Ψ_k Newsletter

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

Number 69 June 2005

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

Contents

1 Editorial

We start this newsletter with a call for registrations and abstracts to the Psi-k2005 Conference. This is followed by a call for workshop proposals in 2006. In this newsletter we have two reports on the recent workshops, one in the ESF section, and another in the UK's CCP9 section. There are a few workshop/conference announcements in this newsletter, and in particular the one of the NANOQUANTA Network of Excellence is on **"40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges"**. The announcements of available positions and abstracts of recently published or newly submitted papers are in their usual sections. In the section on **Presenting Other Initiatives** we advertise a special issue of the "Computational Crystallography" journal.

The scientific highlight of this issue is on **"Many-body perturbation theory using the density-functional concept"** by Fabien Bruneval (*Paris*), Francesco Sottile (*Paris* and *Donostia*), Valerio Olevano (*Paris* and *Grenoble*), Rodolfo Del Sole (*Roma*), and Lucia Reining (*Paris*).

Please check the table of contents for further details on the newsletter.

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

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

The above contains information on the Psi-k 2005 workshops and hands-on courses (subject to funding). In these pages you can also find information on how to apply for funding to make collaborative visits.

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-k2005 Conference

2.1.1 Call for abstracts and registration

"Towards atomistic materials design"

September 17-21, 2005

Schwäbisch Gmünd, Germany

Like the two previous Psi-k meetings (1996, 2000), Psi-k 2005 will cover widely theoretical and computational research of electronic structure and properties of condensed matter, ranging from new materials and nanoscience to systems of biological interest. The conference carries the motto "Toward atomistic materials design", and is supported by the Psi-k Programme and Network of the European Science Foundation.

The scientific programme is based on plenary sessions and parallel symposia organised in part by the Working Groups of the Psi-k Network. There will be close to 100 invited and plenary speakers.

The conference website is at

http://www.fyslab.hut.fi/psik2005/

where more details of the programme are presented.

The conference website now accepts registrations, abstract submission and hotel registration. The registration deadline is July 15, 2005. However, due to limited hotel capacity early registration is strongly recommended.

Looking forward to seeing you in Schwaebisch Gmuend.

Risto Nieminen
Psi-k 2005 Chairman

3 News from the ESF Programme

”Towards Atomistic Materials Design”

3.0.2 Call for Workshop Proposals for 2006

Here we would like to announce the call for workshops, hands-on tutorials and small conferences to be held in 2006 for partial funding by the ESF Psi-k Programme.

A proposal should be submitted by e-mail (in the form of a simple e-mail letter, just plain ASCII) to the Psi-k Programme secretary, Walter Temmerman, at

psik-coord@dl.ac.uk

Since the Steering Committee will meet at the Psi-k 2005 Conference in Schwaebisch-Gmuend, the final **deadline** is already on

15 August 2005

The guide lines for proposals are given below. Here we want to add some general information concerning future workshops and tutorials.

General Information about Psi-k Workshops etc.

The coming years 2006 and 2007 will be the last ones of the present Psi-k Programme ”Towards Atomistic Materials Design”. Since due to excellent planning the finances are in good shape we can fund in the next two years a total of about **35 workshops, tutorials and smaller conferences**. Therefore I ask all Psi-k members, in particular the working groups, to consider and carefully plan activities for the next two years. Besides the large Psi-k Conference and some other activities in 2005, we have organised in 2003 and 2004 28 workshops and 6 tutorials. Therefore the next two years can be equally successful.

Collaboration with CECAM:

During the last half-year we had intensive discussions with CECAM/Lyon, in particular with the director Berend Smit. Both sides have decided to collaborate much stronger together in the future, which would also mean a collaboration of the two large European bottom-up networks on molecular simulations (MOLSIMU) and ab-initio calculations (Psi-k). In this way Psi-k would gain a solid base of funding and CECAM would become the European center for Computational Materials Science.

For these reasons we want to encourage you, to submit in the future more **joint Psi-k/ CECAM** proposals for Workshops. Usually these workshops will take place at CECAM in Lyon, which supplies the lecture rooms and secretarial support. However well-founded requests for other locations will be considered. For you the joint workshops have the advantage that with Psi-k *and* CECAM funding the workshop expenses will be more or less fully covered.

The collaboration with CECAM will also allow for a limited number of **small conferences** with say 50-60 participants. The workshops at CECAM are usually limited to about 40 participants, but facilities for small conferences with up to 70 participants exist. For such a conference Psi-k would increase the usual amount of funding, while CECAM would contribute the normal amount for workshops.

As a rough rule of thumb, we would consider it as ideal, if about half the Psi-k proposals are funded jointly with CECAM. Since this intensive collaboration is new and since we aim at a balanced amount of Psi-k and joint Psi-k/CECAM activities, I would like you to inform me (p.h.dederichs@fz-juelich.de) about your plans for 2006, if possible before August 15. Information about CECAM and guidelines for CECAM proposals you will find under www.cecam.fr. The deadline for CECAM proposals is Oct. 1, 2005. At present the announcement is not yet on the web.

Guidelines for Psi-k Proposals

For joint Psi-k/CECAM proposals you can follow the CECAM guidelines, which will soon appear on the web. The Psi-k proposals should include the following points (preferably numbered in this order).

1. Title and purpose of the workshop, with names and addresses (including email) of the organisers. See item (9) about an American or Japanese co-organiser.
2. The scientific content and why a workshop would be useful at this time.
3. A tentative list of speakers whom it is hoped to have.
4. The number of participants it is planned to invite or attract, and their scientific involvement, e.g. as simulators, related experimentalists, code developers, etc., and young scientists in the subject.
5. Plans for a tutorial element and for attracting new researchers into the subject of the workshop. (If this is thought inappropriate for this workshop, please explain why.) The purpose of the ESF Psi-k Programme is to help everyone in our community to do good quality research, and in our expanding field this implies some outreach and tutorial activity.
6. Budget, expressed in Euro, and how much is being applied for from the ESF Psi-k Programme. In the past, this has been limited to about 9k Euro.
7. A statement about other organisations which will be applied to for co-sponsorship and additional funding, e.g. any EU Network, CECAM, CCP-9 in the UK, etc.
8. Where it is hoped the workshop would be held.

9. Plans about inviting and financing any participants from America. See the announcement of Volker Heine in the June 2003 Newsletter about having an appropriate American co-organiser of the workshop. For plans to invite Japanese scientists or co-organisers in 2006, please contact me or directly Hiroshi Katayama-Yoshida (hiroshi@sanken.osaka-u.ac.jp).

Peter H. Dederichs
Chairman of ESF Psi-k Programme

Institut fuer Festkoerperforschung
Forschungszentrum Juelich
D-52425 Juelich
Germany

Tel.: +49 2461 61 4351
Fax: +49 2461 61 2620
E-Mail: p.h.dederichs@fz-juelich.de

3.1 Reports on ESF Workshops/Conferences

3.1.1 Report on the Twelfth International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

ICTP - Trieste

13 - 15 January 2005

Sponsors:
International Centre for Theoretical Physics (ICTP) - Trieste
International School for Advanced Studies (SISSA) - Trieste
Lawrence Livermore National Laboratory (LLNL) - US
European Science Foundation, Psi-k network
INFM - DEMOCRITOS, National Simulation Center
Material Computation Center (UIUC), Travel Program for Young Scientists

Organizers:
Giulia Galli (LLNL - US)
Emilio Artacho (University of Cambridge, UK)
Andrea Dal Corso (SISSA and DEMOCRITOS, Trieste, Italy)
Web page:
`http://cdsagenda5.ictp.trieste.it/full_display.php?smr=0&ida=a04178#`

Summary

This Workshop followed the series started in Oxford (1983) and continued in Braunschweig (1984) and in Trieste (1987, 1989, 1991, 1993, 1995, 1997, 1999, 2001 and 2003). Following the tradition of the previous meetings, the Workshop has been devoted to recent advances in computational condensed matter physics and materials science, based on realistic calculations of the electronic structure of polyatomic systems.

The Workshop consisted of 28 invited talks, a special section on code development with 5 invited talks and a poster session with about 90 posters. The meeting was focused on methodological aspects, supplemented by sessions devoted to recent important applications. Its format was the one of a Workshop among specialists, with ample space for discussion and personal interaction. This edition, with a total attendance of 206 people, has seen a large number of young participants who could benefit from the interaction with more experienced scientists. Thanks to the ICTP funds we could also support (partially or in full) 9 participants from developing countries.

The Workshop has been followed by a one-week tutorial on the use of the Quantum ESPRESSO package, an open source package for electronic structure calculation. (See the web page `http://www.democritos.it/events/espresso-tutorial.php`). Many participants to this tutorial could follow the discussions at the Workshop and be exposed to the advanced applications of electronic structure methods presented here.

Description of the scientific content

The complete program of the Workshop is given at the end of this document. As can be seen from the program the addressed topics were very broad, ranging from formal theoretical developments in Quantum Monte-Carlo, ab-initio transport theory, ab-initio theory of superconductivity, linear scaling methods and density functional perturbation theory, to applications to nano and biological structures, to complex materials problems, and to surfaces and catalysis.

As in the tradition of the Workshop we had a section on the development of DFT beyond the local density formulation and related topics with contributions by S. Louie (US) and M. Head-Gordon (US).

We had a section devoted to the study of solids in an electric field (static and time dependent) and a related section devoted to density functional perturbation theory with contributions by I. Souza (US), O. Diéguez (US), F. Giustino (Switzerland), S.Y. Savrasov (US), M. Veithen (Belgium), and M. Lazzeri (France).

A section was devoted to linear scaling density functional theory calculations with contributions by M. Challacombe (US), M. Seijo (Spain) and J.L. Fattebert (US).

The ab-initio theory of superconductivity was illustrated by E.U.K. Gross (Germany) and applications were presented by S. Massidda (Italy).

Developments and applications of Quantum Monte Carlo methods were presented by C. Filippi (Netherlands), J.C. Grossman (US) and M. Fuchs (Germany).

Novel methods to deal with the ballistic transport in nanostructures were presented by N. Marzari (US) and by A. Smogunov (Italy).

Applications of the ab-initio methods to the study of nano and biological structures were presented by W. Andreoni (Switzerland), X. Blase (France), A. Oshiyama (Japan) and N. Manini (Italy).

Applications to complex material problems were presented by D. Alfè (UK), F. Willaime (France) and S.A. Bonev (Canada), while applications to surfaces and catalysis were presented by F. de Angelis (Italy), J.M. Soler (Spain) and N. Bonini (Italy).

Moreover, a special section was devoted to the modern methods for code development. Speakers in this section were P. Murray Rust (UK), A. Garcia and J. Wakelin (UK), P. Giannozzi (Italy), J. Junquera (Spain) and J.J. Mortensen (Denmark).

A lively poster section with about 90 posters allowed young participants to present their work and to interact with more experienced scientists. The Workshop had a very international character and it contributed to strengthen contacts between scientists of US, Europe, Asia, and Africa and to continue the strong international attitude of this community. Speakers, committee members, organizers, and chairpersons (47 in total) were from North America (12), from Europe (33), and from Asia (2). Participants (159 in total) were from North America (10), Brasil (1), Europe (113), Eastern Europe (6), Asia (22), Africa (6), and New Zealand (1). 121 among the 159 participants were less than 35 years old.

More information on the event and a booklet of abstracts can be found at the webpage.

Assessment of the results and impact of the event in the future direction of the field

The format of this Workshop has been tested and refined over the years, and the ICTP has provided the ideal framework for the meeting of scientists coming from all over the world, solving almost seamlessly the practical problems that arise in the organization of these meetings. This edition saw a very active and motivated participation of many researchers from several countries, witnessing the interest in many parts of the world to pursue, expand or also to start activities in computational condensed matter physics and materials science based on the electronic structure. This Workshop was a very good occasion for many young people to present their work and to meet more experienced scientists. The quality of the talks and of the posters was very high and very much appreciated. In particular, the number of young participants demonstrates the vitality of this field that is now a mature field that is helping to give a sound theoretical basis to many very rapidly developing areas such as the study of nano and biological structures, the study of complex materials and of materials at extreme conditions, and the microscopic understanding and control of chemical reactions. The Workshop gathered a very active community that struggle to improve and extend the numerical methods based on the electronic structure, increasing their accuracy and the number of properties that they can tackle. The participation of scientists from US, Europe, and Asia shows that these efforts are really international. The availability of open-source codes is a very important aspect for the growing of this community and this Workshop contributed to show the potentiality of these codes and to improve their future developments.

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The Abdus Salam International Centre for Theoretical Physics

12th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods

Co-sponsored by:

- International School for Advanced Studies (SISSA)
- Lawrence Livermore National Laboratory (LLNL)
- European Science Foundation's Psi-k Programme (ESF)
- INFM DEMOCRITOS National Simulation Center
- Materials Computation Center (UIUC), Travel Program for Young Scientists

Organizers: G. Galli, E. Artacho, A. Dal Corso

Trieste - Italy, 13 - 15 January 2005
Venue: Main Building Lecture Hall

Final programme

THURSDAY, 13 JANUARY 2005

REGISTRATION AND OPENING REMARKS

08:00 - 09:00	— Registration and administrative formalities —
09:10 - 09:20	Opening remarks

BEYOND LOCAL DENSITY FORMULATIONS

Chairperson: S. de Gironcoli

09:20 - 10:00	S. Louie / *UC Berkeley & Lawrence Berkeley National Lab., USA* Ab-initio study of the photo-excited state: nanotubes to self-trapped excitons
10:00 - 10:30	M. Head-Gordon / *UC Berkeley & Lawrence Berkeley National Lab., USA* Fast electron correlation methods for molecules
10:30 - 11:00	— — Coffee break — —

AB-INITIO CALCULATIONS IN ELECTRIC AND MAGNETIC FIELDS

Chairperson: D. Vanderbilt

11:00 - 11:30	I. Souza / *UC Berkeley, USA* Dynamics of Berry-phase polarization in time-dependent electric fields
11:30 - 11:50	O. Diéguez / *Rutgers University, USA* First-principles simulations at constant electric polarization
11:50 - 12:10	F. Giustino / *EPFL & IRMMA, Switzerland* Dielectric permittivity across interfaces in the atomic-scale limit
12:10 - 14:10	— — Break — —

LINEAR SCALING DENSITY FUNCTIONAL THEORY CALCULATIONS

Chairperson: G. Galli

14.10 - 14.40	M. Challacombe / *LANL, USA* New developments in linear scaling electronic structure theory: the perturbed projector for ab-initio response theory and exact Hartree-Fock exchange in the condensed phase
14:40 - 15:10	L. Seijo / *UNAM, Spain* Mosaico: a parallel, linear-scaling method for large molecules and embedded clusters
15:10 - 15:40	J.-L. Fattebert / *LLNL, USA* Linear scaling first-principles molecular dynamics with controlled accuracy
15:40 - 16:10	— — Coffee break — —

SUPERCONDUCTIVITY WITHIN DENSITY FUNCTIONAL THEORY

Chairperson: R. Resta

16:10 - 16:40	E.K.U. Gross / *Freie Univ. Berlin, Germany* DFT for superconductivity (theory)
16:40 - 17:10	S. Massidda / *INFM SLACS, Università di Cagliari, Italy* DFT for superconductivity (applications)

SPECIAL SESSION ON CODES

Chairperson: E. Artacho

17:10 - 17:30 P. Murray-Rust / *University of Cambridge, UK*
Modular approaches to computational chemistry

17:30 - 18:00 A. Garcia & J. Wakelin / *Univ. del País Vasco, Bilbao, Spain & Cambridge Univ., UK*
Software tools for data interchange

18:00 - 18:20 P. Giannozzi / *Scuola Normale Superiore Pisa & DEMOCRITOS, Italy*
The Quantum-Espresso software distribution

18:20 - 18:35 J. Junquera / *Universidad de Cantabria, Spain*
Software tools for data interchange

18:35 - 18:55 J.J. Mortensen / *Technical University of Denmark*
An XML-format for atomic PAW setups

POSTER SESSION

FRIDAY, 14 JANUARY 2005

DENSITY FUNCTIONAL PERTURBATION THEORY

Chairperson: R. Resta

09:00 - 09:30 S.Y. Savrasov / *New Jersey Institute of Technology, USA*
Spectral density functionals for electronic structure calculations

09:30 - 09:50 M. Veithen / *University of Liege, Belgium*
Computation of non-linear optical properties from density functional theory

09:50 - 10:10 M. Lazzeri / *LMCP Paris, France*
Kohn anomalies and electron-phonon interactions in graphite

10:10 - 10:40 — — Coffee break — —

QUANTUM MONTE CARLO

Chairperson: R. Needs

10:40 - 11:10 C. Filippi / *Inst.-Lorentz Univ. Leiden, the Netherlands*
Excitation energies of photoactive molecules from Quantum Monte Carlo

11:10 - 11:40 J.C. Grossman / *LLNL, USA*
Efficient Quantum Monte Carlo energies for molecular dynamics simulations

11:40 - 12:10 M. Fuchs / *Max-Planck-Gesellschaft Berlin, Germany*
Diffusion Monte Carlo study of hydrogen bonded systems

12:10 - 14:10 — — Break — —

NANO AND BIO STRUCTURES

Chairperson: E. Tosatti

14:10 - 14:40	W. Andreoni / *IBM Research, Zürich, Switzerland* The role of ab-initio molecular simulations in computational biology
14:40 - 15:10	X. Blase / *CNRS & Univ. Claude Bernard, Lyon, France* From plastic to superconducting properties of covalent clathrates
15:10 - 15:40	A. Oshiyama / *University of Tsukuba, Japan* Nano-shapes and electronic properties of carbon materials
15:40 - 16:10	N. Manini / *Università di Milano, Italy* Jahn-Teller spectral fingerprint in molecular photoemission: C60
16:10 - 16:40	— — Coffee break — —

TRANSPORT PROPERTIES

Chairperson: J. Ihm

16:40 - 17:10	N. Marzari / *MIT, USA* Electronic structure and quantum conductance of nanostructures: the case of functionalized nanotubes
17:10 - 17:30	A.N. Smogunov / *SISSA & INFM DEMOCRITOS, Trieste, Italy & Voronezh State University, Russia* Electron transport in magnetic nanocontacts
17:30 - 19:00	Free time - Posters up — — Conference dinner — —

