of the interesting properties of kaolinite with regard to water adsorption and ice nucleation, revealing that the behavior of water on kaolinite is more complex and interesting than previously thought to be and highlighting the need for further theoretical and experimental work.

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

The Far-Infrared Spectra of Neutral and Cationic Niobium Clusters: $\mathrm{Nb}_5^{0/+}$ to $\mathrm{Nb}_9^{0/+}$

André Fielicke,[1] Christian Ratsch,[1,2] Gert von Helden[1] and Gerard Meijer[1]

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

[2] *Department of Mathematics, UCLA and California NanoSystems Institute,*
UCLA, Los Angeles, CA 90095-1555, USA

Abstract

Far-infrared absorption spectra of small neutral and cationic niobium clusters containing 5 to 9 Nb atoms have been obtained by multiple photon dissociation spectroscopy of their argon complexes. The experimental far-IR spectra are recorded in the 85–600 cm^{-1} region and cover the range of the structure-specific vibrational fundamentals, i.e., the finger-print range, for these metal clusters. The experiments are accompanied by quantum chemical calculations employing density-functional theory. A comparison of the experimental and calculated far-IR spectra spectra allows to identify the cluster structures. Although the experimental spectra for clusters containing 5, 6, 8, and 9 Nb atoms are very different for cationic and neutral clusters, the comparison with theory reveals that, nevertheless, the overall geometries for cations and neutrals are very similar, except for $\mathrm{Nb}_6^{0/+}$.

(submitted to: J. Chem. Phys.)

Contact person: André Fielicke (fielicke@fhi-berlin.mpg.de)

Screening in 2D: GW calculations for surfaces and thin films using the repeated-slab approach

Christoph Freysoldt,[1] Philipp Eggert,[1] Patrick Rinke,[1]
Arno Schindlmayr,[1,2] and Matthias Scheffler[1]

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

[2]*Institut für Festkörperforschung, Forschungszentrum Jülich,*
52425 Jülich, Germany

Abstract

In the context of photoelectron spectroscopy, the *GW* approach has developed into the method of choice for computing excitation spectra of weakly correlated bulk systems and their surfaces. To employ the established computational schemes that have been developed for three-dimensional crystals, two-dimensional systems are typically treated in the repeated-slab approach. In this work we critically examine this approach and identify three important aspects for which the treatment of long-range screening in two dimensions differs from the bulk: (1) anisotropy of the macroscopic screening (2) **k**-point sampling parallel to the surface (3) periodic repetition and slab-slab interaction. For prototypical semiconductor (silicon) and ionic (NaCl) thin films we quantify the individual contributions of points (1) to (3) and develop robust and efficient correction schemes derived from the classic theory of dielectric screening.

(submitted to: Phys. Rev. B)

Contact person: Patrick Rinke (rinke@fhi-berlin.mpg.de)

Alloy surface segregation in reactive environments: A first-principles atomistic thermodynamics study of $Ag_3Pd(111)$ in oxygen atmospheres

John Kitchin, Karsten Reuter, and Matthias Scheffler

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

Abstract

We present a first-principles atomistic thermodynamics framework to describe the structure, composition and segregation profile of an alloy surface in contact with a (reactive) environment. The method is illustrated with the application to a $Ag_3Pd(111)$ surface in an oxygen atmosphere, and we analyze trends in segregation, adsorption and surface free energies. We observe a wide range of oxygen adsorption energies on the various alloy surface configurations, including binding that is stronger than on a Pd(111) surface and weaker than that on a Ag(111) surface. This and the consideration of even small amounts of non-stoichiometries in the ordered bulk alloy are found to be crucial to accurately model the Pd surface segregation occurring in increasingly O-rich gas phases.

(submitted to: Phys. Rev. B)

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

CO oxidation on Pd(100) at technologically relevant pressure conditions: A first-principles kinetic Monte Carlo study

Jutta Rogal, Karsten Reuter, and Matthias Scheffler

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

Abstract

The possible importance of oxide formation for the catalytic activity of transition metals in heterogenous oxidation catalysis has evoked a lively discussion over the recent years. On the more noble transition metals (like Pd, Pt or Ag) the low stability of the common bulk oxides suggests primarily sub-nanometer thin oxide films, so-called surface oxides, as potential candidates that may be stabilized under gas phase conditions representative of technological oxidation catalysis. We address this issue for the Pd(100) model catalyst surface with first-principles kinetic Monte Carlo (kMC) simulations that assess the stability of the well-characterized $(\sqrt{5} \times \sqrt{5})R27^\circ$ surface oxide during steady-state CO oxidation. Our results show that at ambient pressure conditions the surface oxide is stabilized at the surface up to CO:O_2 partial pressure ratios just around the catalytically most relevant stoichiometric feeds ($p_{\rm CO} : p_{\rm O_2} = 2 : 1$). The precise value depends sensitively on temperature, so that both local pressure and temperature fluctuations may induce a continuous formation and decomposition of oxidic phases during steady-state operation under ambient stoichiometric conditions.

