Ψ_k Newsletter

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

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1 Editorial

The holiday season is reflected in this issue of the Psi-k newsletter, as it is rather short and contains mostly position and workshop announcements, and some abstracts of the recent or newly submitted papers. One item we would like to turn our readers' attention to is the "Call for Psi-k Workshop Proposals for 2007" which can be found at the beginning of the section "News from the ESF Psi-k Programme".

We highly recommend the scientific highlight of this issue which is on "Density functional theory for superconductors" by M. Lüders (Daresbury, U. K.), M. A. L. Marques (Coimbra, Portugal), A. Floris (Berlin, Germany, and Cagliari, Italy), G. Profeta (Cagliari, Italy), N. N. Lathiotakis (Berlin, Germany), C. Franchini (Cagliari, Italy), A. Sanna (Cagliari, Italy), A. Continenza (L'Aquila, Italy), S. Massidda (Cagliari, Italy), E. K. U. Gross (Berlin, Germany).

For more details please check the table of contents of this 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 2006 workshops and hands-on courses (subject to funding).

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

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

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

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

2 News from the ESF Programme

"Towards Atomistic Materials Design"

2.1 Call for Psi-k Workshop Proposals for 2007

Here we would like to repeat the call of Walter Temmerman for workshops, hands-on tutorials and small conferences to be held in 2007 for partial funding by the ESF Psi-k Programme and would like to give you some more detailed information.

The deadline for proposals is

15 September, 2006.

General Information about Psi-k

The coming year will be the last funding year of the present Psi-k Programme "Towards Atomistic Materials Design". Due to good financial planning we will also in this year be able to fund up to 20 Psi-k activities. Therefore I ask all Psi-k members, in particular the working groups, to consider and carefully plan activities for the last year of the ESF Programme. At present we have no funding for 2008, but remaining money can still be spend in 2008.

Collaboration with CECAM

During this year the collaboration of Psi-k with CECAM has been strongly intensified. A total of 11 CECAM/Psi-k Workshops will take place at CECAM in Lyon, jointly funded by Psi-k and CECAM. In addition three Psi-k tutorials on electronic structure calculations will be organized within the Marie Curie Tutorial Series at CECAM, funded by the EU-contract of the Molecular Simulation Network. Thus the collaboration with CECAM is working very well and has increased our funding substantially which will be very important in the future. For these reasons we strongly encourage you to plan joint Psi-k/CECAM activities in 2007. The deadline for CECAM proposals is

15 October, 2006.

Several remarks are worthwhile to add. CECAM likes very much discussion workshops on well focussed topics. Conferences will not be supported. The workshops will take place at CECAM/Lyon. Only well-founded requests for other locations have a chance to be considered. Moreover, CECAM proposals have to be competitive; last year, about 10 proposals were rejected. Therefore, you should give the proposal some attention.

Funding from other sources

There is the possibility for joint workshops with CCP9 in the UK (contact: James Annett, (james.annett@bristol.ac.uk) chairman of CCP9). There is also the possibility for 1 or 2 workshops at the Research Center Juelich, funded jointly by Psi-k and Juelich (contact: Stefan Bluegel, (s.bluegel@fz- juelich.de) or myself (p.h.dederichs@fz-juelich.de)). Finally, I want to mention the German Heraeus-Foundation (www.we-heraeus.stiftung.de) which organises every year about 15 workshops and small conferences at Bad Honneff. Please contact me for more information (next deadline: Sept. 1, 2006; 2 deadlines per year). Having an American co-organiser could allow you to get additional NSF- funding.

Submission of Psi-k proposals

Concerning proposals for ESF-funded workshops, the ESF has last year changed its policy and requires now in all cases a detailed proposal. Therefore we take this over already for the Sept. 15 call, since otherwise you have to write two proposals, one for Psi-k and one for ESF. Therefore submit your proposal by Sept. 15 directly to the ESF-website:

`http://212.234.224.239/asp/form/scmeetings/sc\_form.asp?id=47`.