SATURDAY, 15 JANUARY 2005

COMPLEX MATERIAL PROBLEMS

Chairperson: M. Gillan

09:20 - 09:40	D. Alfe' / *London, UK* The melting curve of MgO from first principles calculations
09:40 - 10:00	F. Willaime / *CEA Saclay, France* Kinetics of radiation defects in iron from first principles
10:00 - 10:20	S.A. Bonev / *Dalhousie University, Canada* Ab-initio simulations of phase transitionds in dense hydrogen
10:20 - 10:50	— — Coffee break — —

SURFACES AND CATALYTIC PROCESSES

Chairperson: M. Bernasconi

10:50 - 11:10	F. De Angelis / *ISTM - CNR, Università di Perugia, Italy* A time-dependent DFT study of [Fe(CN)6]4- sensitization of TiO2 nanoparticles
11:10 - 11:40	J.M. Soler / *UNAM, Spain* Fast and reliable STM/STS simulations
11:40 - 12:00	N. Bonini / *SISSA & INFM DEMOCRITOS, Trieste, Italy* Engineering the reactivity of metal catalysts: a model study of methane dehydrogenation on Rh(111)
12:00 - 12:00	R. Martin / *University of Illinois, Urbana, USA* Closing remarks

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The Abdus Salam International Centre for Theoretical Physics

SMR Number: 1641

12th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods

— International School for Advanced Studies (SISSA) —INFM DEMOCRITOS National Simulation Center —European Science Foundation

13 - 15 January 2005

Final List of Participants

Total number of visitors for this activity: 206

Directors

ARTACHO Emilio	Spain	emilio@esc.cam.ac.uk
DAL CORSO Andrea	Italy	
GALLI Giulia	Italy	

Speakers

ALFE' Dario	Italy	
ANDREONI Wanda	Italy	and@zurich.ibm.com
BALDERESCHI Alfonso	Italy	
BLASE Xavier	France	
BONEV Stanimir	Bulgaria	
BONINI Nicola	Italy	bonini@sissa.it
CHALLACOMBE Matt	United States of America	
DE ANGELIS Filippo	Italy	
DIEGUEZ LOPEZ Oswaldo	Spain	dieguez@physics.rutgers.edu
FATTEBERT Jean-Luc	Switzerland	
FILIPPI Claudia	Italy	filippi@lorentz.leidenuniv.nl
FUCHS Martin	Germany	
GARCIA ARRIBAS Alberto	Spain	
GIANNOZZI Paolo	Italy	giannozzi@nest.sns.it, p.giannozzi@sns.it
GILLAN Michael John	United Kingdom	
GIUSTINO Feliciano	Italy	
GROSS Eberhard Kurt Ulrich	Germany	
GROSSMAN Jeffrey C.	United States of America	
HEAD-GORDON Martin Paul	Australia	
IHM Jisoon	Republic of Korea	
JUNQUERA QUINTANA Francisco Javier	Spain	javier.junquera@ulg.ac.be
KOCH Erik	Germany	
KUNC Karel	France	kunc@ccr.jussieu.fr

LAZZERI Michele	Italy	
LOUIE Steven Gwon Sheng	United States of America	sglouie@berkeley.edu
MANINI Nicola	Italy	
MARTIN Richard Mc Fadden	United States of America	
MARZARI Nicola	Italy	
MASSIDDA Sandro Salvatore	Italy	
MORTENSEN Jens Jorgen	Denmark	jensj@fysik.dtu.dk
MURRAY-RUST Peter		
NEEDS Richard James	United Kingdom	rn11@phy.cam.ac.uk
ORDEJON RONTOME Pablo Jesus	Spain	
OSHIYAMA Atsushi	Japan	
RESTA Raffaele	Italy	
SAVRASOV Sergej - Serguei Y. Savrassov	Russian Federation	savrasov@njit.edu
SEIJO Luis	Spain	
SMOGUNOV Alexander	Russian Federation	
SOLER Jose Maria	Spain	
SOUZA Ivo Nuno - Saldanha do Rosario e Souza Ivo Nuno	Portugal	
TOSATTI Erio	Italy	
VANDERBILT David Hamilton	United States of America	
VEITHEN Marek	Belgium	marek.veithen@ulg.ac.be
WAKELIN Jon		
WILLAIME Francois	France	

Participants

ADEAGBO Waheed Adeniyi	Nigeria	deagbo@thp.uni-duisburg.de
AKANDE Akinlolu	Nigeria	babcock@infoweb.abs.net
AKBARZADEH Hadi	Islamic Republic of Iran	
ALMEIDA Jailton	Brazil	jailton.almeida@fysik.uu.se
ALONSO PRUNEDA Jose Miguel	Spain	
ANGHEL Alexandra Teodora	Romania	
ANTONELLI Alex	Brazil	
BALETTO Francesca	Italy	
BANO Fouzia	Pakistan	fouzia_933@hotmail.com
BARNARD Amanda Susan	Australia	amanda.barnard@anl.gov
BAYAZID Ammar - Baiazid Amnmar	Syrian Arab Republic	
BEDOYA MARTINEZ Olga Natalia	Colombia	natalia@icmab.es
BENNECER Badis	Algeria	b_bennacer@hotmail.com, bennecer@univ-guelma.dz
BERGERMAYER Wolfgang	Austria	wolfgang@fukui.kyoto-u.ac.jp
BERNASCONI Marco	Italy	marco.bernasconi@mater.unimib.it
BIANCHETTIN Laura	Italy	
BJORKETUN Marten Emanuel	Sweden	martebjo@fy.chalmers.se
BRAKO Radovan	Croatia	
BRAMANTI Giovanni	Italy	
BUFFA Raffaele	Italy	
CALZOLARI Arrigo	Italy	calzolari.arrigo@unimore.it

CAPELLO Manuela	Italy	
CARACAS Razvan	Romania	r.caracas@gl.ciw.edu
CARNEIRO Nuno Filipe	Portugal	nfc103@york.ac.uk
CASTELLANA Carlo	Italy	castella@sissa.it
CASTRONOVO Matteo	Italy	castronovo@tasc.infm.it
CASULA Michele	Italy	
CERESOLI Davide	Italy	ceresoli@physics.rutgers.edu
CHARLIER Jean-Christophe	Belgium	charlier@pcpm.ucl.ac.be
CHIS Vasile	Sweden	cvasse@fy.chalmers.se
CHOUDHURY Rathin	United Kingdom	r.choudhury@ucl.ac.uk
CIUCHI Sergio	Italy	sergio.ciuchi@aquila.infn.it
COSLOVICH Daniele	Italy	coslo@ts.infn.it
CRLJEN Zeljko	Croatia	
CUCINOTTA Clotilde Silvia	Italy	c.cucinotta@unimo.it
CUDAZZO Pierluigi	Italy	
D'AVEZAC DE CASTERA Mayeul	France	
DE GIRONCOLI Stefano	Italy	degironc@sissa.it
DEBERNARDI Alberto	Italy	
DETRAUX Francois Christian	Belgium	
DIEP Vinh Quang	Viet Nam	dqvinh@phys.hcmuns.edu.vn
DRUMMOND Neil David	United Kingdom	
DUAN Xiangmei	People's Republic of China	
DUBOIS Simon Mutien-Marie	Belgium	

F.N.		
ELLOH Van Wellington	Ghana	
FABRIS Stefano	Italy	fabris@democritos.it
FERNANDEZ SEIVANE Lucas	Spain	
FERNANDEZ-SANCHEZ Julio Juan	Spain	julio@etsit.upm.es
FERNANDEZ-SERRA Maria Victoria	Spain	
FERRETTI Andrea	Italy	ferretti.andrea@unimo.it
FRATESI Guido	Italy	
GARCIA DE GURTUBAY Idoia	Spain	
GARCIA GIL Sandra	Spain	
GAVA Paola	Italy	
GEBAUER Ralph	Germany	
GIACOMAZZI Luigi	Italy	luigi.giacomazzi@epfl.ch
GROSSO Caterina	Italy	grosso@sissa.it
GULIN-GONZALEZ Jorge	Cuba	
HERNANDEZ Eduardo Robert Rafael	United Kingdom	ehe@icmab.es
HERRERA Fernando Enrique	Argentina	herrera@sissa.it
HINE Nicholas Daniel Mark	United Kingdom	nicholas.hine@imperial.ac.uk
HUANG Lunmei	People's Republic of China	lunmei@fysik.uu.se
ISPAS Simona	Italy	simona.ispas@ldv.univ-montp2.fr
JAHNATEK Michal	Slovak Republic	michal.jahnatek@savba.sk

JONES Glenn	United Kingdom	
JOSHI Kavita Purushottam	India	kjoshi@cea.fr
JOYCE Sian Ann	Ireland	
KACZMARSKI Marcin	Poland	
KANHERE Dilip Govind	India	
KHAKIMOV Zokirkhon Muydinkhonovich	Uzbekistan	
KHELIFA Brahim El Khalil	France	
KIM Gunn	Republic of Korea	gkim@phya.snu.ac.kr
KLAVENESS Arne	Norway	
KOKALJ Anton	Slovenia	
KROTSCHECK Eckhard	Austria	eckhard.krotscheck@jku.at
LABORA VIOLANDA Marites Jaberina	Philippines	marites.labora@up.edu.ph, mariteslabora@yahoo.com
LAZIC Predrag	Croatia	
LEE Kwan-Woo	Republic of Korea	lee@physics.ucdavis.edu
LEE Young-Su	Republic of Korea	lee0su@mit.edu
LIANG Yunfeng	People's Republic of China	
LISENKOV Sergey Victorovich	Russian Federation	lisenkov@sky.chph.ras.ru
LOPEZ RIOS Pablo	Spain	pl275@cam.ac.uk
LU Gang	People's Republic of China	

LUGAS Massimo	Italy	lugas@sissa.it
MACHADO CHARRY Fabio Eduardo	Colombia	machado@icmab.es
MAMAT Mamatrishat - Maimati Maimaitirexiati	Peoples's Republic of China	mamatrishat@163.com
MARCHETTI Riccardo	Italy	marchetr@sissa.it
MARTIN-SAMOS Layla	Spain	
MARTINEZ CANALES Miguel	Spain	
MCGILL Philip Robert	New Zealand	
MEHTA Shailesh	United Kingdom	
MESKINI Noureddine	Tunisia	
MIRANDA Caetano Rodrigues	Brazil	cmiranda@ifi.unicamp.br
MIURA Yoshio	Japan	
MIYAZAKI Tsuyoshi	Japan	miyazaki.tsuyoshi@nims.go.jp
MONTOYA MARTINEZ Javier Antonio	Colombia	amontoya@sissa.it
MORARI Ioan Cristian	Romania	
MOSCA CONTE Adriano	Italy	moscac@sissa.it
MOSTOFI Arash Abolhassan	United Kingdom	aam24@cam.ac.uk
MUNOZ JIMENEZ Adriana	Colombia	
MURDACHAEW Garold	United States of America	garold@physics.udel.edu
NARASIMHAN Shobhana	India	
NATARAJAN Gana - Natarajan Ganapati		
NAZARINIA Mojtaba -	Islamic	

Nazari-nia Mojtaba	Republic of Iran	nazarinia@basu.ac.ir, nazarynia@yahoo.com
NGUYEN Viet Huy	Viet Nam	vnguyen@ictp.trieste.it
NIQUET Yann-Michel	France	
ONIDA Giovanni	Italy	
ONO Tomoya	Japan	ono@upst.eng.osaka-u.ac.jp
PALACIOS CLEMENTE Pablo	Spain	pablop@etsit.upm.es
PAOLINI Stefano	Italy	paolini@sissa.it
PAZ Oscar	Spain	scar.paz@uam.es
PEZZOLI Maria Elisabetta	Italy	pezzoli@sissa.it
PICKARD Christopher James	United Kingdom	
PIERLEONI Carlo	Italy	
PIETRUCCI Fabio	Italy	fabio.pietrucci@mater.unimib.it
PONTIGGIA Francesco	Italy	pontiggi@sissa.it
POUILLON Yann	France	pouillon@pcpm.ucl.ac.be
PRENDERGAST David	Ireland	
QTEISH Abdallah	Jordan	aqteish@yu.edu.jo
RADNAI Zoltan	Hungary	
RAGHANI Pushpa Nihalchand	India	
RIGNANESE Gian-Marco	Belgium	rignanese@pcpm.ucl.ac.be
ROCCA Dario	Italy	
ROHLFING Michael	Germany	m.rohlfing@iu-bremen.de
ROMA Guido	Italy	
SATTA Alessandra	Italy	alessandra.satta@dsf.unica.it
SBRACCIA Carlo	Italy	sbraccia@sissa.it

SCEMAMA Anthony	France	scemama@lorentz.leiden.univ.nl
SEITSONEN Ari Paavo	Finland	ari.p.seitsonen@iki.fi
SHAWAGFEH Naseem Taleb A.	Jordon	nassha63@yahoo.com, eande@bau.edu.jo
SILVESTRELLI Pier Luigi	Italy	psil@pd.infn.it
SIMONA Fabio	Italy	
SKRBIC Tatjana	Serbia and Montenegro	skrbic@sissa.it
SKYLARIS Chris-Kriton - Skylaris Christos-Kriton	Greece	chris-kriton.skylaris@chemistry.oxford.ac.uk
SOROURI KHORASHAD Arash	Islamic Republic of Iran	a.sorouri@imperial.ac.uk
SPITALER Jurgen	Italy	
STROPPA Alessandro	Italy	astroppa@ts.infn.it
SUGIHARTONO Iwan Iwan	Indonesia	iwan@fisika.ui.ac.id
TAYLANOV Nizam (Nizom) A.	Uzbekistan	taylanov@yandex.ru
THYGESEN Kristian Sommer	Denmark	thygesen@fysik.dtu.dk
TOBIK Jaroslav	Slovak Republic	tobik@sissa.it
TOCCHIO Luca Fausto	Italy	tocchio@sissa.it
TOWLER Michael David	United Kingdom	
TRAIL John Robert	United Kingdom	jrt32@cam.ac.uk
TRIMARCHI Salvatore	Italy	trimarchi@ts.infn.it
UMARI Paolo	Italy	umari@mit.edu
VERSTRAETE Matthieu	Belgium	verstraete@pcpm.ucl.ac.be

VICARIO Gianpaolo	Italy	
VILLAGONZALO Cristine de Los Reyes	Philippines	cvillagonzalo@nip.upd.edu.ph
VON BOEHM Juhani	Finland	
WADE Abdou Ciss	Senegal	abouwade@yahoo.com
WALKER Brent Graham	New Zealand	
WALKINGSHAW Andrew David	United Kingdom	adw27@esc.cam.ac.uk
YALEW YIMER Yeneneh	Ethiopia	
ZIPOLI Federico	Italy	federico.zipoli@mater.unimib.it
ZYKOVA-TIMAN Tatyana - Tetyana Zykova	Ukraine	

4 News from UK's CCP9 Programme

UK's Collaborative Computational Project 9 on "Computational Studies of the Electronic Structure of Solids"

4.1 Report on the LSIC-Meeting

Novotel, Manchester, UK

12-13 May 2005

http://www.ccp9.ac.uk/data/L-SIC_Meeting/index.html

Organizers:

Walter M. Temmerman (Daresbury Laboratory) and James F. Annett (Bristol)

The meeting was held in the Novotel in Manchester and brought together researchers of the UK CCP9 KKR community with some researchers of the German and US KKR communities. The main topic of the meeting was the recently proposed multiple-scattering implementation of the self-interaction corrected local spin-density approximation (SIC-LSD), called the local SIC (LSIC). The emphasis of the meeting was to discuss technical issues of the implementation and the way of taking it forward.

The meeting was opened by an overview of SIC-LSD, given by Dzidka Szotek, followed by Martin Lüders, who gave an introduction into the LSIC, and explained how the L SIC, combined with the coherent potential approximation (CPA) may form the foundation for an ab-initio method for strongly correlated electron systems. Also a first application to the Ce phase diagram has been discussed. Arthur Ernst explained computational details of the actual implementation of LSIC in the KKR code, and Markus Däne presented applications to transition metal oxides. Julie Staunton and Ian Hughes reported on preliminary results of interfacing the LSIC code with the disordered local moment code to calculate spin susceptibilities for systems including localized states. They showed impressive first results on the magnetic structures and the Curie temperatures of Gd and γ-Ce. Derwyn Rowlands talked about the non-local coherent potential approximation, which facilitates the study of short-range order. Malcolm Stocks and Markus Eisenbach gave an overview of the LSMS code and discussed some issues of how to implement LSIC in the LSMS code. Balazs Gyorffy outlined his ideas towards incorporating dynamical fluctuations in terms of a two level system and discussed their implications. Nektarios Lathiotakis presented the reduced density-matrix functional theory which, when implemented for periodic systems, makes use of localized Wannier orbitals, and therefore has some technical parallels with the SIC approach. Nikitas Gidopoulous gave an introduction into ensemble DFT and pointed out its possible use in connection with the two level system. Last but not least H. Ebert reported on the progress in the implementation of the optimized effective potential method in the Munich SPR-KKR code. The meeting was comcluded by a round table session where strategies how to go beyond the current stage of LSIC were discussed.

The meeting was very successful and triggered many discussions of which some concerned purely technical problems and suggestions of their efficient solutions.

Pdf-files of all presentations can be downloaded at the meetings website.