(submitted to: Phys. Rev. B)

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

7 New Book Announcements

Woodhead Publishing Ltd, Cambridge, England CRC Press LLC, Boca Raton, USA

Multiscale Materials Modelling: Fundamentals and Applications

Ed. by Z. Xiao Guo

- *Comprehensive text on multiscale modelling of materials*
- *General methods illustrated by applications to many specific systems*
- *Of interest to researchers and graduate students in condensed matter physics and in materials science*

The various chapters of the book cover the spectrum of scales in modelling methodologies, including electronic structure calculations, mesoscale and continuum modelling. The book covers such themes as dislocation behaviour and plasticity as well as the modelling of properties of structural materials (metals, intermetallics, polymers and ceramics). With its distinguished editor and international team of contributors, this book will be a valuable reference for both the modelling community and those in industry keen to know more about how multiscale materials modelling can help optimise product and process design.

Contents:

– Z. Xiao Guo, Queen Mary University of London, UK: *Introduction.*

– M. Šob, Masaryk University, Brno, Czech Republic: *The role of ab initio electronic structure calculations in multiscale modelling of materials.*

– K. W. Schwarz, IBM Watson Research Center, USA: *Modelling dislocation behaviour at the continuum level.*

– L.-Q. Chen, Penn State University, USA: *Phase field modelling of material microstructure.*

– D. Moldovan, Louisiana State University & D. Wolf, Argonne National Laboratory, USA: *Mesoscale modelling of grain growth and microstructure in polycrystalline materials.*

– J. Llorca, C. Gonzáles & J. Segurado, Polytechnic University of Madrid, Spain: *Finite element and homogenisation modelling of materials.*

– M.O. Bloomfield & T.S. Cale, Rensselaer Polytechnic Institute, USA: *Grain-continuum modelling of material behaviour.*

– R.E. Miller, Carleton University, Canada: *Coupled atomistic/continuum modelling of plasticity in materials.*

– T.Y. Ng, S.H. Yeak & Y.X. Ren, Nanyang Technological University, Singapore, and K.M. Liew, City University of Hong Kong, Hong Kong: *Multiscale modelling of carbon nanostructures.*

– D. Porter, QinetiQ, UK: *Multiscale modelling of structural materials.*

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8 SCIENTIFIC HIGHLIGHT OF THE MONTH: Local Self-Interaction Correction of a Scattering Resonance: The Atom in Jellium Model

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Local Self-Interaction Correction of a Scattering Resonance: The Atom in Jellium Model

James F. Annett[1], Andrew I. Duff[2,3], Balazs L. Gyorffy[1], Walter M. Temmerman[2], Zdzislawa Szotek[2] and Martin Lüders[2]

1. H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom.
james.annett@bristol.ac.uk

2. Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, United Kingdom

3. Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, Netherlands

Abstract

The atom in jellium model describes a single atom interacting with an infinite homogenous electron gas. It can be thought of as the simplest first principles model which includes all of the essential physics of the Anderson impurity model, namely one or more localized atomic-like states hybridized with a continuum of free electron band states. For example in the case of rare earth elements, such as Ce, one can use the atom in jellium model to examine the valence state of the atom as a function of the jellium density, or r_s. This in turn can be used to understand in simple terms the valence transitions which might occur in bulk materials, for example as a function of pressure. In this highlight we present calculations of a Ce atom in jellium, in which we compare the LSDA results with those of the Local Self-Interaction Correction (LSIC). The LSIC approximation of density functional theory was introduced by Lüders et al.[*Phys. Rev. B*, 71:205109, 2005], and it extends the original self-interaction correction theory to apply the correction to long-lived resonances as well as to bound states. Using the atom in jellium model for Ce we show explicitly how this applies to the $4f$-like states of the Ce atom in jellium. The LSIC has solutions which correspond to different numbers of these f states treated as either SI-corrected or not. This causes these electrons to localize, which within the effective medium theory (EMT) corresponds to a change in the valence of cerium metal as a function of Wigner-Seitz radius.

1 Introduction

The atom in jellium model describes a single atom interacting with an infinite electron gas. It is simply characterized by two parameters, namely the nuclear charge, Z, and the jellium density n_0, or r_s, where $\frac{4\pi}{3}r_s^3 n_0 = 1$. The model has been extensively studied in the past, usually within the local spin density approximation (LSDA), as an illustration of chemical bonding of an atom to a metallic host [1–3]. In this context the key result of the calculation is the immersion energy $E_{imm}(n_0)$, which is the energy of the atom in jellium system compared to the atom in free space and the jellium without the atom. This immersion energy is one of the key ingredients in the semi-empirical Embedded Atom Method (EAM) [4]. Effective medium theory (EMT) provides a fully first principles theory of total energies of solids, in which each atom is viewed as embedded in an effective jellium provided by the electron clouds of its neighbours [5]. This theory gives a very good overall description of the trends in Wigner-Seitz radii across the $3d$ [6] or $4d$ [7] transition metals.