With best regards,

Peter
(Psi-k Chairman)

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2.2 ESF Programme Workshop Announcements

2.2.1 Joint MolSimu-Psi-k Tutorial ”Quantum Simulation of Liquids and Solids”

within the CECAM MC Tutorial Series.

30 October 2006 to 10 November 2006

Location : CECAM 46 allée d’Italie, 69007 Lyon, France

Organizers:
Evert Jan Meijer (University of Amsterdam, Netherlands)
Rodolphe Vuilleumier (Universitet Pierre et Marie Curie France)
Igor Abrikosov (Linkoping Universuty, Sweden)
Sergei Simak (Linkoping Universuty, Sweden)

Description:

This course is aimed at giving an introduction in the simulation of electronic structure in condensed phase materia, solids and liquids. A first series of lectures will be devoted to the basics of Density Functional Theory and to the solution of the electronic structure problem in solids using plane wave basis sets and Green’s function technique. This part of the tutorial was based on the book by R. M. Martin ”Electronic Structure. Basic Theory and Practical Methods” (Cambridge University Press, Cambridge, 2004). A second series of lecture will then focus on the simulation of liquid systems using ab initio Molecular Dynamics. These will also include an introduction to advanced techniques including simulation of reactive processes in liquids and coupling of quantum and classical simulations (so-called QM/MM).

The morning sessions are lectures introducing the methods and in the afternoons there are computer exercises in which these methods will be applied. During these practical classes the students will run a few simulations using existing packages, like CPMD, KKR-ASA and VASP, to apply the techniques discussed in the morning lectures and be acquainted with these packages. They will also write a simple program to solve a one dimensional Schrodinger equation with a periodic potential using a plane wave basis set. In addition, a miniworkshop will be organized, where participants can present results of their research.

The course does not assume any previous knowledge in molecular simulations. However, elementary knowledge in quantum and statistical physics is assumed.

Support for participation (travel and lodging) is available via the Marie Curie Action MolSimu.

Registration Deadline : Sep. 30, 2006

2.2.2 CompMag 2006

First announcement

“Conference on Computational Magnetism and Spintronics”
CompMag 2006

Place: Jülich, Germany

Dates: October 2nd-4th 2006

Organizers:
Stefan Blügel (IFF, Forschungszentrum Jülich GmbH, Germany)
Silvia Picozzi (CNR-INFM, L’Aquila, Italy)
Laszlo Szunyogh (Budapest Univ., Hungary and Vienna Univ., Austria)

Abstract submission deadline: July 15th 2006

Contact: theory1@fz-juelich.de or
silvia.picozzi@aquila.infn.it

Web Page: Will be opened soon

Sponsors: ESF Programme Psi-k and Forschungszentrum Jülich GmbH

Scientific motivation and objectives

Spintronics, magnetoelectronics and magnetism are currently among the most active research themes in condensed matter physics. These fields are progressing very fast and continue branching into increasingly wider areas of condensed matter. These include strongly-correlated electron systems as well as the connection to semiconductors in terms of diluted magnetic semiconductors, to organic molecules in terms of molecular magnets, to nanotubes and wires in the field of nano-spintronics and to ferroelectric materials in terms of multiferroics.

The main objective of the Jülich conference is to bring together leading scientists in Europe, including also guests from USA and Japan, being active in different fields of Magnetism, in particular, in state-of-the-art first principles calculations. We would like to overview and discuss recent results as well as consult about common progresses for the future.

Topics and invited speakers

The scope of the conference will cover those fields that have been recently gaining increasing importance in magnetism, such as:

- Diluted Magnetic Semiconductors and Half-Metals
- Spin-dependent Transport

- Electronic Correlations
- Multiferroics
- Molecular Magnetism and Nanomagnetism
- Advances in theoretical methods.