M. Lüders

Programme:

Thursday 12th May: Afternoon Session

12:00 - 13:00	Buffet Lunch	Novotel, Manchester
13:00 - 13:45	Z. Szotek	*Overview of SIC*
13:45 - 14:30	M. Lüders	*Application of LSIC to Ce*
14:30 - 15:15	Coffee Break	
15:15 - 16:00	A. Ernst	*Numerical aspects of LSIC*
16:00 - 16:45	M. Däne	*Application of LSIC to TM oxides*
16:45 - 17:00	Coffee Break	
17:00 - 17:45	J. Staunton, I. Hughes	*Interfacing susceptibility code with LSIC*
19:30	Evening Meal	El Rincon de Rafa (Spanish Restaurant)

Friday 13th May: Morning Session

09:00 - 09:45	D. Rowlands	*NL-CPA calculations*
09:45 - 10:30	G.M. Stocks, M. Eisenbach	*Interfacing LSIC with LSMS*
10:30 - 11:00	Coffee Break	
11:00 - 11:45	B.L. Gyorffy	*Ideas on dynamical fluctuations*
11:45 - 14:00	Buffet Lunch	Novotel, Manchester

Friday 13th May: Afternoon Session

14:00 - 14:45	N. Lathiotakis	*Electronic correlation in periodic systems using the reduced densitymatrix functional theory*
14:45 - 15:30	N. Gidopoulos	*Different ideas on dynamical fluctuations*
15:30 - 16:00	Coffee Break	
16:00 - 16:45	H. Ebert	*The OPM applied to magnetic solids - aspects and present status*

17:00 - 19:00	Round Table Discussion	
19:30	Conference Dinner	Yang Sing (Chinese Restaurant)

List of participants:

James Annett	University of Bristol
Gary Batt	University of Bristol
Markus Däne	Martin-Luther-University Halle-Wittenberg
Andrew Duff	University of Bristol
Paul Durham	CCLRC Daresbury Laboratory
Hubert Ebert	Ludwig-Maximilians-Universität München
Marcus Eisenbach	Oak Ridge National Laboratory
Arthur Ernst	MPI-Halle
Nikitas Gidopoulas	CCLRC Rutherford Appleton Laboratory
Balazs Gyorffy	University of Bristol
Wolfram Hergert	Martin-Luther-University Halle-Wittenberg
Ian Hughes	University of Warwick
Emma Jones	EPSRC
Diemo Ködderitzsch	Ludwig-Maximilians-Universität München
Nektarios Lathiotakis	Freie Universität Berlin
Martin Lüders	CCLRC Daresbury Laboratory
Frank Pinski	University of Warwick
Julian Poulter	Mahidol University, Bangkok
Derwyn Rowlands	University of Bristol
Leonid Sandratskii	MPI-Halle
Thomas Schulthess	Oak Ridge National Laboratory
Julie Staunton	University of Warwick
Malcom Stocks	Oak Ridge National Laboratory
Dzidka Szotek	CCLRC Daresbury Laboratory
Walter Temmerman	CCLRC Daresbury Laboratory
Paul Tulip	University of Warwick
Hand Zenia	CCLRC Daresbury Laboratory

5 NANOQUANTA Network of Excellence

Nanoscale Quantum Simulations for Nanostructures and Advanced Materials

5.1 356th Wilhelm and Else Heraeus Seminar

40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges

12–15 September 2005, Bad Honnef, Germany

http://www.fz-juelich.de/iff/GW2005

Since its original conception in 1965, the GW approximation has become an indispensable tool for ab initio electronic-structure calculations and is now recognised as the most accurate method to study excited states in solids. The last few years, in particular, have seen a marked rise in new applications and theoretical developments. The 356th Wilhelm and Else Heraeus Seminar will focus on the current progress and on the perspectives for the investigation of electronic excitations from first principles.

The seminar topics will include:

- Theoretical Foundations
- Self-Consistency
- Vertex Corrections
- Implementation Strategies
- Large-Scale Applications
- Surfaces and Nanostructures
- Towards Strong Correlation
- Bethe-Salpeter Equation
- Time-Dependent Density-Functional Theory

Speakers from leading international groups will give an in-depth overview of current research activities and place recent results into context. The meeting aims at providing an informal atmosphere for stimulating discussions between researchers working in this exciting field. Young researchers (Ph.D. students and postdocs) are particularly encouraged to present their work.

We are looking forward to lively discussions and exchange of ideas in the inspiring atmosphere of the Physikzentrum Bad Honnef, located near Bonn and Cologne on the beautiful Rhine river.

The deadline for registration and abstract submission is **15 July 2005**.

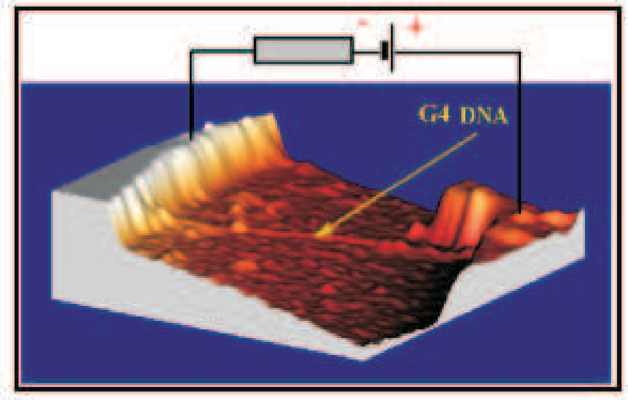
The seminar is financially supported by the Wilhelm und Else Heraeus-Stiftung and the EU's Sixth Framework Programme through the NANOQUANTA Network of Excellence.

Organisers:
Arno Schindlmayr, Pablo García-González, Maurizia Palummo, Olivia Pulci and Nathalie Vast

6 General Workshop/Conference Announcements

6.1 Workshop on DNA-based Nanowires

EC IST-2001-38951 Workshop



DNA-based Nanowires:

On the Way from Biomolecules to Nanodevices

INFM-S3, Modena, Italy

October 7-8, 2005

http://www-dnananowires.uni-r.de/

Introduction

The IST-FET-38951 EC project "DNA-based Molecular Nanowires" (2003-2005) aims at the development of novel DNA-derivatives for the implementation of self-organized molecular nanoelectronics. Native-DNA expresses two essential features demanded from molecular nanowires, i.e. *recognition* and *structuring*; however, its *conductivity* (the third essential feature) is controversial and largely disappointing. To combine the three desired properties, we designed, synthesized, and investigated by multidisciplinary experimental and theoretical tools, specific manipulations of the double-stranded nucleic acids. The main candidates tested in our research were and continue to be: G4-DNA (a quadruple helix made of only guanines), M-DNA (a double helix hybridized with metal ions in the core) and conducting polymer-DNA hybrids. Towards the conclusion of the project, we wish to summarize our concepts and results, and gather a pool of scientists active in related fields worldwide to converse ideas about molecular electronics and the possible role of DNA-based nanowires and nanodevices in this context.

IST-FET-38951 Consortium:

- Alexander Kotlyar (Tel Aviv University, Israel) – biochemistry, synthesis
- Joshua Jortner (Tel Aviv University, Israel) – theory of electron transfer in chemistry and biology
- Amiram Porath (Tel Aviv University, Israel) – project management
- Danny Porath (Hebrew University Jerusalem, Israel) – AFM and STM imaging, spectroscopy, electrical transport measurements
- Shlomo Yitzchaik (Hebrew University Jerusalem, Israel) – surface chemistry, intercalation, polymerization
- Julio Gomez-Herrero (UAM Madrid, Spain) – SPM imaging and spectroscopy and electrostatic polarization experiments
- Eli Kapon & Benjamin Dwir (EPFL Lausanne, Switzerland) – nanofabrication, electrooptical measurements
- Rosa Di Felice & Elisa Molinari (INFM-S3 Modena, Italy) – ab-initio electronic structure calculations
- Angel Rubio Secades (UPV/EHU San Sebastian, Spain) – ab-initio optical properties calculations
- Gianaurelio Cuniberti (University of Regensburg, Germany) – modeling of transport phenomena in nanometer molecular devices

Scope and Topics

The purpose of the workshop is to present and discuss results of ongoing interdisciplinary investigations towards the realization of bio-molecular electronics, with special emphasis on the possible use of DNA to fabricate electrically active molecular wires. We solicit participation of scientists with expertise ranging from biochemistry to device physics, spanning through different branches of chemistry. Topics include, but are not limited to, the following:

- Biomolecular engineering, DNA synthesis, G4-DNA, M-DNA
- Conducting polymers hybridized with DNA, DNA intercalators
- Experimental investigation of conductivity in single native-DNA and DNA-derivative molecules, as well as in DNA layers
- Experimental techniques to measure molecular morphology and conductivity: AFM, EFM, STM, STS, electrical transport

- Attachment of molecules to inorganic substrates and nanoparticles
- Experimental approaches to study charge transfer in DNA in solution
- Theoretical approaches to study quantum transport in molecular wires and junctions
- Understanding the mechanisms for charge transfer in biomolecules and at molecule/surface interfaces
- Concepts for implementing self-organized molecular circuits

Program

The program covers two full days of presentations and discussions, October 7-8, 2005, starting at 9am on October 7th and ending at 7pm on October 8th. There will be several invited speakers, presentations by the project partners‡[1] and a poster session. In addition, few contributed talks will be selected from the abstracts submitted for the poster session.

Program Committee: Rosa Di Felice, Danny Porath, Elisa Molinari, Joshua Jortner.

Tentative list of keynote speakers†[2] (45-min talks): David Bensimon* (ENS Paris), Maria Michel-Beyerle* (Technical Univ. Munich, Germany), Thomas Carell (LMU Univ. Munich, Germany), Jean-Louis Mergny (CNRS Paris, France), Uri Sivan* (Technion Haifa, Israel), Nongjang Tao (Arizona State Univ. Tempe, USA).

Tentative list of invited speakers[] (30-min talks): Emilio Artacho (Cambridge Univ., UK), Lorenzo Berti (INFM-S3 Modena, Italy), Wolfgang Fritzsche (IPHT Jena, Germany), Francesco Luigi Gervasio (ETH Lugano, Switzerland), Avraham Nitzan (TAU Tel Aviv, Israel), Dragan Mihailovic (Stefan Institute Ljubljana, Slovenia), Ross Rinaldi (INFM-NNL Lecce, Italy), Bruno Samorì (Univ. of Bologna, Italy), Felix Zamora (UAM Madrid, Spain).

Venue

The workshop will take place at the INFM-S3 National Center on *nanoStructures and bioSystems at Surfaces*, located in the premises of the University of Modena and Reggio Emilia, in Modena, Italy.

How to reach us: http://www.s3.infm.it/address_index.html

Local Organizers: Luisa Neri, Elisa Molinari, Arrigo Calzolari, Manuela Cavallari, Anna Garbesi, Rosa Di Felice. With the help by the project management in Tel Aviv: Keren Tabach, Maya Shahaf, Amiram Porath.

Registration

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[1] ‡ All the research groups participating in the project will be represented in the workshop, with either a poster or an oral presentation.

[2] † Speakers marked with an asterisk are not yet confirmed.

A registration fee of 50 EUR per participant will be collected at the venue to cover lunch buffets, coffee breaks, and the workshop proceedings. Prior web registration is required to figure out the number of participants and arrange at best the rooms, poster session, and entertainment. Please register here (http://www.s3.infm.it/WS_DNA/Registration_index.html).

Abstract Submission

Please send by e-mail a short abstract of your work (maximum 1 page) to the workshop secretariat segreterias3@unimore.it, using the template that can be downloaded from the webpage. All the abstracts can be presented in the poster session (October 7, 2005): some of them will be selected for short oral presentations. The abstracts will be collected and edited as the proceedings of the workshop, together with a selection of papers by the speakers.

6.2 International Conference on Research Advances in Rational Design of Catalysts and Sorbents

14-16 December 2005, IFP-Lyon (France)

First announcement and call for papers

IFP is pleased to announce the "Research Advances in Rational Design of Catalysts and Sorbents" international conference to be held in IFP-Lyon (France) from 14 to 16 December 2005, under the auspices of the French Academy of Sciences.

The objectives of this conference is to highlight and discuss the recent achievements of combined experimental and molecular modeling approaches in research on catalysts and sorbents. The presentations should contribute to the growing awareness of the scientific community of the key issue of rational design of these materials.

We encourage you to download the first circular from the IFP web site (see below), and submit abstracts before **18 June 2005** for either oral or poster presentations in line with one of the 4 sessions proposed:

- Active sites, mechanisms and kinetics
  keynote speakers: **Pr. J-M. Basset** (Member of the French Academy of sciences, LCOMS, CPE Lyon, France), **Dr. K. Reuter** (FHI Berlin, Germany)
- Chemical trends and the discovery of new catalysts
  keynote speakers: **Pr. J. K. Nørskov** (CAMP - Technical University of Denmark), **Dr. R. R. Chianelli** (University of Texas at El Paso, USA)
- Support effects in catalysis
  keynote speakers: **Pr. K. P. de Jong** (Utrecht University, The Netherlands), **Dr. C. Wolverton** (Ford Research and Advanced Engineering, USA)
- Adsorption and confinement
  keynote speakers: **Pr. A. Corma** (ITQ, UPV-CSIC, Valencia, Spain), **Pr. B. Smit** (University of Amsterdam, The Netherlands, and CECAM, France)

Information, preliminary program and abstract template are available on IFP web site: http://events.ifp.fr and click on "Seminars and Conferences"
or direct access at
`http://www.ifp.fr/IFP/en/IFP00EVE.nsf/VFODocumentCON/2A3861D502F9566580256FE300532C4D?OpenDocument`

We are looking forward to your visit in Lyon.

Best Regards,

On behalf of the organizing committee,

Pascal Raybaud (readicats@ifp.fr),
and IFP Communications Division (frederique.leandri@ifp.fr)

6.3 Meeting on Spin-Dependent Transport through Nanostructures - SPINTRONICS'05

25 - 30 September, 2005 - Poznan, Poland

website: http://www.ifmpan.poznan.pl/spintronics05

Organized by the European "Spintronics" Research Training Network

TOPICS include

- Giant and Tunneling Magnetoresistance,
- Quantum Computing, Quantum Coherence and Decoherence,
- Strongly Correlated Systems, Quantum Criticality,
- Current-Induced Magnetization Reversal, Spin-Orbit Effects,
- Hybrid Ferromagnetic-Superconducting Structures,
- Diluted Magnetic Semiconductors, Molecular Spintronics.

INVITED SPEAKERS (preliminary list)

G. Abstreiter* (München)
B. Altshuler (Princeton)
G. Bauer (Delft)
H. Bouchiat* (Orsay)
P. Bruno (Halle)
T. Dietl (Warszawa)
K. Ensslin (Zürich)
V. Falko (Lancaster)
R. Fazio (Pisa)
A. Fert (Orsay)
J. Folk (British Columbia)
Y. Gefen (Weizmann)
D. Goldhaber-Gordon (Stanford)
G. Güntherodt* (Aachen)
A. MacDonald (Austin)
S. Maekawa (Sendai)
C. Marcus (Harvard)
L. Molenkamp* (Würzburg)
Y. Nazarov* (Delft)
Y. Oreg (Weizmann)
S. Parkin (San Jose)
D. Ralph (Cornell)
H. Schoeller (Aachen)
G. Schön (Karlsruhe)
C. Schönenberger (Basel)
S. Tarucha (Tokyo)
B. van Wees (Groningen)
R. Wiesendanger (Hamburg)

L. Kouwenhoven* (Delft)
J. König (Bochum)
D. Loss (Basel)
A. Yacoby* (Weizmann)
G. Zaránd (Budapest)

(*) To be confirmed

SCOPE

This event intends to bring together multidisciplinary groups of experts from the fields of mesoscopic physics, nanotechnology and magnetism, that have a common interest in spintronics. The main experimental and technological challenges to be addressed involve creating, maintaining, measuring and manipulating spin currents in mesoscopic electronic systems, as well as spin entanglement in semiconductor quantum dots in the context of quantum computation. Such active control of spin dynamics is envisioned to make possible the development of new devices and novel technologies, such as spin transistors, spin-valves, ferromagnetic single-electron transistors, spin filters and modulators, current-induced magnetization reversal devices, new memory elements, and possibly new devices for quantum information processing and quantum computation. The aim of the Meeting is to give a state of the art overview of the important aspects regarding these problems.

LOCATION

The conference site is at a neogothic palace near Pozna in Poland, built in the 19th century and beautifully renovated in recent years (for which they won a prize for the "best modernization project in 2002"). There is a conference room (with modern facilities like built-in beamer, etc.) that can host around 100 people. In addition, many nice amenities are available, like fitness room, sauna, restaurant-bar, billiard room, etc. All participants would be accommodated in the palace complex together, which is ideal for stimulating lots of discussions. The palace is located in a very big park, with opportunities for hiking, cycling, canoeing, horse-riding, etc.

APPLICATIONS

Besides the invited talks, contributed talks and poster can be presented. Deadline for registration is June 15, 2005. The meeting is limited to about 90 participants, so organizers recommend early registration. For members of the Spintronics RTN network all local expenses will be covered. For non-members, limited funds for financial assistance are available.

For more information and application details please visit the website

http://www.ifmpan.poznan.pl/spintronics05

Yours sincerely,

The Organizing Committee

Jozef Barnas (Adam Mickiewicz University, Poznan, Poland)
Jan von Delft (Ludwig-Maximilians-Universität, München, Germany)
Jan Martinek (Institute of Molecular Physics, PAS, Poznan, Poland)

6.4 International Conference on Computational Methods in Science and Engineering (ICCMSE)

Loutraki, Korinthos, Greece

21 to 26 of October 2005

The International Conference on Computational Methods in Science and Engineering (ICCMSE) will be held in Loutraki, Korinthos, Greece, from 21 to 26 of October 2005. This year the ICCMSE has a strong computational chemistry and physics component as you can see from the partial list of symposia below. If you wish to participate or have any question, feel free to contact one of the symposium organizers. The list of symposia follows below.

You can register on-line at

`http://www.uop.gr/~iccmse/` .