In this highlight we examine the atom in jellium model from a quite different point of view. Namely, it can be thought of as the simplest first principles model which includes all of the essential physics of the Anderson impurity model [8]. This model is the central model in "quantum impurity" problems, including the theory of the Kondo effect. It is characterized by one or more localized atomic states, with an energy ϵ_f and an on-site repulsion U, which are hybridized with a free electron band of states $\epsilon_{\mathbf{k}}$, by the matrix element $V_{\mathbf{k}}$,

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \epsilon_f f^{+}_{\sigma} f_{\sigma} + U \hat{n}_{f\uparrow} \hat{n}_{f\downarrow} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} \left(c^{+}_{\mathbf{k}\sigma} f_{\sigma} + h.c. \right), \qquad (1)$$

where $c^{+}_{\mathbf{k}\sigma}$ is the usual creation operator for electrons in band states and f^{+}_{σ} is the creation operator for the localized state, with $\hat{n}_{f\sigma} = f^{+}_{\sigma} f_{\sigma}$. As well as modelling a single atomic impurity in a metallic host, this model is central to Dynamical Mean Field Theory (DMFT) [9]. In DMFT the free particle band of states $\epsilon_{\mathbf{k}}$ is replaced with a suitably chosen effective medium, obtained self-consistently from the many-body solution of the Hamiltonian of Eq. 1. Implemented together with LDA+U or other means to estimate the Anderson model parameters this is now one of the most widely used first principles approaches to the theory of d and f-electron metals and their compounds [10, 11].

Our motivation for studying the atom in jellium model is to find an alternative route to an effective quantum impurity problem, i.e. without mapping onto the Anderson impurity problem explicitly, and without invoking an additional parameter, U. Although effective Hubbard parameters, U, can be estimated from constrained density functional theory [12] our aim is to solve the atom in jellium model directly without requiring this additional step. For example, one possible approach is to solve the atom in jellium model directly using quantum Monte Carlo (QMC). We have recently shown that this approach is feasible, at least for an atom embedded in a finite size jellium sphere. For a Hydrogen in jellium we were able to obtain reasonable immersion energies, $E_{imm}(n_0)$, using a Variational-QMC approach based on a trial wave function previously used by Sottile and Balone [13]. Our results [14] show a minimum in $E_{imm}(n_0)$ of about $1eV$ at a jellium density of about $n_0 = 0.0025a_B^{-3}$. In contrast the LSDA result for the same system is a minimum of about $2eV$ at the same density. We interpret this as evidence for overbinding in LSDA compared to the more exact QMC results.

Unfortunately the QMC approach is currently too expensive to apply to a more interesting case, such as rare earth atoms embedded in an electron gas. For these atoms we have applied the Local Self-Interaction-Correction (LSIC) method, first developed by Lüders *et al.* [15]. In particular we have demonstrated explicitly the ability of the LSIC method to self-interaction correct both bound states and states within scattering resonances. This then leads to a theory which can describe valence transitions between different valence states of the rare earth atom as a function of jellium density, or Wigner-Seitz radius within the EMT theory [5]. The remainder of this highlight describes the LSIC method, and its application to a Ce atom in jellium.

2 Local Self-interaction Correction (LSIC)

The self-interaction correction (SIC) [16] approximation to density functional theory (DFT) was proposed by Perdew and Zunger to ensure that the exchange correlation functional becomes exact for a single electron in a bound state. Other widely used approximations, such as the local spin density approximation or the generalized gradient approximation (GGA) do not obey this constraint, and therefore make an error when applied to a single electron. The Perdew-Zunger SIC adds a correction term to the LSDA, which subtracts the unphysical Hartree self-interaction of each single electron generalized Kohn-Sham orbital spin density, $n_{i\sigma}(\mathbf{r})$ and the corresponding erroneous LSDA exchange and correlation energy, $E_{xc}[n_{i\sigma}, 0]$. The resulting energy functional is a functional of the generalized Kohn Sham orbital densities, $n_{i\sigma}(\mathbf{r})$, and becomes exact when only one electron bound state is occupied. The original Perdew-Zunger SIC functional was shown to improve significantly the descriptions of atoms, for example giving the correct asymptotic $-1/r$ form of the Kohn Sham potential $V(\mathbf{r})$, and providing improved ionization energies and electron affinities. For systems where all the Kohn Sham states are extended the SIC correction vanishes and so the functional again becomes equal to the usual LSDA (or GGA).

The application of SIC to bulk periodic crystals leads to an improved description of systems with tightly localized electron states, such as 3d transition metal oxides and the lanthanide and actinide f-electron metals [17]. In these cases the SIC functional allows electronic states to be either band-like or localized, and both kinds of states are treated together within the same *ab initio* approach. In general the self-consistent minimization of the total energy functional leads to solutions with different numbers of localized states, and the lowest energy solution found is taken as the global ground state. If no states are found to be localized the method is equivalent to standard LSDA. These different localization states can be interpreted physically as representing different chemical valence states of the d or f shell states. In particular for Cerium it was found that the isostructural transition between the α and γ phases arose naturally from the SIC methodology as a valence transition between trivalent and tetravalent Ce [18].