A tentative list of invited speakers includes:

David J. Singh (Oak Ridge National Lab., Tennessee)
Mark van Schilfgaarde (ASU, Tempe, Arizona)
Olle Eriksson (Uppsala Univ., Sweden)
Paul J. Kelly (Univ. Twente, The Netherlands)
Balazs L. Györffy (Univ. Bristol, UK)
Tamio Oguchi (Hiroshima Univ., Japan)
Josef Kudrnovsky (Academy of Sciences of the Czech Republic, Prague)
Stefano Sanvito (Trinity College Dublin, Ireland)

3 General Workshop/Conference Announcements

3.1 2nd Annual CNF Fall Workshop: *Building Nanostructures Bit by Bit*

Cornell Nanoscale Science and Technology Facility, Ithaca, NY

October 23th-25th, 2006

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

Sponsored by the National Science Foundation

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

`http://www.cnf.cornell.edu/cnf_fallworkshop2006.html`

Overview: The nanoscale regime provides an important arena where scientific disciplines converge to study systems that can have tremendous fundamental and commercial impact. Modeling and simulation techniques play a crucial role in guiding nanoscale research and interpreting data. However, in order to successfully integrate these computational approaches with experimental tools, researchers must learn about the principles and applications associated with each code.

Format: This workshop will provide morning lectures on the theory behind different approaches followed by *hands-on* sessions on each code. In some cases, the participants will be able to learn directly from the code's creator. Graduate students and young researchers with theory or experimental backgrounds are encouraged to attend. More seasoned members of the field are also encouraged to come and share their knowledge.

Materials, Deposition, Nanoscale Chemistry

Tenative Code List: Quantum Espresso Package (plane wave DFT), Meep (FDTD), MIT Photonic Bands, LAMMPS (Molecular Dynamics), Parsec (Real space DFT), Siesta (Order-N DFT), Elmer (fluidics), Layered KKR (multiple scattering DFT)

Important Dates:
Poster Abstract Deadline: September 15th, 2006
Registration deadline: **September 29, 2006**
Seating is limited to 30-40 participants. Please register early!

3.2 CASTEP Workshop

11th - 15th September 2006

Imperial College London, U. K.

The CASTEP developer's group and the EPSRC National Service for Computational Chemistry Software are pleased to announce a five-day training workshop on the ab-initio simulation package CASTEP. The workshop will be held in the Chemistry Department at Imperial College London from the 11th to 15th September 2006.

Lecturers will be

Dr Stewart Clark (Durham University)
Dr Matt Probert (York University)
Dr Matt Segall (Ltd)
Dr Phil Hasnip (York University)
Dr Chris Pickard (St. Andrews University)
Dr Keith Refson (CCLRC Rutherford Appleton Laboratory)
Dr Barbara Montanari (CCLRC Rutherford Appleton Laboratory)
Professor Nic Harrison (Imperial College)

The aim is to teach the basics of ab-initio atomistic materials simulation using the CASTEP plane-wave pseudopotential code. The workshop will consist of 50% lectures and 50% practical sessions. Topics to be covered include:

* Fundamentals of density functional theory
* DFT in the solid state, kpoints, Brillouin zones
* Plane-wave basis sets
* Pseudopotentials, ultrasoft, norm-conserving and self-consistent
* Simulations using plane-wave DFT

- geometry optimization
- molecular dynamics in various ensembles
- quantum path-integral molecular dynamics
- ab-initio lattice dynamics and spectroscopy
- dielectric properties
- Electric fields, Berry phase and Wannier functions
- NMR properties and chemical shifts

* Ab-initio beyond the LDA and GGA, EXX, hybrid functionals
* Practical aspects of ab-initio calculations
* Application to structural and surface calculations
* Convergence - how to get accurate results.

The workshop is suitable for postgraduate students and researchers who wish to learn the methods of plane-wave pseudopotential simulation and CASTEP. We will assume a reasonable knowledge of quantum mechanics applied to the electronic structure of atoms and molecules and a basic knowledge of solid-state physics.

Further information about CASTEP can be found at the CASTEP web site

http://www.castep.org.

The workshop is open to all users and potential users of CASTEP, and both academic staff and students are welcome. Registration is free for UK academics but participants are expected to pay for their own travel and accommodation. There will be a charge of £150, $280 or 220 Euro for non-UK academics." For more information and to register for the workshop, please visit

`http://www.nsccs.ac.uk/castep_workshop.php`

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3.3 Workshop on "Simulations of Novel Carbon Materiels"

25 - 28 of October

CECAM, Lyon, France

We would like to draw your attention to the workshop "Simulations of Novel Carbon Materiels" organized 25 - 28 of October at CECAM in Lyon.