The ICCMSE conference will be held at the Poseidon hotel

http://www.greekconference.com/club-hotel/poseidon/index.html

which is in a wonderful location, on the outskirts of Loutraki and opposite the historic city of Corinth. There is plenty to do and see in and around Loutraki, see

http://www.city-of-loutraki.gr/

Sincerely yours,

Theodore Simos, Department of Computer Science and Technology, University of Peloponnese,

George Maroulis, Department of Chemistry, University of Patras

List of Symposia

Electric (hyper)polarizability: From atoms and molecules to the nonlinear optics of materials. A celebration of David Bishop's contribution
Organizer: G. Maroulis (maroulis@upatras.gr)

Electron densities and density functionals
Organizer: Ajit Thakkar (ajit@unb.ca)

Computational Methods for Atomic and Molecular Clusters

Organizer: R. Fournier (renef@yorku.ca)

Open-shell organic molecules. Electric and magnetic properties

Organizers: B.Champagne (benoit.champagne@fundp.ac.be) and M. Nakano (mnaka@cheng.es.osaka-u.ac.jp)

Trends and perspectives in Computational Chemistry

Organizer: G. Maroulis (maroulis@upatras.gr)

Computational molecular science: hybrid classical-quantum and force field methods

Organizer: P.O. Åstrand (per-olof.aastrand@chem.ntnu.no)

Applications of Computational and Mathematical Chemistry: From structure to biology

Organizer: K. Balasubramanian (kbala@ucdavis.edu)

QSPR and QSAR modeling

Organizer: Sonja Nikolic (sonja@irb.hr)

Electronic Structure Calculations on Embryonic Metallic and Intermetallic Clusters

Organizer: C.A. Tsipis (tsipis@chem.auth.gr)

Theoretical and experimental methods applied to development of new medicines. The arise of new era of drug delivery systems based upon cyclodextrins molecular structure

Organizers: Antonio Lino and Carlos Jaime (antonio.lino@uab.es)

Aspects of Computational Chemistry in Rational Drug Design and Development

Organizer: T. Mavromoustakos (tmavro@eie.gr)

Explicit density functional of the kinetic energy in computer simulations at atomistic level

Organizer: T. Wesolowski (Tomasz.Wesolowski@chiphy.unige.ch)

Quantum Mechanical Calculations for Molecules

Organizers: Vitaly Glushkov (`v_n_glushkov@yahoo.com`) and Andreas K. Theophilou (theo@ims.demokritos.

New algebraic tools in computational chemistry: conceptual and practical advances

Organizers: P. Cassam-Chenai (cassam@unice.fr) and F. Patras (patras@math.unice.fr)

Optimizing structures of larger, finite systems
Organizer: Michael Springborg (mcs@springborg.pc.uni-sb.de)

The full list of symposia can be seen at

`http://www.uop.gr/~iccmse/Sessions_Minisymposia.htm`

7 General Job Announcements

IMPERIAL COLLEGE LONDON

Condensed Matter Theory Group
Department of Physics

Research Associate in Theory and Simulations of Non-Adiabatic Processes in Irradiation Damage of Metals

A postdoctoral research position has become available on modelling non-adiabatic processes in materials with correlated electron-ion dynamics (CEID), funded for up to 4 years by the Materials Modelling Initiative of EPSRC. You will be joining a distinguished consortium of researchers at Imperial College London, UCL and Queen's University Belfast led by Professor Adrian Sutton, FRS at Imperial College London. Your work at Imperial College London will focus on irradiation damage in metals where excited electrons play a decisive role in the creation and subsequent healing of damage caused by high energy impacts. You will also be expected to play a significant role in the supervision of a 4-year postgraduate student working on the project with you.

CEID was developed recently by members of the consortium. It is a new paradigm for dynamical atomistic simulations of materials where energy may be exchanged irreversibly between ions and electrons. Like Ehrenfest dynamics these simulations do not make the Born-Oppenheimer approximation, but unlike Ehrenfest dynamics they treat the quantum fluctuations in the positions and momenta of the ions. The latter are essential for certain non-adiabatic processes.

The salary will be in the range of £22,116 – £32,232 per annum, depending on qualifications and experience. You should have a PhD in condensed matter physics or materials science, a strong background in the theory of the electronic structure of solids, and excellent computational skills. The post is available from 1 October 2005 or as soon as possible thereafter.

A job description and an application form can be obtained from the following website:

http://www.imperial.ac.uk/employment/research/index.htm.

Alternatively, please contact Ms Theresa Debono, t.debono@imperial.ac.uk. Completed application forms should be sent, with a full curriculum vitae and list of publications to Ms Theresa Debono, Department of Physics, Blackett Laboratory, Prince Consort Road, Imperial College London SW7 2AZ, UK.

Closing date: 31 July 2005

Interview date: 31 August 2005

Valuing diversity and committed to equality of opportunity

Ph.D Position
Trinity College, Dublin, IRELAND

Two PhD studentships are available in the "Computational Spintronics Group" in the Physics Department at Trinity College Dublin (IRELAND). The project is sponsored by Science Foundation of Ireland and is part of a collaboration between TCD and the group of Prof. K. Burke at Rutgers University (USA).

Both PhD projects will involve the development and the numerical implementation of quantum transport techniques combined with density functional or other electronic structure methods. Most of the implementations will be based on the existing Dublin quantum transport code Smeagol (http://www.smeagol.tcd.ie). Strong collaborations with other groups both in Europe and the USA are envisaged. Both the students will be based in Dublin, although long visiting periods at Rutgers are planned.

The first of the two projects is focused on the investigation of the effects of non-local exchange and correlation functionals on molecular transport. This will define the range of applicability of existing methods, and it will form the basis for a fully quantitative transport theory.

The main aim of the second project is the development of a fully quantitative transport theory incorporating inelastic effects. These are essential for the description of realistic molecular devices under bias. Problems connected with quantum dissipations and current induced forces will be addressed.

The studentships will commence ideally on the 1st August 2005. We are seeking for strongly motivated students with an excellent general background in Physics and good computational skills. A previous experience in electronic structure method or transport theory will be considered as a plus.

Candidates are invited to send a CV together with the full addresses of two potential referees (including e-mail) by post or e-mail to:

Dr. Stefano Sanvito
Department of Physics
Trinity College
Dublin 2, Ireland
Tel: +353-1-6083065
Fax: +353-1-6711759

E-mail: sanvitos@tcd.ie

Information about our research activity may be found at:
http://www.tcd.ie/Physics/People/Stefano.Sanvito/ and
http://www.smeagol.tcd.ie/

POSTDOCTORAL RESEARCH FELLOWSHIP

DEMOCRITOS National Simulation Center
SISSA International School for Advanced Studies, and
ELETTRA Synchrotron Light Laboratory
Trieste, Italy

A postdoctoral position is available immediately at the DEMOCRITOS National Simulation Center (http://www.democritos.it), in the area of catalysis on oxide-supported metallic nanoparticles. The successful candidate will join a newly established theoretical research group based at the ELETTRA synchrotron radiation center (http://www.elettra.trieste.it) with strong links with the SISSA condensed-matter theory group (http://www.sissa.it/cm/), under the supervision of Stefano Fabris and Stefano Baroni. He/She is expected to develop strong links with the local experimental groups and to be able to work in a highly multidisciplinary environment.

Research will involve the development and application of "ab initio" methods for the study of processes and reactions catalyzed by transition metals dispersed on oxide surfaces.

Candidates must hold a PhD in Physics, Chemistry, Materials Science, or related discipline, and have good knowledge of electronic structure theory. Prior experience in first-principles calculations would be an advantage. Initial appointment is for two years, renewable for a third year. Consideration of candidates will begin immediately and continue until the position is filled. Interested applicants should submit a CV, including list of publications and name (with e-mail address) of two referees to:

Prof. Stefano Baroni (baroni@sissa.it) and
Dr. Stefano Fabris (fabris@democritos.it)
INFM-DEMOCRITOS National Simulation Center and
SISSA International School for Advanced Studies
via Beirut 2-4, I-34014 Trieste, Italy

PhD-position

Institute of Theoretical Physics

Frankfurt/Main, Germany

Salary: BATIIa/2 (half a Post-Doc salary)
Starting-time: immediately
Duration: max. 3 years
Subject: complex adaptive systems - neural networks

Requisites: Diploma or master in physics, CV, 1-3 letters of references, skills in theoretical physics, computer simulation, C++

Contact:

Prof.Dr.C. Gros,
`http://www.itp.uni-frankfurt.de/~gros`

Further information:
`http://www.itp.uni-frankfurt.de/~gros/PhD.html`

Post-doctoral position
University of Iceland

A post-doctoral position is available in my research group at the University of Iceland. It is part of a European network of eight theoretical groups studying ammonia synthesis (see `http://rulgla.leidenuniv.nl/network/network_main.htm`). Only a citizen of a European Union country or one of the associated members can be hired. The post-doc would, in particular, continue development of methods for estimating rates of quantum mechanical tunneling in thermal systems using both empirical potential functions to describe interatomic interactions as well as direct use of energy and atomic forces calculated by density functional theory. In addition to the various elementary steps in the industrial process for ammonia formation, the possibility of making ammonia by electrochemical means at ambient temperature and pressure would also be addressed as well as general methodology for the study of electrochemical processes.

For more information and applications, send e-mail to me at hj@hi.is (see also the group web page at http://www.hi.is/ hj).

Hannes Jonsson
Professor of Chemistry
University of Iceland
107 Reykjavik, Iceland

Post-doctoral and PhD positions in ”Electronic excitations at surfaces”

International University Bremen, Germany

Positions for a post-doctoral fellow or for PhD candidates are available at the International University Bremen, in the ”Theory of Condensed Matter” group headed by Prof. Dr. Michael Rohlfing.

The prospective candidates will mainly work on electronic properties of clean and adsorbate-covered surfaces, focusing on excited electronic states, their spectra, and related short-time dynamics (desorption processes and femtosecond charge-carrier dynamics). Possible topics include spectra of PTCDA on metal substrates, laser-induced desorption from insulator surfaces, and excitation-induced dynamics of silicon surfaces. Density functional theory and ab-initio many-body perturbation theory (GW method and Bethe-Salpeter equation techniques) will be employed. A solid background in computational solid-state physics or computational chemistry and solid programming skills in FORTRAN or C will be considered favourable.

International University Bremen (in Bremen, Germany) is a newly founded private university aiming at high-level research and teaching in an international environment. With English as our working language and more than 70 nations on campus, IUB provides excellent research and working conditions and a unique intercultural atmosphere.

The positions are for two years (three to four years for the PhD positions). The salary corresponds to the BAT IIa level (1/2 BAT IIa for the PhD candidates) common at German public universities.

For further information, visit our website at http://www.iu-bremen.de/physics The positions are immediately available and applications will be considered until the positions are filled. Further inquiries and applications (including a CV, names and addresses of three references, summary of research interests, and list of publications) should be directed to Prof. Dr. Michael Rohlfing (m.rohlfing@iu-bremen.de).

Postdoctoral Position

Modeling Laboratory for Nanostructure and Catalysis, Department of Chemistry

University of Salerno, Salerno, Italy

A postdoctoral position is available in the Modeling Lab for Nanostructure and Catalysis, a brand new research group at University of Salerno.

Projects involve the development and application of new molecular simulation methods to problems in chemistry, biochemistry and material science.

Experience in modifying and writing Monte Carlo and/or Molecular Dynamics and/or Quantum Chemistry codes (not simply using packages) and expertise in the maintenance of computer clusters is required.

The research group has good computational facilities, and friendly atmosphere. Computational facilities at Molnac include local workstations, two beowulf clusters, 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 Prof. Luigi Cavallo (lcavallo@unisa.it) or Dr. Giuseppe Milano (gmilano@unisa.it).

Ph.D. Studentship in Computational Nanotechnology

Department of Physics and Astronomy, University College London,

Gower Street, London WC1E 6BT, United Kingdom

The Department of Physics and Astronomy at University College London has an opening for a four year PhD studentship starting October 2005. It is open to citizens of the EU. The project will be to study excited states in polymers using our recently developed state-of-the-art computer modelling technique: Correlated Electron-Ion Dynamics (see the April 2005 edition of the Ψ_K newsletter for a description of CEID).

Interested candidates should send a CV to Andrew Horsfield at a.horsfield@ucl.ac.uk.

Post-Doctoral Position in Atomic Scale Simulation
EPFL/IRRMA (Lausanne), Switzerland

There is currently a post-doctoral position available for a talented and motivated individual in Atomic-Scale Simulation (http://itp.epfl.ch/page13360.html) at EPFL (http://www.epfl.ch/index.html)/IRRMA (http://irrmawww.epfl.ch/index.html) in Lausanne. The position is available immediately but could also start at a later convened date. The position is for one year and could be extended for a second one depending on mutual agreement and available funding. The selected individual will join a research project in computational condensed matter physics. The research activity will concern materials and interfaces of interest in the nanoelectronic industry. (see here `http://irrmawww.epfl.ch/%7Epasquarello/G3.html`). Previous experience with density-functional calculations based on plane waves and pseudopotentials is requested. The EPFL in Lausanne benefits from outstanding computational facilities.

The interested candidates should send (in PDF-format) their (1) curriculum vitae (including nationality, date of birth, civil state, and achieved degrees), (2) publication list, and (3) one or two reprints representative of previous research. The interested candidate should also express his/her motivation in a cover letter, including the prospected date of availability, and arrange confidential letters of recommendation to be sent to the address below. Only complete applications will be processed.

Professor Alfredo Pasquarello
(http://personnes.epfl.ch/cgi-bin/people/)
Chair of Atomic Scale Simulation
CSEA-ITP-SB-EPFL and IRRMA
Station 13 / PPH340
CH-1015 Lausanne
Switzerland
Tel. : +41 21 693 44 16
Fax : +41 21 693 66 55
E-mail : Alfredo.Pasquarello@epfl.ch

PhD STUDENTSHIPS IN CONDENSED MATTER & MATERIALS THEORY/MODELING

UNIVERSITY OF SOUTH FLORIDA

Applications are invited for several PhD research studentships in computational condensed matter & materials physics in the group of Prof. I. Oleynik in the Physics Department at the University of South Florida. Successful candidates will work on one of several exciting research projects in the following areas: first-principles theory of tunneling in condensed matter and molecular systems, atomistic modeling of matter at extreme conditions and nanostructured materials.

We are seeking bright, creative and highly motivated individuals with solid theoretical background in physics, chemistry, materials science or closely related fields with genuine interest to conduct interdisciplinary research in a close collaboration with experimentalists. You will obtain a practical experience in electronic structure theory including density functional theory, tight-binding, molecular dynamics, empirical potentials, and novel theoretical methods such as Green's function theory of tunneling and analytic bond order potentials. Our activities rely heavily on using computers. Therefore, you will acquire strong programming skills and knowledge of advanced large scale parallel computations. This unique combination of skills will open up exceptional employment opportunities at academia, industry and national laboratories in the areas of computational condensed matter & materials physics, and nanotechnology.

You will be working in intellectually stimulating and supportive environment that will help you to succeed in your learning and research endeavors. Additional possibilities to gain teaching experience exist for individuals interested in pursuing career in academia. The University of South Florida is located in Tampa, Florida, which is consistently rated as one of the best major metropolitan areas for quality of life, vibrant arts, and cultural, recreational and outdoor opportunities. You will also be offered a generous stipend.

Applicants should have a good bachelor's or master's degree in physics, chemistry or related subjects. They should send curriculum vitae, a statement of career goals and general research interests, and names, phone numbers and e-mail addresses of two references to Prof. Ivan Oleynik (oleynik@shell.cas.usf.edu). You are also welcome to email informal inquiries. Additional information about research activities can be found at `http://shell.cas.usf.edu/~oleynik/`.

Ivan I. Oleynik
Department of Physics
University of South Florida
4202 East Fowler Avenue
Tampa, Florida 33620-5700
E-mail : oleynik@shell.cas.usf.edu
Tel : (813) 974-8186
Fax : (813) 974-5813
WWW : `http://shell.cas.usf.edu/~oleynik/`

Post-doctoral and assistant professor positions in theoretical solid state physics

University of Erlangen-Nürnberg, Germany

Positions for a post-doctoral fellow (three-year term) and at an assistant professor level (initially one-year term) are available at the University of Erlangen-Nürnberg, the Solid state theory chair.

The candidates will work on density-functional-theory studies of electron correlation effects on surfaces, in particular, a metallized SiC or graphite surfaces. Another research direction is a study of electron excitations in a framework of time-dependent density functional theory. An adequate knowledge of DFT and many-body perturbation theory, as well as a background in a computational solid-state physics is required.

The assistant professor position assumes a regular teaching load at a graduate level.

The salary is at BAT IIa level common at German public universities.

For further information, visit our website at

http://www.tfkp.physik.uni-erlangen.de/ .

The positions are immediately available and applications will be considered until the positions are filled. Further inquiries and applications (including a CV, names and addresses of three references, summary of research interests, and list of publications) should be directed to Prof. Dr. Oleg Pankratov (Oleg.Pankratov@physik.uni-erlangen.de).

Two open staff scientist positions

Condensed Matter Sciences Division

Oak Ridge National Laboratory, USA

The Condensed Matter Sciences Division is expanding the Theory group through a series of recent and future hires. Applications are invited for two open staff scientist positions in connection with this expansion. Current interests include correlated electron materials, density functional methods, nanoscience, complex systems, surface science, optical and excited state properties, magnetism and superconductivity. Further details about the group may be found on the web page http://www.ornl.gov/sci/cmsd/theory.

We are seeking theorists who will complement current research, establish exciting new research areas, and interact strongly with ORNL research activities, such as those associated with the new Center for Nanophase Materials, the neutron scattering facilities (SNS and HFIR), and the leadership computational facilities.

A Ph.D. in Condensed Matter Theory or closely related field is required. We invite applications from candidates at all levels. These are open positions emphasizing fundamental research. U.S. citizenship is not required. Qualified candidates should use the on-line application process to send a complete CV with publication list, a brief statement of research interests or research plan, and the names of three references by attaching a Word or PDF file. Any questions related to the position should be sent to: Dr. David J. Singh, Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6032, U.S.A. or by e-mail to singhdj@ornl.gov. Applications should be via the ORNL web site: http://www.ornl.gov and position number 50231009.

Fellowship at Isfahan University of Technology (IUT), Iran

The computational condensed matter group in physics department of Isfahan University of Technology (IUT) has expanded its regional scientific character by acting as an ICTP Affiliated Centre during the last two years. Following such a mission, the ICTP and IUT have agreed to support the below mentioned fellowships for the year 2005:

a). Six fellowship to young researchers (possess a PhD degree or at the final stage of getting it) from the Regional countries (Western South Asia, Central Asia, Middle East) to come and work in the Centre as medium term visitors (10-12 weeks).

b). Two fellowship to young researchers from former Soviet Union countries which are supported by the OEA: see list at the web site http://oea.ictp.it/supportes/ to come and work in the Centre as medium term visitors (10-12 weeks).

c). Three fellowship to young researchers from less developed universities in Iran to come and work in the Centre as short term visitors (4-8 weeks).