An important feature of the original SIC formulation by Perdew and Zunger was that the SIC should vanish for the case of extended quantum states. However, recently Lüders *et al.* [15] proposed an extension of the SIC to strongly bound resonances. They argued that it is reasonable to apply the SIC for resonances, provided that the time for which the electron is bound in the resonance (the Wigner delay time) is longer than other characteristic timescales in the quantum many-body scattering problem. In practice this new formulation of SIC, named local-SIC (LSIC), has the advantage of being compatible with the multiple scattering KKR approach to electronic structure calculations. Unlike the original Perdew Zunger formulation of SIC, it can also be applied for finite temperature calculations, and combined with the coherent potential approximation (CPA) for disorder and with the disordered local moment (DLM) model of finite-temperature magnetism [19]. The LSIC has been successfully applied to a wide range of different systems, including the α and γ phase transition of Ce [15].

We first show that the LSIC functional proposed and developed by Lüders et al. [15] can be readily adapted to the case of an atom in jellium. In the original formulation of SIC, the correction would be applied to all the bound states, but not to any extended states, as for example in the embedded atom calculations of Puska and Nieminen [20]. However, demonstrably within the model, the electron density due to a resonance in the continuum states is just as well-localized as the density due to a discrete state. Therefore it is reasonable to assume that the self-interaction for such a resonance does not vanish, and so the corresponding self-interaction energy terms for this density should also be subtracted from the LSDA energy functional. In what follows we shall demonstrate this with explicit calculations.

3 LSDA solution of an atom in jellium

We consider an atom of atomic number Z, embedded in a uniform jellium of background electron density n_0. Within the LSDA the ground-state solution is obtained by solving the self-consistent Kohn-Sham (KS) equations

$$\left(-\frac{1}{2}\nabla^2 + V^\sigma(r)\right)\phi_i^\sigma(\mathbf{r}) = E_i^\sigma \phi_i^\sigma(\mathbf{r}) \tag{2}$$

where, assuming spherical symmetry, the potentials are

$$V^\sigma(r) = \int \frac{\Delta n(r')}{|\mathbf{r}' - \mathbf{r}|} d\mathbf{r}' - \frac{Z}{r} + V_{xc}^\sigma(n^\uparrow(r), n^\downarrow(r)) - V_{xc}(\frac{n_0}{2}, \frac{n_0}{2}). \tag{3}$$

where $\Delta n(r) = n(r) - n_0$ is the atom induced electron density. In principle the Kohn-Sham potentials, $V^\sigma(\mathbf{r})$, and spin-densities, $n^\sigma(\mathbf{r})$, may become non-spherical, however in the work described below we have imposed spherical symmetry on the spin densities, and hence the KS equations reduce to the radial Schrödinger equations. The final term in Eq. 3 defines the potential energy to be zero far from the ion.

The total energy of the atom in jellium is defined by

$$\begin{aligned} E_{tot} \quad = \quad & \sum_{n,l,\sigma} (2l+1) E_{nl}^\sigma + \int_0^{E_F} E \Delta n(E) dE - \\ & \sum_\sigma \int n^\sigma(r) V^\sigma(r) d\mathbf{r} + \\ & \int \left(\frac{1}{2} \int \frac{(\Delta n(r'))}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - \frac{Z}{r}\right) (\Delta n(r))\, d\mathbf{r} + \\ & E_{xc}\left[n^\uparrow(r), n^\downarrow(r)\right] - E_{xc}\left[\frac{n_0}{2}, \frac{n_0}{2}\right] \end{aligned} \tag{4}$$

where the E_{nl}^σ are the KS eigenvalues of the atom induced bound states ($E_{nl}^\sigma < 0$) of quantum numbers n and l, and $\Delta n(E)$ is the atom-induced density of states in the continuum ($0 < E < E_F$, where E_F is the Fermi energy of the jellium). The Hartree and exchange-correlation energy terms are defined to subtract out the (infinite) energy of the jellium background, ensuring that

$E_{tot} = 0$ in the absence of the atom. Note that the continuum eigenvalue energy term above can be re-written in terms of the scattering phase-shifts, $\delta_l^\sigma(E)$ for angular momentum channels l,

$$\int_{E=0}^{E_F} E\Delta n(E)dE = \frac{1}{\pi}\sum_{\sigma,l}(2l+1)E_F\delta_l^\sigma(E_F) - \frac{1}{\pi}\sum_{\sigma,l}(2l+1)\int_0^{E_F}\delta_l^\sigma(E)dE. \tag{5}$$