Scope of the Workshop

The aim of this workshop is to address the computational challenges posed by the continously increasing number of carbon structures. A number of different methods, such as simulations based on empirical potentials, tight-binding calculations or DFT are being used today and it is becoming evident that a combination of these methods is needed to make new progress in the carbon field. The goal of this workshop is therefore to bring researcher working with different aspects of carbon and using a variety of methods together. The workshop is intended to present the latest results on carbon materials, to discuss how different methods can be combined and to address how we can predict new carbon structures.

Time and Place

The Workshop will take place at the CECAM in Lyon from Wednesday 25th to Saturday 28th October 2006. The program will start in the early afternoon of Wednesday and finnish by lunch time on Saturday.

Form of the workshop

The workshop will contain lectures by invited speakers who are listed below. The workshop is also open for contributions and there will be a poster session, where all participants can present recent results in poster form.

List of Invited speakers

Bernard, Stephane, CEA-DAM, France
Blas, Xavier, Universit Claude Bernard-Lyon 1, France
Bolton, Kim, Goteborg University, Sweden
Charlier, Jean-Christophe, Universit Catholique de Louvain, Belgium
Colombo, Luciano, INFM-SLACS, Italy
Crespi, Vincent, Penn State University, USA
Galli, Guilia, University of California, Davis, USA
Gillet, Phillipe, Ecole Normale Suprieure de Lyon, France
Heggie, Malcolm, University of Sussex, UK

Katsnelson, Mikhail I., Radboud University Nijmegen, Netherlands
Kaxiras, Efthimos, Harvard University, USA
Lindan, Phil, University of Kent UK
Los, Jaan H., Radboud University Nijmegen, Netherlands
Louie, Steven G., University of California, Berkeley, USA
Marks, Nigel A., University of Sydney, Australia
Meijer, Evert J., University of Amsterdam, Netherlands
Buongiorno Nardelli, Marco, North Carolina State University, USA
Nieminen, Risto, Helsinki University of Technology, Finnland
Scandalo, Sandro, The Abdus Salam ICTP, Italy
Seifert, Gotthard, TU Dresden, Germany
Tomanek, David, Michigan State University, USA

van Duin, Adri, California Institute of Technology, USA

Application

Application for participation can be made through the CECAM webpage. Deadline for application for participation is 1st of July. Applications after this date can only be accepted if place is still available.

More information about the workshop can be found on the CECAM webpages:

http://www.cecam.fr .

On behalf of the Organizers

Dr. Johan M. Carlsson and Prof. Annalisa Fasolino

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3.4 3rd International Workshop on DFT in Algeria

2 - 4 May 2007

Eden Airport Hotel, Oran, Algeria

Website: http://adft.univ-tlemcen.dz

The Algerian Materials Research Society jointly with the CMSL laboratory of the University of Sidi Belabbes, and the LEPM Laboratory of the University of Tlemcen, are organizing the third International Workshop on DFT applied to metals and alloys. The workshop will take place at Eden Airport Hotel, Oran, Algeria, on the 2nd to 4 th of May 2007.

DFT calculations now commonly play an important role in materials research programs, where they provide qualitative insights into physical processes and quantitative information used in simulations of macroscopic systems. The prevalence of DFT calculations has better revealed deficiencies in metals and alloys. At the same time, the increasing capability and importance of DFT calculations has created greater urgency fro developing more accurate techniques. Because and DFT and related techniques are expected to play an increasingly important role in the future research programs, we feel timely to bring together leading theorists and practitioners to learn about DFT and related techniques in metals and alloys and discuss ideas for developing improved approaches.