The applicants are expected to have keen interest in computational condensed matter physics, with hands on experience on first principle methods. Applications including, a full CV, a list of publications, an abstract of research achievements within one A4 page), a proposal of about 500 words explaining the details of the research project that the applicant is going to perform during the stay in the Centre, and names and addresses (email) of two referees should be send to the following address:

Professor Hadi Akbarzadeh
Department of Physics,
Isfahan University of Technology,
Isfahan, Iran
Email: akbarzad@cc.iut.ac.ir,
Tel +98-311-3912375 (or 3913700),
Fax: +98-311-3912376.

Accepted candidates within items (a) and (b) are entitled for the following supports:

1. Travel expenses by economy round air ticket.
2. Accommodation in IUT Guest House.
3. 300 Euro per month for living expenses.

Regarding the accepted candidates within item (c) the Affiliated Centre will only cover the accommodation expenses in IUT Guest House.

Current research interests of the Centre

Electronic structure calculations are the main current activity in the computational condensed matter group in physics department of Isfahan University of Technology.

Our calculations are within density functional theory using FP-LAPW as well as PP-PW methods. We have access and hands on experience to work with WIEN2k and PWSCF codes.

The ongoing research projects in the group are as follow:

1. Co_2MnSi and other Huesler alloys as novel materials for spintronic applications.

2. Ab-initio study of spin density waves in Chromium.

3. First principle study of structural, electronic, and magnetic properties of $Cr_{15}X$ alloys (X=Fe, Rh, Cd, Sn).

Post-doctoral scientist

University of Notre Dame Radiation Laboratory

Department of Chemical and Biomolecular Engineering

The University of Notre Dame Radiation Laboratory (http://www.rad.nd.edu/) and Department of Chemical and Biomolecular Engineering (`http://www.nd.edu/~chegdept/`) have an opening for a post-doctoral scientist to contribute to a research program in radiation chemistry at water/metal oxide interfaces. The candidate will have primary responsibility for applying first-principles DFT tools to simulate radiation chemical (and photochemical) reactions of water on the surfaces of bulk and nanoparticle metal oxides, and will interact closely with complimentary experimental efforts to synthesize and characterize well-defined, nanoscale metal oxide particles and photocatalysts. The Radiation Laboratory is a Department of Energy-supported facility on the campus of the University of Notre Dame that offers access to state-of-the-art computational facilities and outstanding capabilities in photo- and radiation chemistry. The post-doctoral appointment will be for one year with the possibility of extensions for subsequent years. Interested candidates should submit a CV and three references to Prof. Bill Schneider, Department of Chemical and Biomolecular Engineering (mailto to: wschneider@nd.edu, tel. (574) 631-8754), or Prof. Ian Carmichael, Radiation Laboratory (mailto to: carmichael.1@nd.edu, tel. (574)631-4502).

Postdoctoral Research Associate

Department of Materials Science and Metallurgy

University of Cambridge

Advanced Atomistic Modelling of Multi-Layer Optical Coatings

Applications are invited for a Postdoctoral Research Associate to perform advanced quantum mechanical modelling of the mechanical and optical properties of multi-layer coatings. Using density functional methods the successful applicant will study from first principles the adhesion of the interfaces between the layers and the effect of the interfacial structures on the dielectric properties of the coating. Typical optical coatings are nanostructures consisting of several different oxide or metal layers deposited on a glass or polymer substrate. They are used as anti-reflective films on spectacle lenses, UV and infra-red blockers, lighting filters, conductive oxides for flat screen displays and solar control coatings on windows. In order to optimise the performance of these coatings it is essential to understand the reasons for interfacial failure and the influence of defects and lattice strain on the optical constants of the materials.

The project forms part of an EPSRC Materials Modelling Consortium on Functional Coatings with collaborating researchers from 6 universities and 2 industrial partners.

Suitable candidates should have a PhD in condensed matter physics or materials science and have experience with density functional calculations and large scale computing. He/she should be able to help supervise research students, interact closely with other members of the consortium including experimentalists and help maintain the local computing facilities. Most of the large scale computing will be performed on the HPCx system at the Daresbury Laboratory.

The position is funded by the EPSRC and is available from the 1st October 2005 for up to 3 years. The starting salary will be on the University RA1A scale (£19,460 - £29,127) depending on experience.

Information about the Atomistic Simulation Group at Cambridge is available at

http://www.msm.cam.ac.uk/asg/index.shtml.

Informal enquiries can be made to Dr Paul Bristowe, e-mail: pdb1000@cam.ac.uk.

Applications should be sent by post to Dr P. D. Bristowe, Department of Materials Science and Metallurgy, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK, and should include a full CV and list of publications with the names and addresses of two referees. E-mail applications will not be considered.

Closing date: 31 July 2005.

PhD position

Laboratoire de Métallurgie Physique (LMP) Université de Poitiers (France)

Application deadline: June 5, 2005

Field(s): computational physics, material science

Contact: Dr. BROCHARD Sandrine
Tel.: +33 5 49 49 68 33
email: sandrine.brochard@univ-poitiers.fr

Job description: Applications are invited for a PhD. research position in material science at the Laboratoire de Mtallurgie Physique of the University of Poitiers, France. The candidate should have a Diploma M.S. in Physics with an excellent academic background. Computational skills are welcome, but not essential.

The focus of the work will be the study of dislocations formation in nanostructured materials thanks to large scale Molecular Dynamics simulations. More details on the subject can be found here:

`http://ed-spia.univ-poitiers.fr/ACTUALITES/Recrutement/Recrutement_sujets_Materiaux.htm`

(click on English version of the 4th proposal).

The appointment will be for three years, starting in fall 2005. The financing (about 1300 euros monthly) is not yet established, since it depends on the candidate qualifications. Administrative details (in French) can be found here:

`http://ed-spia.univ-poitiers.fr/ACTUALITES/Recrutement/Recrutement_modalites.htm`

Interested applicants should submit a curriculum vitae and letter in support to Dr. Sandrine Brochard (sandrine.brochard@univ-poitiers.fr) before June 5, 2005.

The final deadline is June 10, 2005 for application to the "Ecole Doctorale Sciences pour l'Ingénieur et Aéronautique".

8 Abstracts

Multiple scattering formalism for correlated systems: A KKR+DMFT approach

J. Minár[1], L.Chioncel[2], A. Perlov[1], H. Ebert[1], M.I. Katsnelson[3],
and A.I. Lichtenstein[4]
[1] *Dep. Chemie und Biochemie, Physikalische Chemie, Universität München,*
Butenandtstr. 5-13, D-81377 München, Germany
[2] *Institute for Theoretical Physics and Computational Physics,*
Graz University of Technology, A-8010 Graz, Austria
[3] *University of Nijmegen, NL-6525 ED Nijmegen, The Netherlands*
[4] *Institut für Theoretische Physik, Universität Hamburg,*
20355 Hamburg, Germany

Abstract

We present a charge and self-energy self-consistent computational scheme for correlated systems based on the Korringa-Kohn-Rostoker (KKR) multiple scattering theory with the many-body effects described by the means of dynamical mean field theory (DMFT). The corresponding local multi-orbital and energy dependent self-energy is included into the set of radial differential equations for the single-site wave functions. The KKR Green's function is written in terms of the multiple scattering path operator, the later one being evaluated using the single-site solution for the t-matrix that in turn is determined by the wave functions. An appealing feature of this approach is that it allows to consider local quantum and disorder fluctuations on the same footing. Within the Coherent Potential Approximation (CPA) the correlated atoms are placed into a combined effective medium determined by the dynamical mean field theory (DMFT) self-consistency condition. Results of corresponding calculations for pure Fe, Ni and $\mathrm{Fe}_x\mathrm{Ni}_{1-x}$ alloys are presented.

(Phys. Rev. B, 2005 in print (cond-mat/0504760))
Contact person: Jan.Minar@cup.uni-muenchen.de

Spin-polarized surface states close to adatoms on Cu(111)

B. Lazarovits[1], L. Szunyogh[1,2], P. Weinberger[1]

[1] *Center for Computational Materials Science, Technical University Vienna, A-1060, Gumpendorferstr. 1.a., Vienna, Austria*

[2] *Department of Theoretical Physics and Center for Applied Mathematics and Computational Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1521, Budapest, Hungary*

Abstract

We present a theoretical study of surface states close to *3d* transition metal adatoms (Cr, Mn, Fe, Co, Ni and Cu) on a Cu(111) surface in terms of an embedding technique using the fully relativistic Korringa-Kohn-Rostoker method. For each of the adatoms we found resonances in the s–like states to be attributed to a localization of the surface states in the presence of an impurity. We studied the change of the s–like densities of states in the vicinity of the surface state band-edge due to scattering effects mediated via the adatom's d-orbitals. The obtained results show that a magnetic impurity causes spin-polarization of the surface states. In particular, the long-range oscillations of the spin-polarized s–like density of states around an Fe adatom are demonstrated.

Manuscript available under `cond-mat/0505505`
Contact person: szunyogh@heisenberg.phy.bme.hu

When Seeing is Not Believing: Oxygen on Ag(111), a Simple Adsorption System?

Angelos Michaelides, Karsten Reuter and Matthias Scheffler

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

Abstract

A number of recent studies indicate that, under the oxygen rich conditions of oxidation catalysis, some transition metal catalysts may be covered by thin oxide overlayers. Moreover, it has been suggested that such "surface-oxide" layers are catalytically active, possibly more active than the pure metal surfaces as was traditionally assumed. This contemporary picture can be traced back to Ag catalysis, where over 30 years ago it was suggested that the top layer of Ag(111) reconstructed to an epitaxial Ag2O-like overlayer upon exposure to oxygen (Rovida *et al.*, Surf. Sci. 43, 230 (1974)). Extensive experimental work, including scanning tunneling microscopy studies in which the oxide was apparently imaged with atomic resolution, as well as density-functional theory calculations, largely confirmed this interpretation. However, a review of published experimental data and new density-functional theory results presented here indicate that previous conclusions are significantly incomplete and that the structure of this original surface-oxide must be reconsidered.

(Submitted to: Journal of Vacuum Science and Technology A)
Contact person: Angelos Michaelides (michaeli@fhi-berlin.mpg.de)

Structural, electronic, and chemical properties of nanoporous carbon

Johan M. Carlsson and Matthias Scheffler

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

Abstract

Nanoporous carbon (NPC), exhibits unexplained chemical properties, making it distinct to other graphene-like materials, as, e.g. graphite, fullerenes, or nanotubes. In this paper we analyze the properties of NPC in terms of its structural motifs, which are derived from defects in distorted graphene sheets. Our density-functional theory calculations show that these motifs can be present in high concentration (up to 1 %). Some of them induce localized levels close to the Fermi level, therefore leading to local charging and controlling the material's chemical function, for example as a catalyst.

(Submitted to: Phys. Rev. Lett.)

Contact person: Johan M. Carlsson (johanc@fhi-berlin.mpg.de)

First-principles study of thin magnetic transition-metal silicide films on Si(001)

Hua Wu, Peter Kratzer, and Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft,
D-14195 Berlin-Dahlem, Germany

Abstract

Ferromagnetic (FM) metal/semiconductor heterojunctions are promising materials for anticipated technological applications in the field of magnetoelectronics or spintronics. In this work, we present density-functional theory calculations addressing the thermodynamic stability and magnetism of both pseudomorphic CsCl-like MSi (M=Mn, Fe, Co, Ni) thin films and Heusler alloy M_2MnSi (M=Fe, Co, Ni) films on Si(001). It is our goal to provide hints to the experimentalist which of these films are stable or at least metastable, and could possibly have interesting properties. We find that the energy for forming such films on the Si(001) surface from elemental reservoirs quickly (after two monolayers) becomes a linear function of film thickness, with the slope determined by the enthalpy of formation of the bulk compound. Moreover, the calculations show that Si-termination of the MSi films is energetically preferable during epitaxy since it minimizes the energetic cost of broken bonds at the surface. Furthermore, we identify chemical trends, e.g., the energy of formation of MSi compounds with six- or sevenfold coordinated metal atoms increases as M varies from Mn to the late transition metals. This is helpful to understand a number of experimental observations. From our calculations, we predict that ultrathin MnSi films are FM with sizable spin magnetic moments at the Mn atoms, while FeSi and NiSi films are nonmagnetic. However, CoSi films display itinerant ferromagnetism due to the Fermi level crossing a flat electronic band. For the M_2MnSi films formed by substituting a manganese atom for every second Si atom in each Si layer of the CsCl-like MSi films the MnSi termination is found to have the highest thermodynamic stability. In the FM ground state, the calculated strength of the effective coupling between the magnetic moments of Mn atoms within the same layer approximately scales with the measured Curie temperatures of the bulk M_2MnSi compounds. In particular, the Co_2MnSi/Si(001) thin film has a robust FM ground state as in the bulk, and is found to be stable against a phase separation into CoSi/Si(001) and MnSi/Si(001) films. Hence such films are interesting in the context of possible applications and deserve further experimental investigations.

(Submitted to: Phys. Rev. B)

Contact person: Peter Kratzer (kratzer@fhi-berlin.mpg.de)

Structural Transitions in the Polyalanine α-Helix under Uniaxial Strain

Joel Ireta, Jörg Neugebauer[†], Matthias Scheffler

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

Arturo Rojo, Marcelo Galván

Departamento de Química, División de Ciencias Básicas e Ingeniería,
Universidad Autónoma Metropolitana-Iztapalapa, A.P. 55-534,
México D. F. 09340

Abstract

We analyzed the response to strain of an infinite polyalanine chain in the α-helical conformation using density-functional theory. Under compressive strain the α-helix is found to undergo structural transitions to a π-helix when the length of the helix is reduced by more than 10 %. Under tensile strain the structure changes into a 3_{10}-helix when the length is stretched by more than 10 %. Our analysis of these transitions shows that they proceed essentially in two steps: At first there is mainly a length change, and only with some delay the helix twist adjusts.

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Contact person: Joel Ireta (ireta@fhi-berlin.mpg.de)

[†] Permanent address: Max-Planck-Institut für Eisenforschung,
Max-Planck-Str. 1, 40237 Düsseldorf

Spectroscopic Analysis of Small Organic Molecules: a comprehensive NEXAFS study of C_6 ring containing molecules

C. Kolczewski[1], R. Püttner[2], M. Martins[2,3], A. S. Schlachter[4], G. Snell[4,5],
M. Sant'anna[4,6], K. Hermann[1], G. Kaindl[2]

[1] *Fritz-Haber-Institut der Max-Planck-Gesellschaft,*
Faradayweg 4–6, 14195 Berlin, Germany
[2] *Institut für Experimentalphysik, Freie Universität Berlin,*
Arnimallee 14, D-14195 Berlin-Dahlem, Germany
[3] *Universität Hamburg, Institut für Experimentalphysik,*
Luruper Chaussee 149, D-22761 Hambrug, Germany
[4] *Advanced Light Source, Lawrence Berkeley National Laboratory,*
Berkeley, CA 94720, USA
[5] *Department of Physics, Western Michigan University, Kalamazoo,*
MI 49008-5151, USA
[6] *Instituto de Fysica, Universidade Federal do Rio de Janeiro,*
Caixa Postal 68528, Rio de Janeiro, RJ 21941-972, Brazil

Abstract

We report high resolution C 1*s* NEXAFS spectra of the C_6-ring containing molecules benzene (C_6H_6), cyclohexadiene (C_6H_8), cyclohexene (C_6H_10), cyclohexane (C_6H_12), styrene (C_8H_8), and ethylbenzene (C_8H_10) which allow us to examine the gradual development of delocalization of the corresponding π electron systems. Due to the high experimental resolution vibrational progressions in the spectra can be partly resolved. The experimental spectra are compared with theoretical NEXAFS spectra obtained from density functional theory (DFT) calculations where electronic final state relaxation are accounted for. The comparison yields very good agreement between theoretical spectra and experimental results. In all cases, the spectra can be described by excitations to π- and σ-type final state orbitals with valence character while final state orbitals of Rydberg character make only minor contributions. The lowest C 1s to $1\pi^*$ excitation energy is found to agree in the (experimental and theoretical) spectra of all C_6H_n molecules except for 1,3 cyclohexadiene (C_6H_8) where an energy smaller by about 0.6 eV is obtained. The theoretical analysis can explain this result by different binding properties of this molecule compared to the others.

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Contact person: Christine Kolczewski (kolczew@fhi-berlin.mpg.de)

Oxygen 1s NEXAFS spectra of the V_2O_5(010) Surface: theoretical studies using ab initio DFT cluster models

C. Kolczewski and K. Hermann
Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4–6, D-14195 Berlin, Germany

Abstract

The (010) surface of vanadium pentoxide, V_2O_5, contains 1-, 2-, and 3-fold coordinated oxygen centers which can participate as active sites in specific surface reactions. In the present work we use ab initio density functional theory (DFT) together with cluster models to calculate 1s core excitation spectra of the different oxygen centers. Excitation energies and intensities are characterized by details of local V-O binding where the data depend strongly on coordination. As a result, strong coordination dependence of the angle-resolved NEXAFS spectra of different oxygen centers is found. The differences can also be seen in the total spectrum obtained from a superposition of the atom specific spectra. A comparison of our theoretical spectra with experimental NEXAFS data yields good agreement and allows an assignment of the experimental peaks to the differently coordinated oxygen centers.

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Contact person: Christine Kolczewski (kolczew@fhi-berlin.mpg.de)

Competition Between Delocalization and Spin- Orbit Splitting in the Actinide $5f$ States

J.G. Tobin, K.T. Moore, B.W. Chung, M.A. Wall, A.J. Schwartz
Lawrence Livermore National Laboratory,
Livermore, California 94550, USA
G. van der Laan
Synchrotron Radiation Source, Daresbury Laboratory,
Warrington, WA4 4AD, UK
A.L. Kutepov
Russian Federation Nuclear Center, Institute of Technical Physics (VNIITF),
Snezhinsk, Chelabinsk Region, Russia

Abstract

We have solved the Pu puzzle. Synchrotron-radiation-based X-ray absorption, electron energy-loss spectroscopy in a transmission electron microscope, multi-electronic atomic spectral simulations and improved first principles calculations (Generalized Gradient Approximation in the Local Density Approximation, GGA/LDA) have been used to investigate the electronic structure of the light actinides: α-Th, α-U and α-Pu.