4 LSIC solution for an atom in jellium

In the LSIC formalism, we minimize the energy functional

$$\begin{aligned} E_{tot} \quad = \quad & \sum_{l,m,\sigma} E_l^\sigma + \frac{1}{\pi}\sum_{\sigma,l}(2l+1)E_F\delta_{l,m}^\sigma(E_F) - \\ & \frac{1}{\pi}\sum_{\sigma,l,m}\int_{E=0}^{E_F}\delta_{l,m}^\sigma(E)dE - \sum_\sigma \int n^\sigma(r)V^\sigma(r)d\mathbf{r} + \\ & \int\left(\frac{1}{2}\int\frac{(n(r)-n_0)}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' - \frac{Z}{r}\right)(n(r)-n_0)\,d\mathbf{r} + \\ & E_{xc}\left[n^\uparrow(r), n^\downarrow(r)\right] - E_{xc}[\frac{n_0}{2},\frac{n_0}{2}] - \\ & \sum_\alpha\left(\frac{1}{2}\int_{r=0}^{R^\alpha}\int_{r'=0}^{R^\alpha}\frac{n_{SIC}^\alpha(r)n_{SIC}^\alpha(r')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}' + E_{xc}[n_{SIC}^\alpha(r), 0]\right) \end{aligned} \tag{6}$$

where n_{SIC}^α is the density of the channel α, which in this case is one of the $l = 3$, m, σ channels for which the SI-correction is applied. α denotes the spin and angular momentum quantum numbers, and in the case of bound states also the principal quantum number. In this functional, the radii R^α are either set equal to the neutral sphere radius [5], or are set by the condition

$$\int_{r=0}^{R^\alpha} n_{SIC}^\alpha(r)d\mathbf{r} = 1 \tag{7}$$

We show below that our results are independent of this choice.

Minimizing the energy functional with respect to the orbitals gives the following generalized KS equations for the SI-corrected electrons:

$$\left(-\frac{1}{2}\nabla^2 + V_{SIC}^\alpha(r)\right)\phi_{SIC}^{\alpha,(b.s)}(\mathbf{r}) = E_{SIC}^\alpha\phi_{SIC}^{\alpha,(b.s)}(\mathbf{r}) \tag{8}$$

for the bound-state solution, and

$$\left(-\frac{1}{2}\nabla^2 + V_{SIC}^\alpha(r)\right)\phi_{SIC}^{\alpha,(s.s)}(k,\mathbf{r}) = \frac{k^2}{2}\phi_{SIC}^{\alpha,(s.s)}(k,\mathbf{r}) \tag{9}$$

for the scattering-state solutions. The quantity $n_{SIC}^\alpha(r)$ is then obtained as the density contributions from the bound and scattering state SIC solutions,

$$n_{SIC}^\alpha(\mathbf{r}) = |Y_{lm}(\theta,\phi)|^2R^\alpha(r)^2 + \frac{1}{2\pi^2}|Y_{lm}(\theta,\phi)|^2\int_0^{k_f}k^2R^\alpha(k,r)^2dk, \tag{10}$$

where $\phi^{\alpha}_{SIC}(\mathbf{r}) = Y_{lm}(\theta,\phi)R^{\alpha}(r)$ for both bound and scattering states in a given SIC angular momentum channel, $lm\sigma$. As illustrated in Fig. 1, the first term refers to the negative energy contribution while the second one accounts for positive energy contributions within a given SIC channel. In the case of a partially filled sub-shell, we spherically average the corresponding SIC densities $n^{\alpha}_{SIC}(\mathbf{r})$.

For the non-SI-corrected electrons we obtain the LSDA KS equations

$$\left(-\frac{1}{2}\nabla^2 + V^{\sigma}(r)\right)\phi^{\sigma}_i(\mathbf{r}) = E^{\sigma}_i\phi^{\sigma}_i(\mathbf{r}) \tag{11}$$

which also contain bound and scattering state solutions.

5 Self-interaction correction of scattering resonances for Ce in jellium

In order to test whether the above generalization of SIC adds useful physical insight, we consider the case of a cerium atom embedded in a jellium host. Cerium is an interesting case because of its mixed valency, having different valence states depending on the $4f$ orbital occupation. In a jellium host the LSIC formalism allows the $4f$ state of Ce to be either bound or a scattering state. In fact we find both possibilities occur as we vary the jellium density n_0. This is illustrated in Fig. 1 which shows the phase-shifts $\delta^{\sigma}_{lm}(\epsilon)$ for a cerium atom in jellium, with one electron SI-corrected, for two background densities of the jellium. For the low density of $n_0 = 0.0014a_B^{-3}$ ($r_s \sim 5.5a_B$), the SIC potential generates a bound-state, whereas for a high density $n_0 = 0.04a_B^{-3}$ ($r_s \sim 1.8a_B$) the SIC potential generates a resonance in the continuum. The figure shows that in both cases the f-wave phase shift jumps by π in the SI-corrected channel, lm. In Fig. 1 one can see that the phase shifts for the non-SI-corrected f channels show a sharp resonance located just above the Fermi energy, while the d channels show a broad resonance above ϵ_F and the s and p channels are non-resonant. In a pure LSDA calculation all of the f states would have been resonant above ϵ_F, corresponding to a pinning of the partially filled $4f$ shell states at the Fermi energy. The SIC allows one (or more) of the f states to become pulled below the Fermi energy, giving a full electron charge in a $4f$ pseudo-atomic state. It is this ability to treat localized and extended states with different orbital dependent effective potentials, $V^{\alpha}_{SIC}(\mathbf{r})$, which is at the heart of the success of SIC in treating narrow band materials [17]. One can see from Fig. 1 that the LSIC also has this ability, treating some of the Ce $4f$ states as atomic-like and SI-corrected, while treating the remaining $4f$ states in the same way as standard LSDA.