Topics Covered:

1) Development of Ab initio electronic- structure methods
2) First principles calculations of structural and electronic properties of metals and alloys
3) Atomistic calculations of defect structures
4) Development of equation of state models
5) Dynamical field theory calculations
6) Dynamic fracture and plasticity in metals
7) Multiscale modelling of Metals and Alloys behaviour
8) Atomistic simulations of metals and alloys under extreme conditions of pressure and/or temperature
9) Atomistic simulation of rapid solidification , molecular dynamics
10) Quantum Monte Carlo
11) Mechanical properties of metals and alloys using DFT calculations
12) Liquid and amorphous metals and alloys
13) Design and development of graphical user interface and data analysis tools
14) Data Mining
15) Topology Theory, charge density, Bader critical point approach

Professor Aourag Hafid
Physics Department
University of Tlemcen, Algeria

http://heberge.univ-tlemcen.dz/˜aourag/

4 General Job Announcements

Postdoctoral Position

”Ab-initio Calculations in Mineral Physics” Condensed Matter Physics Department, Universidad del Pais Vasco, Bilbao (Spain)

A postdoctoral position to perform ab-initio calculations in mineral physics will become available soon at the Condensed Matter Physics Department of the Universidad del Pais Vasco, in Bilbao (Spain).

The position is funded by the Spanish Ministry of Education in the framework of the European Science Foundation EUROCORES Eurominsci program. The project, ”Ordering of Ions in Minerals”, involves researchers from:

- Bilbao (JM Perez Mato, K. Friese, A. Grzechnik): ab-initio calculations, superspace analysis methods, high-pressure research, state-of-the art crystallographic structure determination.
- Innsbruck (V. Kahlenberg): high-pressure synthesis, structural analysis.
- Bochum (M. Fechtelkord): NMR spectroscopy.
- Prague (V. Petricek): refinement of non-standard structures.
- Copenhaguen (T. Balic-Zunic): mineralogical analysis.

The project is led by Alberto Garcia (soon to move to the Materials Science Institute in Barcelona, but with close ties with the Bilbao group).

The successful candidate will join the group in Bilbao, performing ab- initio or in general first-principles-based calculations to analyse the relative stability of different ionic orderings in representative minerals, to predict and suggest new structural configurations, and to study related properties. It is expected that there will be strong interaction with the other nodes in the project, including short stays.

Prospective applicants must hold a Ph. D. degree in physics, chemistry, materials science, or related field. Experience with density functional calculations, numerical methods, and programming using Fortran, is essential. Familiarity with other relevant methods (such as the Monte Carlo simulation of effective hamiltonians) is a plus.

Salary is at the level of a starting associate professor (around 30,000 EUR gross p.a.), through a contract which also includes the standard Spanish health benefits and social-security contributions. The appointment is in principle for two years, with an initial period of one year extended by mutual agreement.

Interested candidates should contact Alberto Garcia (wdpgaara@lg.ehu.es) or J.M Perez Mato (wmppemam@lg.ehu.es), attaching a CV and the names and contact information of two references.

Ph. D. Position

King's College London (KCL), U.K.

Applications are invited for a Ph. D. position related to ab initio and semiclassical modelling of large organic molecules on crystal surfaces, the kinetics of their self-assembly and theoretical investigation of their manipulation with scanning probe methods. The project is a part of a bigger EPSRC project on *Supramolecular Self-assembly of 1-10nm templates for biofunctional surfaces, quantum information processing and nanoelectronics. Our partners include a number of well-known theoretical and experimental groups in the UK, and the work on the project will be done in a close collaboration with them.*

The Ab Initio Modelling of Complex Systems group at KCL has an attractive working environment in the centre of London and excellent computational facilities.

The position can be filled immediately. The funding is available for the period of up to 4 years.

Informal inquiries are welcomed and should be directed to Dr. Lev Kantorovich (email: lev.kantorovitch@kcl.a
tel: (+44) (0)20-78482160, fax: (+44) (0)20-8482420).

The closing date for applications is 31st August 2006.

Equality of opportunity is College policy.