It is shown that the spin-orbit interaction can be used as a measure of the degree of localization of valence electrons in a material. The spin-orbit interaction in the light actinide metals, α-Th, α-U and α-Pu, has been determined using the branching ratio of the white line peaks of the $N_{4,5}$ edges, which correspond to $4d \rightarrow 5f$ transitions. Examination of the branching ratios and spin-orbit interaction shows that the apparent spin-orbit splitting is partially quenched in α-U, but is strongly dominant α-Pu. These results are fully quantified using the sum rule. This picture of the actinide $5f$ electronic structure is confirmed by comparison with the results of electronic structure calculations for α-Th, α-U and α-Pu, which in turn are supported by a previous Bremstrahlung Isochromat Spectroscopy (BIS) experiment.

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Energy-loss near-edge structure changes with bond length in carbon systems

J. T. Titantah and D. Lamoen
TSM, Departement Fysica, Universiteit Antwerpen,
Groenenborgerlaan 171, 2020 Antwerpen, België

Abstract

We show that as the graphene planes of graphite are uniformely expanded thereby increasing the C−C bond length to 1.7 Å, the σ^* edge onset of the energy-loss near-edge structure (ELNES) spectrum shifts to lower energies by almost 5 eV meanwhile the π^*edge onset shifts by a value lower than 0.2 eV. The shift of the σ^* edge demonstrates that at some bond lengths which are typical of some carbon systems like the amorphous carbon, it is possible to find σ^* features in the ELNES spectra at energies as low as 286-288 eV. Most of the sp^2/sp^3 quantification techniques that are available often overlook this issue and assume that all features within this energy range are entirely of π^* origin. We show that the effect of bond length variation on the π^* spectrum of graphite is minor thereby supporting the reliability of the use of this spectrum for sp^2/sp^3 quantification purposes as was recently demonstrated [See J. T. Titantah and D. Lamoen, Phys. Rev. B **70**, 075115 (2004)].

(Submitted to Physical Review B (Brief Reports))
Contact person: Dirk Lamoen (Dirk.Lamoen@ua.ac.be)

Temperature effects on the electronic, bonding, optical and mechanical properties of sp^3-rich amorphous carbon

J. T. Titantah and D. Lamoen
TSM, Departement Fysica, Universiteit Antwerpen,
Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Abstract

The thermal properties of dense tetrahedral amorphous carbon (ta-C) made of ~80-85% sp^3-bonded atoms at a density of 3.4 g/cm^3 are theoretically investigated by looking at the structural, bonding, mechanical, electronic and optical properties as the formed ta-C is heated up. A low temperature structural transformation accompanied by a minor decrease of the sp^3 fraction (less than 10%), but leading to an abrupt pressure build up is evidenced above a temperature of about 600 °C. Below this temperature it is found that the equilibrium density (density at which the ta-C becomes stress-free) is 0.6% lower (than 3.4 g/cm^3) while beyond it a drastic decrease in density (about 2.4%) is recorded. A considerable amount of sp^2 sites that cluster together is also seen near this temperature. Considering the fact that it is at such temperatures that stress-relieve is reported in non-equilibrium as-deposited ta-C, this study suggests that, for highly ta-C, while clustering of the sp^2 sites is responsible for stress relieve, this is accompanied by an increase in the atomic volumes of such sites. This work is based on ta-C structures generated using the Tersoff potential whose cut-off distance was set at 2.45 Å in order to accurately locate the second coordination structure of amorphous carbon. We have also found that the choice of the range of the Tersoff potential is crucial to locate the correct temperature $T_1' \sim 1200°C$ above which there is a transformation from sp$^3-$ to sp$^2-$rich amorphous carbon.

(Submitted to Carbon)
Contact person: Dirk Lamoen (Dirk.Lamoen@ua.ac.be)

N-representability theorem of the fermion p-order reduced density matrix

Thierry Deutsch
Département de recherche fondamentale sur la matière condensée,
SP2M/L_Sim, CEA-Grenoble, 38054 Grenoble cedex 9, France

Abstract

The necessary and sufficient conditions to have a N-representable p-order reduced density matrix, i.e. representing a wavefunction of N fermions where p is an integer between 1 and N, are presented: the p-order reduced density matrix has to be semi-definite positive and its diagonal part called the p-body density must be inside a polytope (generalisation of a polyhedron) with a countable known vertices. This result is also directly applicable to the case of bosons. Exact calculations are now tractable for fermions without any many-body wavefunction.

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Contact person: tdeutsch@cea.fr

Ab initio theory of planetary materials

Artem R. Oganov(1), G. David Price(2), Sandro Scandolo(3)
(1) Laboratory of Crystallography, Department of Materials, ETH Hönggerberg,
Wolfgang-Pauli-Strasse 10, Zurich CH-8093, Switzerland
(2) Department of Earth Sciences, University College London,
Gower Str., London WC1E 6BT, UK
(3) The Abdus Salam International Centre for Theoretical Physics (ICTP)
and INFM/Democritos National Simulation Center, I-34014 Trieste, Italy

Abstract

Ab initio simulations play an increasingly important role in the studies of deep planetary interiors. Here we review the current state of this field, concentrating on studies of the materials of the Earth's deep interior (MgO-SiO_2-FeO-Al_2O_3, Fe-Si-S-O) and of the interiors of giant planets (H-He system, H_2O-CH_4-NH_3 sys-tem). In particular, novel phases and phase diagrams, insights into structural and electronic phase transitions, melting curves, thermoelasticity and the effects of impurities on physical properties of planet-forming materials are discussed.

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Contact person: A.R. Oganov (a.oganov@mat.ethz.ch)

New high-pressure phase of alumina and implications for Earth's D" layer

Artem R. Oganov$^{(1)}$ and Shigeaki Ono$^{(2)}$
(1) Laboratory of Crystallography, Department of Materials, ETH Hönggerberg,
Wolfgang-Pauli-Strasse 10, Zurich CH-8093, Switzerland
(2) Institute for Research on Earth Evolution,
Japan Agency for Marine-Earth Science and Technology,
2-15 Natsushima-cho, Yokosuka-shi, Kanagawa 237-0061, Japan

Abstract

Using ab initio simulations and high-pressure experiments in a diamond anvil cell, we show that alumina (Al_2O_3) adopts the $CaIrO_3$-type structure above 130 GPa. This finding completely changes the picture of high-pressure behaviour of alumina, in particular we find that perovskite structure is never stable for Al_2O_3 at zero Kelvin. The new phase suggests a re-interpretation of previous shock-wave experiments and has important implications for the use of alumina as a window material in shock-wave experiments. In particular, the conditions of the stability of this new phase correspond to those at which shock-wave experiments indicated an increase of the electrical conductivity. If this increase is due to high ionic mobility in the $CaIrO_3$-type phase of Al_2O_3, similar effect can be expected in the isostructural post-perovskite phase of $MgSiO_3$ (which is the dominant mineral phase in the Earth's D" layer). The effect of the incorporation of Al on the perovskite/post-perovskite transition of $MgSiO_3$ is discussed.

(Proc. Natl. Acad. Sci., under review (2005))
Contact person: A.R. Oganov (a.oganov@mat.ethz.ch)

Ab initio thermodynamics of $MgSiO_3$ perovskite at high pressures and temperatures

Artem R. Oganov$^{(1)}$, G. David Price$^{(2)}$
(1) Laboratory of Crystallography, Department of Materials, ETH Hönggerberg,
Wolfgang-Pauli-Strasse 10, Zurich CH-8093, Switzerland
(2) Department of Earth Sciences, University College London,
Gower Str., London WC1E 6BT, UK

Abstract

Using quantum-mechanical simulations based on density-functional perturbation theory, we address the problem of stability of $MgSiO_3$ perovskite to decomposition into MgO and SiO_2 at pressures and temperatures of the Earth's lower mantle. We show that $MgSiO_3$ perovskite sand its post-perovskite phased is more stable than the mixture of oxides throughout the pressure-temperature regime of the Earth's mantle. Structural stability and lattice dynamics of phases in the system MgO-SiO_2 are discussed.

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Contact person: A.R. Oganov (a.oganov@mat.ethz.ch)

Crystal morphology and surface structures of the orthorhombic $MgSiO_3$ perovskite

Alfredsson M., Dobson D.P., Oganov A.R., Catlow C.R.A., Brodholt J.P.,
Parker S.C., Price G.D.

Abstract

Orthorhombic $MgSiO_3$ perovskite is thought to be the most abundant mineral in the mantle of the Earth. Its bulk properties have been widely studied, but many geophysical and rheological processes are also likely to depend upon its surface and grain boundary properties. As a first step towards modelling these geophysical properties, we present here an investigation of the structures and energetics of the surfaces of $MgSiO_3$-perovskite, employing both shell-model atomistic effective-potential simulations, and density-functional-theory (DFT) calculations. Our shell-model calculations predict the 001 surfaces to be the energetically most stable surfaces: the calculated value of the surface energy being 2.2 J/m2 for the MgO-terminated surface, which is favoured over the SiO_2-terminated surface (2.7 J/m2). Also for the polar surfaces 111, 101 and 011 the MgO-terminated surfaces are energetically more stable than the Si-terminated surfaces. In addition we report the predicted morphology of the $MgSiO_3$ perovskite structure, which is dominated by the energetically most stable 001 and 110 surfaces, and which appears to agree well with the shape of grown single crystals.

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Contact person: A.R. Oganov (a.oganov@mat.ethz.ch)

In situ observations of phase transition between perovskite and $CaIrO_3$-type phase in $MgSiO_3$ and pyrolitic mantle composition

Shigeaki Ono(1), Artem R. Oganov(2), Yasuo Ohishi(3)
(1) Institute for Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology, 2-15 Natsushima-cho, Yokosuka-shi, Kanagawa 237-0061, Japan
(2) Laboratory of Crystallography, Department of Materials, ETH Hönggerberg, Wolfgang-Pauli-Strasse 10, CH-8093 Zurich, Switzerland
(3) Japan Synchrotron Radiation Research Institute,
Mikazuki-cho, Sayo-gun, Hyogo 679-5198, Japan

Abstract

In situ observations of the perovskite-$CaIrO_3$ phase transition in $MgSiO_3$ and in pyrolitic compositions were carried out using a laser-heated diamond anvil cell interfaced with a synchrotron radiation source. For pure $MgSiO_3$, the phase boundary between the orthorhombic Mg-perovskite and $CaIrO_3$-type phases in the temperature range of 1300-3100 K was determined to be P (GPa) = 130 (3) + 0.0070 (0.0030)(T - 2500) (K) using platinum as a pressure calibrant. We confirmed that the $CaIrO_3$-type phase remained stable up to pressures of at least 156 GPa and temperatures of 2600 K. The consistency of our results with previous theoretical calculations leads us to conclude that the 2700 km seismic discontinuity at the bottom of the lower mantle can be attributed to a phase transition to the $CaIrO_3$-type phase. The phase change from an orthorhombic Mg-perovskite to a $CaIrO_3$-type bearing assemblage in a pyrolitic mantle composition was also observed at P = 125 GPa, which corresponds to the same mantle depth as the seismic discontinuity. This transition boundary indicates that the temperature at a depth of 2700 km is about 2600 K, and the adiabatic temperature gradient in the lower mantle is estimated to be 0.31 K/km. The partition coefficients and the effect of some elements on the phase equilibrium between the orthorhombic $MgSiO_3$ perovskite and $CaIrO_3$-type $MgSiO_3$ were estimated from ab initio calculations. Our experimental and theoretical results indicate that the D" layer consists of a $CaIrO_3$-type bearing assemblage which is likely to have significant effect on the chemical and thermal evolution of the Earth's mantle.

(Earth Planet. Sci. Lett., under revision (2005))
Contact person: A.R. Oganov (a.oganov@mat.ethz.ch)

9 Presenting Other Initiatives

9.1 Special Issue "Computational Crystallography" of Zeitschrift fuer Kristallographie

Guest Editor: A.R. Oganov
Publication date: May/June 2005

This special issue is a collection of up-to-date reviews on the methodology and application of simulation methodology (ab initio methods are in the focus) to crystallographic problems:

1. C.Gatti. "Chemical bonding in crystals"
2. X. Gonze , G.-M. Rignanese, R. Caracas. "First-principles studies of the lattice dynamics of crystals, and related properties"
3. S.Y. Savrasov, A. Toropova, M.I. Katsnelson, A.I. Lichtenstein, V. Antropov, G. Kotliar. "Electronic structure and magnetic properties of solids"
4. R. Martonak, A. Laio, M. Bernasconi, C. Ceriani, P. Raiteri and M. Parrinello. "Simulation of structural phase transitions by metadynamics"
5. A. Gavezzotti, "The calculation of lattice energies by the PIXEL point-by-poiint integration method"
6. R. Caracas, X. Gonze. "First-principles study of materials involved in incommensurate transitions"
7. J.S. Tse. "Crystallography of high-pressure elemental solids"
8. A.R. Oganov, G.D. Price, S.Scandolo, "Crystallography of of planetary interiors".

In addition, a number of overviews of popular simulation and visualisation codes are presented.

10 SCIENTIFIC HIGHLIGHT OF THE MONTH

Many-body perturbation theory using the density-functional concept

Fabien Bruneval,[a] Francesco Sottile,[ac] Valerio Olevano,[ad] Rodolfo Del Sole,[b]
and Lucia Reining[a]
[a]*Laboratoire des Solides Irradiés, UMR 7642 CNRS/CEA,*
École Polytechnique, 91128 Palaiseau, France
[b]*Istituto Nazionale per la Fisica della Materia*
e Dipartimento di Fisica dell'Università di Roma "Tor Vergata",
Via della Ricerca Scientifica, 00133 Roma, Italy
[c] *present address: Donostia International Physics Center (DIPC),*
20018 Donostia/San Sebastian, Spain
[d] *present address: Laboratoire d'Études des Propriétés Électroniques des Solides,*
UPR 11, CNRS, F-38042, Grenoble, France

Abstract

Many-body perturbation theory (MBPT) offers a convenient framework for the calculation of electronic excitations. In principle, all kinds of electronic excitations (i.e., neutral or involving a change in particle number) are accessible, and the physics that has to be included is relatively well understood. Also time-dependent density-functional theory (TDDFT) allows one in principle to describe excitations, at a *a priori* lower computational cost. However, in that case it is more difficult to design good approximations for the exchange-correlation contribution, since one does not work in the physically intuitive quasi-particle picture. Moreover, only neutral excitations are accessible. In order to combine the advantages of both approaches, we propose an alternative formulation of many-body perturbation theory that uses the density-functional concept. Variations of many-body quantities upon excitation are expressed through variations with respect to the density. In this way, instead of the usual four-point integral equation for the polarizability (namely, the Bethe-Salpeter equation), we obtain a two-point one (i.e., like in TDDFT), that leads to excellent optical absorption and energy loss spectra. The corresponding three-point vertex function and self-energy are then simply calculated via an integration, for any level of approximation. Moreover, we show the direct impact of this formulation on the time-dependent density-functional theory. With the help of numerical results, we discuss the consequences of exchange-correlation contributions to the response for optical spectra and for the band gap of bulk silicon and solid argon.

1 Introduction

The electronic structure of materials and its response to an external perturbation are key quantities for the interpretation of many experimental results or for the design of technological devices. Electronic excitations enter a wealth of scientific questions or daily-life problems, ranging e.g. from the deformation of molecules upon absorption of radiation in cancer research, to defect creation in nuclear waste, to photosynthesis or to the design of more efficient solar cells. It is therefore highly desirable to be able to describe, understand, and even predict electronic excitations and their consequences.

In this context, *ab initio* electronic structure calculations have become a tool of choice. In the community of solid-state physicists the widely used Kohn-Sham (KS) framework of the density-functional theory (DFT) [1] is a convenient starting point. Although DFT is in principle a ground state theory and KS eigenvalues are not meant to represent measurable electron addition and removal energies, the KS band structure already yields much useful information, and occupied bands are often in quite reasonable agreement with, e.g., photoemission results. In order to describe the response to an external perturbation, such as it is measured for example in optical absorption experiments, one can then construct a response function using an independent particle Fermi's golden rule, eventually including the self-consistent variations of the Hartree potential (which is equivalent to the Random Phase Approximation (RPA) including crystal local-field effects).

Beyond this, one should try to improve the description of exchange-correlation effects, both in the band structure and in the self-consistent variation of the corresponding potential. State-of-the-art calculations for solids are based on the many-body perturbation theory (MBPT). Concerning the band structure, in that case, quasi-particle (QP) energies are obtained from the solution of an equation similar to the Kohn-Sham one, but with the KS exchange-correlation (xc) potential v_{xc} replaced by the electron self-energy Σ. The last quantity is most often calculated in Hedin's GW approximation [2], where Σ is equal to the product of the one-particle Green's function G and the screened Coulomb interaction W calculated in the RPA. The resulting band structures, and in particular the band gap, are generally much closer to the measured ones than the KS results [3]. In order to include the self-consistent variation of Σ (which is the corresponding xc "potential") upon excitation, and hence to get improved response functions, one can then add the so-called "vertex corrections" beyond the RPA. This is done in practice by solving the four-point Bethe-Salpeter equation (BSE) for the polarizability P; the kernel of this integral equation expresses the electron-hole interaction (whereas electron and hole are non-interacting when the RPA is adopted and local-field effects are neglected). The BSE leads in general to excellent absorption and electron energy-loss spectra [4]. In particular, one correctly describes the important excitonic effects.

Unfortunately, calculations of vertex corrections are cumbersome essentially because of the four-point (electron-hole scattering) nature of the BSE (see e.g. [4]). Calculations of the response functions in this framework have therefore been limited to relatively simple systems. Moreover, attempts to go beyond the GW approximation through vertex corrections (see e.g. [6, 7, 8, 9]) are rare and restricted to relatively simple systems, even though it is well known that the precision of the standard GW approximation is limited, and that the approximation often fails for moderately to strongly correlated materials (see e.g. [10]). Again, this lack of examples is essentially due to the above-mentioned computational difficulties.