The key feature of the LSIC is that it treats bound states and resonances on an equal footing. Therefore there is no discontinuity in the generalized KS potentials $V^{\alpha}_{SIC}(\mathbf{r})$ when a bound state becomes a scattering resonance. This is confirmed in Fig. 2 where we plot the f resonance energy for a single LSIC corrected state in Ce as a function of jellium density n_0. The range of densities corresponds to typical metallic values of r_s. At low densities the f state is bound, crossing over smoothly to a sharp resonance which moves up and gradually broadens as the jellium density increases. However, at some jellium density the total energy corresponding to a delocalised f electron, i.e. the LSD energy, becomes more favourable and hence the ground state.

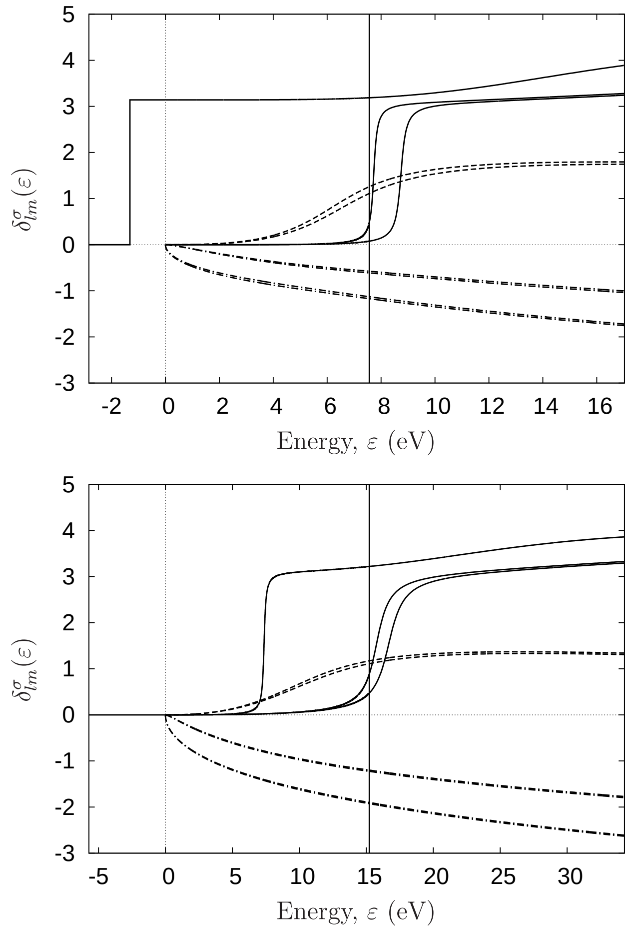

Figure 1: Phase-shifts for cerium in jellium with one electron SI-corrected. The two background densities are: (a) $0.0014a_B^{-3}$, and (b) $0.032a_B^{-3}$. In the first case the SIC potential binds an electron and in the second the SI-corrected state appears as a resonance in the scattering states. Here the solid lines are f channel phase shifts (both SI-corrected and not corrected), the dashed lines are d-channels, and the dot-dashed lines are s and p channels. Splitting of up and down spin states is also visible in the d and the non SI-corrected f channels.

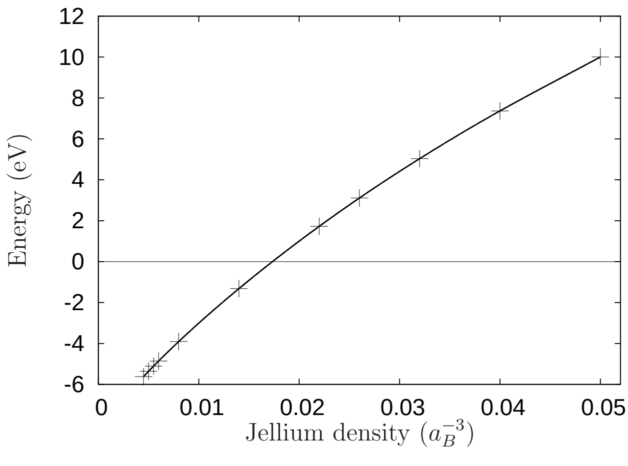

Figure 2: Position of the bound-state/resonance generated by the SIC potential as a function of the background density of the jellium. The system is a cerium atom in jellium with one electron SI-corrected.