However, at least concerning response functions, it is known that *in principle* one could obtain the polarizability directly from a two-point equation: this is the case when one works in the framework of time-dependent DFT (TDDFT) [11], since one propagates the density (a function that is local in time and space) instead of the one-particle Green's function (which is non-local both in time and in space). TDDFT could therefore clearly be a prominent computational alternative to the BSE for the calculation of P. The drawback resides in the fact that up to recently, and contrary to the MBPT framework, reliable approximations for the xc potential $v_{xc}(\mathbf{r}, t)$ and its first density-variation, the xc kernel $f_{xc}(\mathbf{r}, \mathbf{r}', t, t')$, were missing in particular concerning absorption spectra of solids. Several attempts were therefore made to derive the unknown, but two-point, xc kernel of the TDDFT linear response equation for P from the known, but four-point, BSE, in order to combine the precision of the latter with the computational advantages of TDDFT [12, 13, 14]. Various different approaches have lead to quite similar expressions that, tested for real materials, have turned out to be extremely successful in reproducing the underlying BSE via a TDDFT-like equation. While recalling below some of these recent results, we will however focus on some more general questions that, we believe, are answered by the present work. These are (i) a physical explanation for the unexpected success of these approaches, (ii) a prescription of how one can use this MBPT-TDDFT combination in order to get response functions beyond the approximations that are currently made for the BSE, and (iii) the use of the TDDFT concept within MBPT (instead of the use of MBPT quantities within TDDFT). In fact, since TDDFT is not designed to access one-QP properties, like the band structure, this enlarges significantly the range of problems that can be addressed by such a combination.

The ultimate goal of this line of research can be summarized as the hope to combine the density-functional and the QP concepts in such a way that systematic and efficient improvements to the spectroscopic quantities of interest could be obtained. We believe that this work shows how this goal can be reached [15].

2 Many-body perturbation theory and time-dependent density-functional theory: two approaches, in part to the same problem

2.1 Hedin's equations

In the field of electronic excitations, it is convenient to work with Green's functions. The time-ordered one-particle Green's function is defined

$$G(1,2) = -i\langle\Phi_0|T\left[\hat{\psi}(1)\hat{\psi}^{\dagger}(2)\right]|\Phi_0\rangle, \qquad (1)$$

where $|\Phi_0\rangle$ is the many-body N-particle ground state, $\hat{\psi}(1)$ ($\hat{\psi}^{\dagger}(1)$) is the annihilation (creation) operator of an electron, T is the time-ordering operator and 1 stands for the set of the real space and time coordinates plus the spin degree of freedom, $1 = \mathbf{r}_1, t_1, \sigma_1$. The Green's function G has poles that correspond to electron addition and removal energies. Since the many-body ground state $|\Phi_0\rangle$ is another unknown of the problem, the calculation of this quantity is not straightforward. One has to search either for a diagrammatic expansion or for a set of equations governing G that eventually may be somehow approximated. Here we adopt the second line, developped in its present form by Lars Hedin [2]. For the sake of comprehension of all our subsequent developments, we estimate useful to summarize it in the following.

The main idea is that one starts by writing the equation of motion for the one-particle Green's function G via its time derivative. It is not astonishing to find that this gives rise to an expression involving a two-particle Green's function $G^{(2)}$: the particle propagating in the system polarizes the system. This polarization corresponds to the creation of electron-hole pairs, hence two particles. The problem of calculating the one-particle Green's functions is then translated into the problem of calculating the two-particle Green's function which, in its turn, would imply an higher order Green's function, and so on. In order to obtain a closed description, one introduces a potential-like operator that is however nonlocal in time and space, namely the self-energy Σ. By definition, G and Σ are linked through the Dyson equation

$$G^{-1}(1,2) = G_0^{-1}(1,2) - V(1)\delta(1,2) - \Sigma(1,2) \tag{2}$$

where G_0 is the free-particle Green's function, and $V(1) = U(1) + V_H(1)$, the total classical potential, (U is an external potential and V_H is the Hartree potential). Now, one wishes to introduce the above-mentioned two-particle Green's function $G^{(2)}$ via some known quantity. Since $G^{(2)}$ is responsible for the response to a perturbation, one can in fact also create it by applying an external potential. To this purpose in Hedin's approach a small time-dependent contribution is added to the external potential. The resulting U is constructed such that it goes to the static physical potential $V_{ext}(\mathbf{r})$ at times $\pm\infty$; its fictious time-dependent part will be made vanishing at the end of the derivation. One can then express the self-energy in terms of variations of the Green's function with respect to the external potential, $\Sigma = -ivG\delta G^{-1}/\delta U$ [2], or

$$\Sigma(1,2) = iG(1,4)\Gamma(4,2;5)\frac{\delta V(5)}{\delta U(3)}v(3,1^+), \tag{3}$$

with the irreducible vertex function

$$\Gamma(1,2;3) = -\frac{\delta G^{-1}(1,2)}{\delta V(3)} = \delta(1,3)\delta(2,3) + \frac{\delta\Sigma(1,2)}{\delta V(3)} \tag{4}$$

and v the bare Coulomb interaction (integration over indices not present on the left is implicit throughout the equations).

The derivative $\delta\Sigma/\delta V$ is then usually replaced by the chain rule $(\delta\Sigma/\delta G)(\delta G/\delta V)$. Using the relation $(\delta G/\delta V) = -G(\delta G^{-1}/\delta V)G$, Eq. (4) is transformed into and integral equation

$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \int d4567\,\frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\Gamma(6,7;3). \tag{5}$$

In the same way one obtains the remaining Hedin's equations

$$\Sigma(1,2) = i\int d34\, G(1,3)\Gamma(3,2;4)W(4,1) \tag{6}$$

$$W(1,2) = v(1,2) + \int d34\, v(1,3)P(3,4)W(4,2) \tag{7}$$

$$P(1,2) = -i \int d34\, G(1,3)G(4,1)\Gamma(3,4;2) \tag{8}$$

in terms of the time-ordered polarization operator $P(1,2)$, and the dynamical screened interaction $W(1,2) = \delta V(1)/\delta U(3)v(3,2)$.

Disregarding Σ on the right-hand side of Eq. (4) would yield the GW approximation,

$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) \qquad \Longrightarrow \qquad \Sigma(1,2) = iG(1,2)W(2,1) \tag{9}$$

Equation (5), or an equivalent form, with its four-point kernel dominated by $\delta\Sigma(1,2)/\delta G(3,4)$, has to be solved in order to get the irreducible polarizability $P = -iGG\Gamma$ [3] and an improved self-energy from Eq. (6). Equation (5) is the main obstacle on the way to a calculation of polarizabilities or self-energies beyond the RPA.

2.2 Response functions in Time-dependent density-functional theory

As pointed out above, in principle also TDDFT allows one to calculate the excitation energies and transition probabilities of a many-body system, for constant particle number. In the time-dependent approach, one studies how the system behaves when subject to a time-dependent external perturbation that gives rise to density variations. In this case, the system's response is directly related to the N-particle excited states of an N-particle system, in a similar manner that the one-particle Green's function is related to the $(N+1)$- and $(N-1)$-particle excited states of the same system.

In TDDFT, the linear density response of an interacting many-electron system [16]

$$\chi(\mathbf{r},t,\mathbf{r}',t') = \frac{\delta\rho(\mathbf{r},t)}{\delta U(\mathbf{r}',t')} \tag{10}$$

is obtained from the non-interacting Kohn-Sham response to a change in the total Kohn-Sham potential v_{KS}

$$\chi_0(\mathbf{r},t,\mathbf{r}',t') = \frac{\delta\rho(\mathbf{r},t)}{\delta v_{KS}(\mathbf{r}',t')}. \tag{11}$$

via

$$\chi(\mathbf{r},\mathbf{r}';\omega) = \chi_0(\mathbf{r},\mathbf{r}';\omega) + \int d\mathbf{r}_1 d\mathbf{r}_2\, \chi_0(\mathbf{r},\mathbf{r}_1;\omega)K(\mathbf{r}_1,\mathbf{r}_2,\omega)\chi(\mathbf{r}_2,\mathbf{r}';\omega)\,, \tag{12}$$

where the kernel K has been introduced as

$$K(\mathbf{r}_1,\mathbf{r}_2,\omega) = \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} + f_{xc}(\mathbf{r}_1,\mathbf{r}_2,\omega)\,. \tag{13}$$

with the exchange-correlation contribution

$$f_{xc}(\mathbf{r},t,\mathbf{r}',t') = \frac{\delta v_{xc}[\rho](\mathbf{r},t)}{\delta\rho(\mathbf{r}',t')}. \tag{14}$$

---

[3] The irreducible polarizability P defined in this work is a time-ordered quantity. From the time-ordered P one can then obtain a physical (causal) response function with the usual conversion rules. It should be noted that in the following we do not make a distinction between time-ordered and causal quantities. However, one has to be careful because this apparent "subtlety" could cause severe errors in practice when not properly accounted for. One possible way is represented by the Keldysh formalism. In this scheme all the quantities are consistently defined on the Keldysh contour and pseudo-time-ordered. At the end, projecting from the pseudo-time to the physical time, causal physical response functions are restored.

The exact time–dependent exchange-correlation kernel is of course unknown, and practical calculations must rely on some approximation. The most commonly used, due to its simplicity but also its success mostly in finite systems, is the adiabatic local-density approximation also called time-dependent LDA (TDLDA), where $f_{xc}(\mathbf{r}_1, \mathbf{r}_2, \omega)$ is approximated with the (ω-independent) functional derivative of the LDA exchange-correlation potential:

$$f_{xc}^{\mathrm{TDLDA}}(\mathbf{r}_1, \mathbf{r}_2, \omega) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \frac{dv_{xc}^{\mathrm{LDA}}(\rho(\mathbf{r}_1))}{d\rho(\mathbf{r}_1)}. \tag{15}$$

Apart from this approximation for f_{xc}, another approximation has to be done in practical calculations: the static Kohn–Sham orbitals and eigenvalues used to construct χ_0 are in fact calculated with an approximate exchange-correlation potential v_{xc}, typically the same as the one used in ground state calculations.

If all quantities were evaluated exactly, the retarded version of the time-ordered P calculated via Eq. (8) should yield the retarded response function χ (Eq. (12) via $\chi = P + Pv\chi$. However, whereas it has turned out that the commonly used GW approximation for Σ *together with* its variation ($\delta\Sigma/\delta G$) are successful in describing response functions (via the today standard Bethe-Salpeter equation), TDLDA often does not properly account for excitations. In particular absorption spectra in solids are badly described, even though LDA usually yields satisfactory ground state properties. Moreover, important quantities such as the measurable bandstructure are not accessible through TDDFT (at least not considering closed systems). For all these reasons, the idea consisting in keeping the substantial accuracy of MBPT while at the same time introducing the density degree of freedom concept, could lead to a more convenient framework where the computational advantages of density-functional play a fundamental role. Further on this route, indications on how to improve upon the well established many-body approximations, could constitute an important subproduct of this derivation.

3 MBPT and TDDFT: a successful combination

3.1 MBPT quantities in TDDFT: a summary of some previous works

During the last years, the scientific community has made a major effort trying to find reliable approximations for the exchange-correlation kernel of TDDFT. One important line of research has been the attempt to use MBPT as a starting point. This is in a sense, the opposite direction of the present work (where we aim at using TDDFT to improve within MBPT), but the two are of course tightly linked. We will therefore very briefly summarize some of the MBPT-TDDFT work that is of direct importance for the present approach.

Already in the eighties Streitenberger has suggested [5] to exploit the very fact that both TDDFT and MBPT should yield, at least in principle, the same (exact) polarizability, in order to define an effective xc-kernel for the homogeneous electron gas. Later on, the inclusion of approximate vertex functions in the self energy has been addressed by Mahan and Sernelius [6] for the homogeneous electron gas and, in the mid nineties, by Del Sole, Reining and Godby for silicon [7].

More recent work has focused on the extraction of an effective TDDFT xc-kernel by comparison with the macroscopic dielectric function resulting from BSE calculations [17]. This yields some information on the analytic structure of the xc correlation kernel in extended systems, for instance about its long range behavior in real space, but does not avoid the cumbersome solution of the BSE. Very recently, approaches have been developed by a few groups to this aim. In one case, a perturbative expansion in W of the xc kernel obtained from the equality of the two macroscopic dielectric functions, namely the one calculated with the Bethe-Salpeter equation and the one calculated with the TDDFT screening equation, has yielded a result that already in first order turned out to yield excellent optical spectra in solids [13]. Another approach is based on the formal replacement of TDDFT kernel matrix elements taken in a basis of Kohn-Sham transitions with Bethe-Salpeter matrix elements, and arrives to the same formula and of course to numerical results of similar quality [12]. Finally, by recognizing that the same physics should be represented by the MBPT and the TDDFT equations, Stubner, Tokatly and Pankratov have developed a diagrammatic approach to the derivation of improved exchange-correlation kernels [14]. Again the same result for the effective xc kernel is obtained.

A final point to notice is that the xc correlation kernel derived above has a long range (1/r) tail in real space, and hence a small-q behavior of type α/q^2, clearly visible from the equations. Hence it is possible to avoid the cumbersome calculation of α, that is of the kernel itself, looking instead for the α values which yield the best optical spectra. Even this very simple approach works well, and leads to good optical spectra using α values ranging from -0.2 for semiconductors to -1 for insulators. It is found that these values are roughly inversely proportional to the dielectric constant [18].

In conclusion, at present, at least three seemingly completely different approaches have hence led independently to the same expression for the effective xc correlation kernel, Eq. (27), which yields optical and energy loss spectra very close to those derived within the BSE approach. The present work sheds light on the deep reasons for their coincidence and success.

3.2 Density variations in MBPT: the idea and the equations

In the way TDDFT and MBPT are hence usually presented, self-consistent linear response in TDDFT is determined by variations of the potential with respect to the *density*, whereas in MBPT variations with respect to the one-particle *Green's function* are the key ingredient. However, in both cases it is a local external potential that actually creates these variations. Therefore, we have suggested that also in the case of MBPT one might rely on the fact that *density variations determine the physics* when the system is polarized. In practice, this means that one can use the Runge-Gross theorem of TDDFT [11] in order to rewrite $\delta\Sigma/\delta V$ in Eq. (4). The one-to-one relation between time-dependent densities and external potentials, or consequently between the densities and the classical potentials V, allows one then to use an alternative chain rule to express $\delta\Sigma/\delta V$, namely $(\delta\Sigma/\delta\rho)(\delta\rho/\delta V)$.

Equation (4) hence becomes

$$\Gamma(1,2;3) = \delta(1,3)\delta(2,3) + \frac{\delta\Sigma(1,2)}{\delta\rho(4)}P(4,3), \tag{16}$$

where $P = \delta\rho/\delta V$ is the irreducible polarizability that, as explained above, is usually calculated by solving the vertex equation. However, by integrating Eq. (16) with two Green's functions G, one directly obtains

$$P(1,2) = P_0(1,2) + P_0(1,3) f_{xc}^{\text{eff}}(3,4) P(4,2), \tag{17}$$

with $P_0(1,2) = -iG(1,2)G(2,1)$ and the two-point kernel

$$f_{xc}^{\text{eff}}(3,4) = -iP_0^{-1}(3,6)G(6,5)G(5',6)\frac{\delta\Sigma(5,5')}{\delta\rho(4)}. \tag{18}$$

In other words, *one can now first determine the two-point irreducible polarizability P from the integral Eq. (17), and subsequently the three-point vertex Γ via the integration of Eq. (16).* From P, the reducible polarizability P^{red} is obtained via $P^{\text{red}} = P + PvP^{\text{red}}$.

Finally, the self-energy becomes

$$\Sigma(1,2) = iG(1,2)W^{\text{TC-TC}}(2,1) + iG(1,4)\frac{\delta\Sigma(4,2)}{\delta\rho(5)}P^{\text{red}}(5,3)v(3,1^+). \tag{19}$$

The first term has the GW form, but with the testcharge-testcharge (TC-TC) screened Coulomb interaction $W^{\text{TC-TC}} = (1 + vP^{\text{red}})v$, instead of the RPA one. In this expression, the term $vP^{\text{red}}v$ creates the induced Hartree potential felt by a classical charge. The additional term $(\delta\Sigma/\delta\rho)P^{\text{red}}$ in Eq. (19) is responsible for the missing induced xc potentials that act on an electron or hole. It is therefore useful to reformulate Eq. (16) as

$$\Gamma(1,2;3) = \delta(1,3)\delta(2,3) + \delta(1,2) f_{xc}^{\text{eff}}(1,4)P(4,3) + \Delta\Gamma(1,2;3) \tag{20}$$

where

$$\Delta\Gamma(1,2;3) = \left(\frac{\delta\Sigma(1,2)}{\delta\rho(4)} - \delta(1,2) f_{xc}^{\text{eff}}(1,4)\right) P(4,3). \tag{21}$$

The "non-locality correction" $\Delta\Gamma$ has no effect on P, as one can see by integrating Eq. (21) with two Green's functions and using Eq. (18). In the self-energy of Eq. (19), the inclusion of the two first terms of Eq. (20) (called $\Gamma^{(2)}$) leads to $\Sigma = iG\tilde{W}$ with a modified screened Coulomb interaction $\tilde{W} = (1 + (v + f_{xc}^{\text{eff}})P^{\text{red}})v$. This is a testcharge-testelectron (TC-TE) screened Coulomb interaction instead of $W^{\text{TC-TC}}$; this expresses the fact that an additional electron or hole in the system cannot be described as a classical charge. $\Delta\Gamma$ yields then in Σ a non-vanishing correction term. One can understand this by the fact that, contrary to the polarizability P that contains the response of the (quantum) system to an external (classical) perturbation, Γ has to contain the information that the screening in Σ has to act on an electron or hole. Hence, the screened object "feels" an exchange-correlation induced potential. Since we are talking about quasi-particles, this potential is necessarily non-local.

Equation (17) is a two-point equation for the polarizability, like in TDDFT; it is however involving the "polarizability" P_0 of independent quasi-particles. It is hence not a TDDFT, but a sort of hybrid equation. The advantage over TDDFT is that the set of equations still leaves accessible the observables of the original equations like QP energies, whereas this would not be the case in pure TDDFT.

3.3 The link to TDDFT

The link with TDDFT can be made by the fact that the diagonal of G yields the exact time-dependent density $-iG(1,1^+) = \rho(1)$ [19]. $\delta G/\delta\rho = -G(\delta G^{-1}/\delta\rho)G$ leads to

$$iG(1,3)G(4,1^+)\frac{\delta G^{-1}(3,4)}{\delta\rho(2)} = \delta(1,2). \tag{22}$$

Since the same exact density, and hence the same Hartree potential, should also be obtained from the Kohn-Sham potential $v_{KS} = V + v_{xc}$ we can write

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \delta(1,2)\,[v_{KS}(1) - v_{xc}(1)] - \Sigma(1,2). \tag{23}$$

As $\delta G_0^{-1}/\delta\rho = 0$, Eq. (22) becomes

$$P_0(1,3)\chi_0^{-1}(3,2) - iG(1,3)G(4,1^+)\frac{\delta\Sigma(3,4)}{\delta\rho(2)} - P_0(1,3)f_{xc}(3,2) = \delta(1,2), \tag{24}$$

where $\chi_0(12) = \delta\rho(1)/\delta v_{KS}(2)$ is the KS independent particle polarizability and $f_{xc}(1,2) = \delta v_{xc}(1)/\delta\rho(2)$ is the xc kernel of TDDFT. This kernel turns out to consist of two terms, namely $f_{xc}^{(1)}$ and $f_{xc}^{(2)}$, with $f_{xc}^{(2)}$ exactly equal to the $f_{xc}^{\rm eff}$ arising from our previous approach and

$$f_{xc}^{(1)}(1,2) = \chi_0^{-1}(1,2) - P_0^{-1}(1,2). \tag{25}$$

$f_{xc}^{(1)}$ has the effect to change the KS response function into the independent QP one, in particular, to solve the so-called band gap problem. $f_{xc}^{(2)}$ accounts for the electron-hole interaction. This splitting [14] is physically intuitive. Altogether, TDDFT yields then for the irreducible polarizability P,

$$P = \chi_0 + \chi_0(\chi_0^{-1} - P_0^{-1} + f_{xc}^{\rm eff})P. \tag{26}$$

This is equivalent to Eq. (17).

3.4 Approximations in practice

Of course, in spite of this apparent simplification, one stills faces an unsolvable problem, unless approximations are made. The big advantage of writing the formula in the present form is in fact that they suggest rather straightforward approximations. In particular, in order to get an explicit expression for $f_{xc}^{\rm eff}$, we choose a starting approximation for the self-energy, and consistent approximations for the functional derivative of Σ and for G, on the right side of Eqs. (18) and (19). A simple choice could be to take Σ, G and P_0 as derived from a *local* and *adiabatic* xc potential, e.g. the LDA one. This leads of course to the TDLDA and the GWΓ approach of Ref. [7]. A better choice is to start from the GW approximation for Σ, taking W as a screened (e.g. static RPA) Coulomb interaction. For the functional derivative, one can now fully use the experience made using the BSE; in particular, this suggests to neglect also in the present framework the derivative of W with respect to ρ. One still has to find a good approximation for the term $\delta G/\delta\rho$. If one would choose a starting Σ obtained from a self-consistent GW calculation, one would have to evaluate $\delta G/\delta\rho = -G(\delta G^{-1}/\delta\rho)G = G(P^{-1} + (\delta\Sigma/\delta\rho))G$: one would again end up with an integral equation now for $\delta\Sigma/\delta\rho$, similar to the one depicted in Fig. 2(b) of Ref. [14]. However, again based on previous experience in MBPT calculations, one can suppose the Green's function on $\Sigma = iGW$ to be obtained from a suitable local potential, preferably with eigenvalues close to the GW ones. This leads approximately to $\delta G/\delta\rho = GP_0^{-1}G$.

We obtain hence from Eq. (18)

$$f_{xc}^{\rm eff}(3,4) = P_0^{-1}(3,6)G(6,5)G(5',6)W(5,5')G(5,7)G(7,5')P_0^{-1}(7,4). \tag{27}$$

The present derivation is not the first attempt that leads to Eq. (27) [12, 13, 14]. Below, we will show results that we have obtained previously using this formula. However, we believe that the approach outlined here sheds light on the question *why* the former derivations had led to such (unexpectedly) good results: *the physics of the variation of the self-energy upon excitation, which gives rise to the electron-hole interaction, can be captured in terms of density variations only.* This is very important, since it encourages the use of the present scheme also for cases where one wishes to go beyond the above approximations. In particular, it is now clear how any improvement made on the approximations with respect to standard Bethe-Salpeter calculations can be straightforwardly extrapolated to the kernel Eq. (18).

4 Numerical results

Results using the approximation of Eq. (27) or similar approximations have been published by ourselves and by other authors concerning absorption and loss spectra [12, 13], and QP lifetimes [9]. Here we give some of our illustrations.

4.1 Optical spectra

It is instructive to apply Eq. (27) to the calculation of optical spectra of realistic materials, to understand the role of the two parts $f_{xc}^{(1)}$ and $f_{xc}^{(2)}$ of the TDDFT kernel. Figure 1 provides calculations of optical absorption spectrum of bulk silicon using the three highest valence bands and the three lowest conduction bands, a regular grid of 512 slightly shifted k-points in the full Brillouin zone, and an imaginary part in the energy denominators $\eta = 0.1\,\text{eV}$.

As the figure shows, the TDLDA approach fails to reproduce the optical absorption, since both the band gap and the oscillator strengths of the main peaks are wrong. On the contrary, following our comparison between TDDFT and Green's functions, we have to evaluate the two contributions to the TDDFT kernel. The first term $f_{xc}^{(1)}$ accounts for the one-quasiparticle xc effects. It transforms the KS response function χ_0 into the GW independent quasiparticle P_0. The corresponding curve in figure 1 gives the correct band gap. At this level, electron-hole interaction xc effects are still absent, as it is evident in the remaining blue shift of the spectrum and the underestimation in the oscillator strength of the first excitonic peak. The second term $f_{xc}^{(2)}$ accounts for the two-particle xc effects. If the same technical approximations as in BSE are used (use of a static W, neglect of the derivative of W with respect to G), the corresponding curve closely reproduces the solution of BSE, which is the current state-of-the-art concerning calculations of optical absorption.

The same considerations also apply to the example of another system, silicon carbide, whose optical absorption is shown in Fig. 2.

4.2 Quasiparticle energies

It is also interesting to see what one obtains when using this scheme to go beyond the GW approximation for the calculation of band gaps in semiconductors and insulators. Since systematic

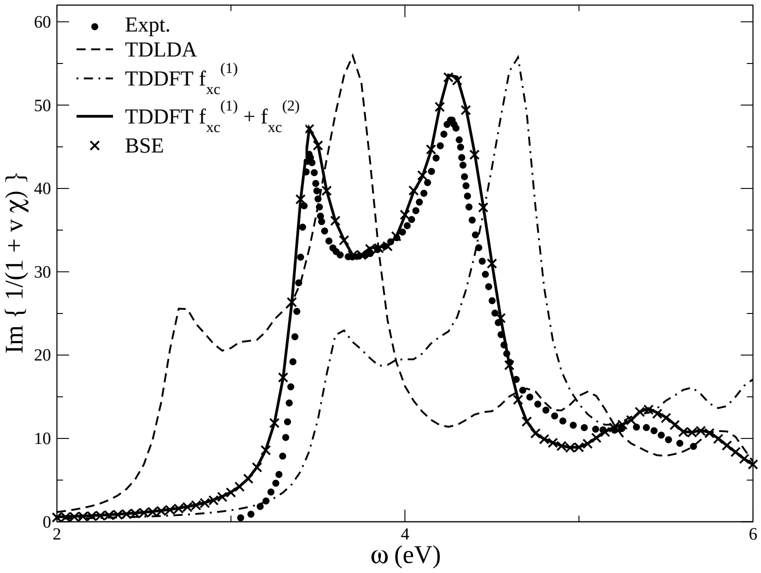

Figure 1: Optical absorption spectrum of bulk silicon calculated within different approximations and compared to experimental data of Ref. [20]. The dashed line represents the TDLDA curve, the dot-dashed line the TDDFT kernel using $f_{xc}^{(1)}$ of the text only, the full line the full TDDFT kernel of the text. The Bethe-Salpeter equation's solution (crosses) and the experimental curve (full circles) are given for comparison.

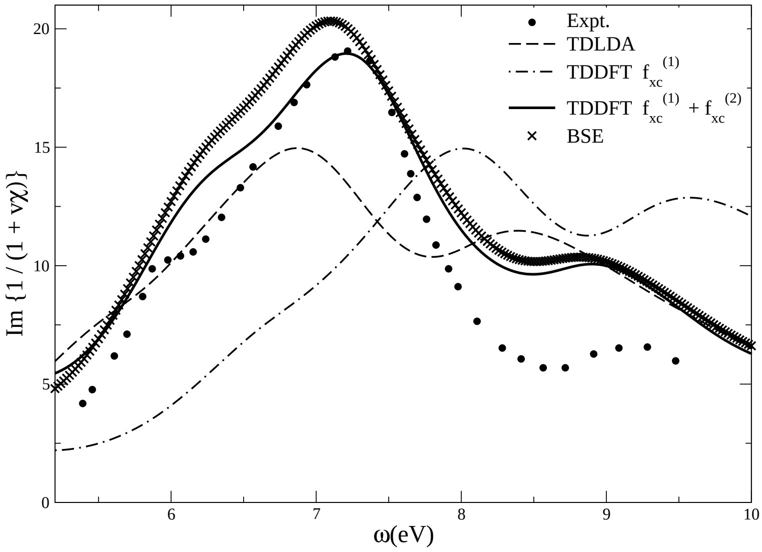

Figure 2: Optical absorption spectrum of bulk silicon carbide calculated within different approximations and compared to experimental data of Ref. [21]. The dashed line represents the TDLDA curve, the dot-dashed line the TDDFT kernel using $f_{xc}^{(1)}$ of the text only, the full line the full TDDFT kernel of the text. The Bethe-Salpeter equation's solution (crosses) and the experimental curve (full circles) are given for comparison.

GWΓ studies in literature are available only for a short-range (LDA) kernel [7], we provide here a discussion on the influence of a *long-range* contribution on QP energies.

For illustration, we present in Tables 2 and 3 results on bulk silicon and solid argon (obviously, the effect of a long-range contribution is particularly interesting in a solid, and silicon and argon represent two extreme cases, the first one with strong screening and continuum excitons, the second one with almost no screening and strongly bound electron-hole pairs).

The first series of results, presented in Table 2, uses LDA as starting approximation for the right-hand side of Eq. (19), whereas the second series in Table 3 uses the static but nonlocal "Coulomb-hole-plus-screened exchange" (COHSEX) approximation to GW [2]. In the latter case, we use the kernel f_{xc}^{eff} given by Eq. (27) which, although approximate, has the correct long-range behavior [12, 13, 22]. Furthermore, LDA wavefunctions are used throughout: we suppose them to be similar to the COHSEX QP ones.

The two tables show the band gap at Γ for both materials under study. The first column gives the band gap that is obtained from the respective starting approximation (i.e. LDA or COHSEX). The second column uses this band structure, and provides the subsequent standard non-self-consistent GW^{RPA}. Columns 3 and 4 show the band gap for the approximations to the self-energy derived in this work, using either $W^{\text{TC-TC}}$ (first part of Eq. (19)) or $\tilde{W}$ (neglect of only $\Delta\Gamma$). Finally, the experimental value is given in the last column [23]. Both materials show similar tendencies. In particular, there is a significant influence of the single-particle energies on the GW^{RPA} (second columns). The choice of COHSEX energies in W simulates the effect of the contribution $f_{xc}^{(1)}$ of Eq. (25). In most cases, the electron-hole vertex correction $f_{xc}^{\text{eff}} = f_{xc}^{(2)}$ in W^{TC-TC} closes the gap (third columns) with respect to RPA. When f_{xc}^{eff} is included according to Eq. (19) in order to evaluate the explicit vertex in $\Sigma = iGW^{TC-TC}\Gamma^{(2)} = iG\tilde{W}$ (fourth columns), there is a strong opening of the gap. Our most complete result is hence determined by a series of cancellations. The overall behavior of both kernels under study (arising from LDA or the non-local COHSEX scheme) is very similar, even though the LDA kernel does not have the crucial, correct long-range contribution [22]. These results roughly justify calculations using the RPA GW form constructed with QP energies instead of KS ones. The $GW\Gamma$ gap turns out to be slightly bigger than the experimental value. In order to obtain improved agreement, one should of course avoid some of the above approximations; in particular we expect the non-locality correction to decrease the gap, since the neglected term should reduce the effect of the external vertex. Those and other more sophisticated numerical calculations (including, e.g., self-consistency in the wavefunctions) are however beyond the scope of this illustration.

5 Conclusions

In conclusion, using the concept of the density as crucial quantity we have derived a complete new set of equations for the many-body vertex, polarizability and self-energy. This approach does not require the solution of integral equations containing a four-point kernel. In particular, the polarizability is directly obtained from a two-point equation, containing a two-point many-body kernel f_{xc}^{eff}, which completely changes the way e.g. excitonic effects can be calculated. The exchange-correlation kernel of TDDFT turns out to differ from f_{xc}^{eff} by a term that is essentially responsible for the gap correction. Our approach explains the success of previously published approximations for the kernel and allows one to go beyond in a systematic way. On top of this progress concerning TDDFT, the approach also opens the way for better approximations to the

	LDA	GW^{RPA}	$GW^{\text{TC-TC}}$	$G\tilde{W}$	Expt.
Si	2.53	3.17	3.08	3.18	3.40
Ar	8.18	12.95	12.64	12.75	14.2

Table 2: Direct gap (in eV) at Γ in bulk silicon and solid argon, calculated using a local approximation (LDA) for the starting self-energy (see text).

	COHSEX	GW^{RPA}	$GW^{\text{TC-TC}}$	$G\tilde{W}$	Expt.
Si	3.64	3.30	3.18	3.32	3.40
Ar	14.85	14.00	14.16	14.76	14.2

Table 3: Same as Table 2, but based on a non-local approximation (COHSEX) for the starting self-energy.

self-energy and other many-body quantities.

These steps forward could be achieved by combining two fundamentally different frameworks. We think that this might be a nice illustration for the strength of a network like Ψ_k, that tries to bring together different communities of people working on similar problems. The present work has in fact benefitted from many formal and informal meetings; in particular, we are grateful for discussions with C.-O. Almbladh, U. von Barth, J. F. Dobson, A. Marini, A. Rubio, G. Stefanucci, R. van Leeuwen, and N. Vast. We also acknowledge support from the the EU's 6th Framework Programme through the NANOQUANTA Network of Excellence (NMP4-CT-2004-500198), and computer time from IDRIS (project 544).

References

[1] P. Hohenberg and W. Kohn, Phys. Rev. **136** B864 (1964); W. Kohn and L. J. Sham, Phys. Rev. **140** A1133 (1965).

[2] L. Hedin, Phys. Rev. **139**, A796 (1965); G. Strinati, Riv. Nuovo Cimento **11**, 1 (1988).

[3] W. G. Aulbur, L. Jonsson, and J. W. Wilkins, Solid State Physics **54**, 1 (1999), and references therein.

[4] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002), and references therein.

[5] P. Streitenberger, Phys. Status Solidi. B **125**, 681 (1984); P. Streitenberger, Phys. Lett. A **106**, 57 (1984).

[6] G. D. Mahan and B. E. Sernelius, Phys. Rev. Lett. **62**, 2718 (1989).

[7] R. Del Sole, L. Reining, and R. W. Godby, Phys. Rev. B **49**, 8024 (1994).

[8] E. L. Shirley and R. M. Martin, Phys. Rev. B **47**, 15404 (1993); R. T. M. Ummels, P. A. Bobbert, and W. van Haeringen, Phys. Rev. B **57**, 11962 (1998).

[9] A. Marini and A. Rubio, Phys. Rev. B **70**, 081103(R) (2004).

[10] F. Aryasetiawan, Phys. Rev. B **46**, 13051 (1992).

[11] E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984).

[12] L. Reining *et al.*, Phys. Rev. Lett. **88**, 066404 (2002); F. Sottile, V. Olevano, and L. Reining, Phys. Rev. Lett. **91**, 056402 (2003).

[13] G. Adragna, R. Del Sole, and A. Marini, Phys. Rev. B **68**, 165108 (2003); A. Marini, R. Del Sole, and A. Rubio, Phys. Rev. Lett. **91**, 256402 (2003).

[14] I. V. Tokatly and O. Pankratov Phys. Rev. Lett. **86**, 2078-2081 (2001); R. Stubner, I. V. Tokatly, and O. Pankratov, Phys. Rev. B **70**, 245119 (2004).

[15] F. Bruneval, F. Sottile, V. Olevano, R. Del Sole, and L. Reining, Phys. Rev. Lett. **96**, 186402 (2005).

[16] E. K. U. Gross and W. Kohn, Phys. Rev. Lett. **55**, 2850 (1985).

[17] R. Del Sole, G. Adragna, V. Olevano and L. Reining, Phys. Rev. B **67**, 045207 (2003).

[18] S. Botti, F. Sottile, N. Vast, V. Olevano, H.-C. Weissker, L. Reining, G. Onida, A. Rubio, R. W. Godby, and R. Del Sole, Phys. Rev. B **69**, 155112 (2004).

[19] R. van Leeuwen, Phys. Rev. Lett. **76**, 3610 (1996).

[20] P. Lautenschlager, M. Garriga, L. Vina, and M. Cardona, Phys. Rev. B **36**, 4821 (1987).

[21] S. Logothetidis and J. Petalas, J. Appl. Phys. **80**, 1768 (1996).

[22] Ph. Ghosez, X. Gonze, and R. W. Godby, Phys. Rev. B **56**, 12811 (1997).

[23] R. R. L. Zucca and Y. R. Shen, Phys. Rev. B **1**, 2668 (1970); R. Haensel, Phys. Rev. Lett. **23**, 1160 (1969).