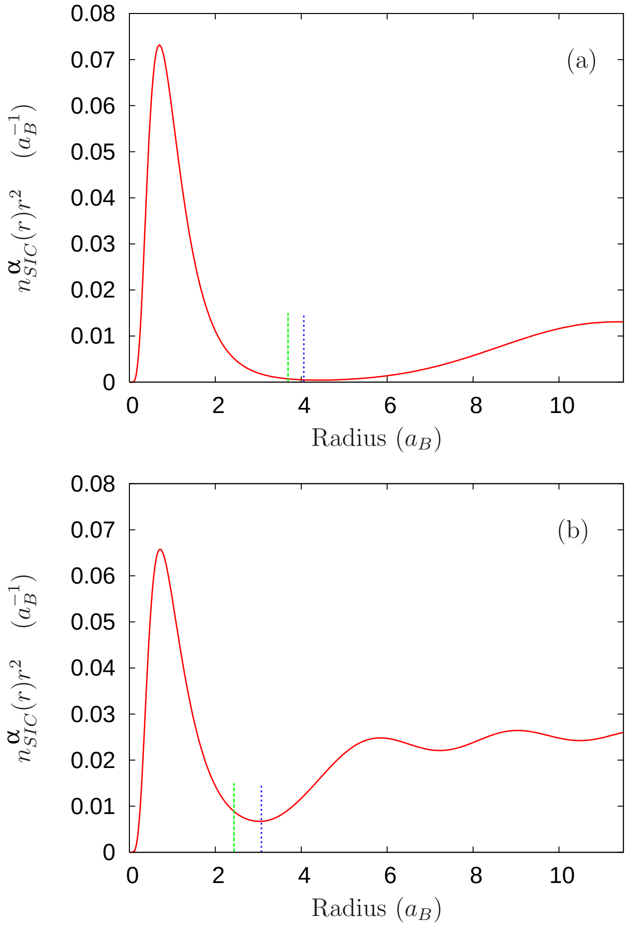

Figure 3: The SIC corrected orbital density $n^{\alpha}_{L}(r)$ is plotted for a cerium atom in jellium with one electron SI-corrected for two background densities, $0.0055a_B^{-3}$ (a) and $0.04a_B^{-3}$ (b). The straight lines indicate the neutral sphere radius (furthest left) and the radius at which the total integrated SIC charge equals one (as defined by Eq. 7).

The physical justification of LSIC requires that the orbital density $n^{\alpha}_{SIC}(\mathbf{r})$ contains one electron within the atomic radius R^{α}, as expressed in Eq. 7. To demonstrate that this is indeed the case we show in Fig. 3 the orbital density, spherically symmetrized, for the case of a bound or resonant SI-corrected $4f$ channel, for two jellium densities $0.0055a_B^{-3}$ and $0.04a_B^{-3}$. For the lower of the two densities the SIC potential localizes a bound-state, while for the higher of the two the SIC potential generates a resonance, as can be seen from Fig. 2. One can see that the orbital density is similar whether the SIC corrected channel contains a bound state or a scattering resonance. Hence the self-interaction for the case of the resonance is just as large as for the bound-state, therefore demonstrating the need for an energy functional which can include scattering states in the SI- correction.

Fig. 3 also shows two possible definitions of the atomic sphere R for the Ce in jellium. One can take either the "neutral sphere radius" of Effective Medium Theory (EMT) [5], defined as the radius for which the atom-induced electron density $\Delta n(\mathbf{r})$ integrates to the nuclear charge Z, or define a radius R^{α} for which Eq. 7 is satisfied exactly for the SI-corrected f channel. In practice it is clear from Fig. 3 that these two definitions give essentially identical results. It is also clear from the figure that the total channel density $n^{\alpha}_{SIC}(r)$ for $r < R^{\alpha}$ contains the localized atomic-like part of the density and very little of the extended jellium-like part. Therefore it does not matter in detail whether one includes only the part of the density associated with the bound state or resonance, or includes all of the density up to ϵ_F within that $L = lm$ channel, as given in Eq. 7.

6 Effective Medium Theory of Ce metal

In the EMT, each atom in a solid is regarded as sitting in an electron density set up by the density tails of all of the other atoms in the solid. The only input parameter in the EMT is the atomic number, Z. The theory has been successfully put to use in the calculation of cohesive properties of solids, amongst other uses. In particular, the theory reproduces trends in the experimental lattice constants, bulk moduli and cohesive energies across the periodic table [5,6,20].

In the EMT, the cohesive energy of the solid is written as

$$\Delta E[n, v] = \sum_i E_c(\bar{n}_i) + \Delta E_{1-el} \tag{12}$$

where

$$E_c(\bar{n}) = E_{imm}(\bar{n}) + \bar{n}\int_{r=0}^{r=s}\left(\int \frac{\Delta n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' - \frac{Z}{r}\right)d\mathbf{r} \tag{13}$$

Here $\Delta n(\mathbf{r})$ is the atom-induced density. The second term is attractive and has the effect of lowering $E_c(\bar{n})$. It can be viewed as the attraction of the sum of the density tails from all other cells ($\bar{n}$) with the Hartree potential from cell a_i.

The ΔE_{1-el} term is the sum of the change of the one-electron energy eigenvalues when we go from the homogeneous electron gas to the real host. This change occurs because of covalent bonding, hybridisation and effects due to wavefunction orthogonalisation. A number of ways

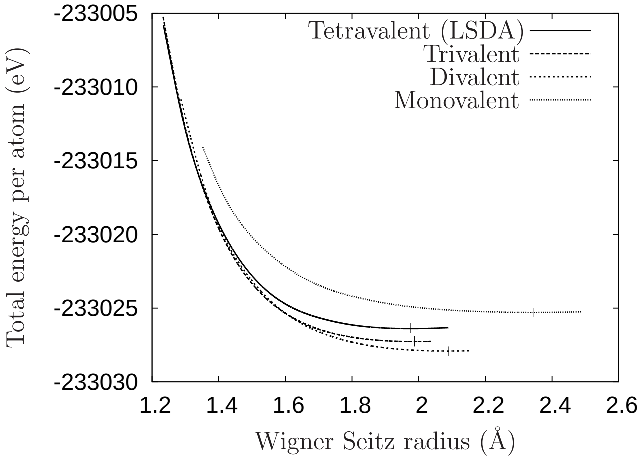

Figure 4: Total energy per atom plotted against the Wigner-Seitz radius (EMT neutral sphere radius) for different choices of the exchange-correlation functional. SI-correcting two electrons, which corresponds to a valence of two in the full solid, gives the lowest energy.

have been proposed to include this term [21–25], however in our calculations we will neglect this term. With this term neglected, $E_c(\bar{n})$ is the cohesive energy per atom.

The procedure in EMT is to solve for some arbitrarily chosen $\bar{n}$, the self-consistent problem of an atom in a homogeneous gas in order to obtain $\Delta n(\mathbf{r})$ and then evaluate $E_c(\bar{n})$. One then varies $\bar{n}$ in order to minimise $E_c(\bar{n})$. This minimum value of $E_c(\bar{n})$ is then the cohesive energy per atom of the solid, and the corresponding value of neutral sphere radius, R^α, is the Wigner-Seitz radius as predicted by the theory.

Fig. 4 shows our results for the total energy of a bulk Ce metal calculated using the effective medium theory (EMT) from our LSIC atom in jellium results. The different curves correspond to: standard LSDA with no SIC correction (tetravalent Ce), one f state SIC corrected (trivalent Ce), two f states corrected (divalent Ce) and three states corrected (monovalent Ce). The curves are plotted as a function of the effective Wigner Seitz atomic radius, obtained within the EMT theory. The fcc-γ phase of Ce is believed to be trivalent, [18] corresponding to one localized f state. Our calculations predict the minimum energy Wigner Seitz radius for trivalent Ce to be 1.99 $\mathring{A}$, in very good agreement with the Wigner-Seitz radius of 2.02 $\mathring{A}$ fcc-γ phase Ce.

One can see in Fig. 4 a series of crossings between the different valence states as a function of the Wigner-Seitz radius. At the smallest Wigner-Seitz radius the LSDA tetravalent state is lowest in energy, crossing over to trivalent and then divalent at the radius is increased. In terms of the phase diagram of Ce this would imply a series of valence state transitions under pressure. If the α-γ transition in bulk Ce is viewed as a crossing between trivalent and tetravalent states, then our EMT results give a small volume “collapse” of a few % in volume, but one which is much smaller than found experimentally or in previous SIC calculations [15, 18]. Nevertheless the SI-corrected calculation appears to capture the essential physics of the valence transition. However our global minimum energy state is the divalent one, with a larger radius of about 2.09$\mathring{A}$, rather than the expected trivalent state. It is most likely that this discrepancy arises from the omission of the covalent terms in the EMT theory, ΔE_{1-el}. The spherical symmetrization of the LSDA and SIC-charge densities is also a possible problem, since recent results of Stengel and Spaldin show a substantial contribution to the energy from the non-spherical terms. [26] We leave further investigation of these important questions to future work.

7 Conclusions

We have demonstrated that the LSIC approach is necessary to correctly treat the self-interaction of resonances in the system of an atom in jellium. We have shown that the electron density corresponding to a resonance is just as localized as that due to a bound-state, and therefore this resonance should also be corrected for in the LSIC energy functional. Using the LSIC, we have shown that as we increase the background density of the jellium, a bound-state of the LSIC potential will increase in energy and will eventually become a scattering state resonance. This resonance will continue to increase in energy as the background density is increased further. This is in contrast with the Perdew-Zunger SIC approach. In this approach, when the electron in the SIC channel enters the continuum of scattering states, it will no longer be treated for its self-interaction and so will become extended and will not form a resonance.

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