Postdoctoral Scholar in Condensed Matter Physics
Department of Physics and Astronomy, Ohio University, Athens

Applications are invited for a post-doctoral scholar in condensed matter theory. An ideal candidate will have knowledge of first principles electronic structure calculations and transport theory. The successful candidate will join an active group working on the physics of disordered materials, perform basic research on transport in amorphous and defective materials, and will apply the techniques to high Temperature Coefficient of Resistance materials including amorphous silicon materials and vanadium oxides. The work will be carried out in collaboration with several experimentalists funded by the same program. The search will continue until the position is filled. Initial appointment will be for one year with an additional year upon joint agreement. A longer term appointment may be possible. The position is available immediately. For additional information, see http://www.phy.ohiou.edu/ drabold/research.html

Please submit a full CV and arrange for three letters of reference to be sent by email to drabold@ohio.edu

Address 19 June to 1 December 2006:

Prof. David A. Drabold
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Post-Doctoral Position
Institute of Nuclear Physics of Orsay, FRANCE

A post-doctoral position in computational materials science for one year (extendable to a second year) is available at the Institute of Nuclear Physics of Orsay (FRANCE, nearby Paris). The starting date is October first, 2006.

The candidates should have deep knowledge in ab initio calculations based on DFT, as well as a good experience with modelling codes as Gaussian03 and/or VASP. Accomplished research work in the field of the adsorbate-surface interactions with cluster and/or periodic approaches is highly desirable.

This project is funded by the French National Research Agency (ANR). The candidate will join the theoretical team of the Nuclear Physics Institute of Orsay and will also have to collaborate with our theoretical French partner groups.

The successful candidate will have to deal with the theoretical part of a general environmental study of the migration of toxic elements in the geosphere (radiotoxic elements are of primary importance in the field of a deep geological storage of nuclear wastes).

In this study, the considered surface is the aluminium hydroxide (Al(OH)3, gibbsite). The adsorbates under interest are water molecules, an oxocation (UO22+) and two oxoanions (SeO32- and SeO42-).

The main goals of the theoretical part of this project are:

1) The modelling of the most stable faces of the Al(OH)3 surface with cluster as well as periodic approaches.

2) The study of the water interaction with these faces.

3) The investigation of the UO22+, SeO_{32}^{-} and SeO_{42} adsorptions.

Theoretical results will be correlated with experimental data obtained by our partner teams (spectroscopic techniques: XPS, DRIFT, SHG, Raman, TRLFS, and XAS).

Interested candidates are invited to send:

(1) a full CV,
(2) a list of publications,
(3) two recommendation letters

to Jerome Roques (roques@ipno.in2p3.fr)

Postdoctoral Research Positions in Computational Materials Physics/Chemistry

National Renewable Energy Laboratory, Golden, Colorado

We at the National Renewable Energy Laboratory (http://www.nrel.gov/cms/) invite applications for a total of three or four theoretical postdoctoral positions, available immediately. Initial assignment is for a year, but renewable upon funding availability, performance, and mutual agreement up to a total of three years. Research direction will be one of the followings: (1) the development of first-principles methods for van der Waals interaction - a new program that requires strong ability both in basic theory and in software development. (2) The application of state-of-the-art first-principles methods to a broad range of impurity and defect related issues in wide-gap, low-dimension, and/or organic semiconductors, and to the storage of hydrogen in solid-state materials. The starting salary is US$45-55K/year depending on the qualification. Candidate should send curriculum vitae, a list of publications, and arrange three reference e-mail letters to one of the following persons:

Yong-Hyun Kim (`yong_hyun_kim@nrel.gov`)
Yufeng Zhao (`yufeng_zhao@nrel.gov`)
Shengbai Zhang (`shengbai_zhang@nrel.gov`)

National Renewable Energy Laboratory
1617 Cole Blvd.
Golden, CO 80401, USA

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

POSTDOCTORAL FELLOWSHIP

Uppsala University, Sweden

A postdoctoral position is available in the Theoretical Magnetism Group, Department of Physics, Uppsala University, Sweden, starting October 1, 2006, for a period of two years.

The research will be on electronic and magnetic properties of novel functional materials, using ab initio Density Functional Theory-based calculations. Theoretical modeling of properties like magneto-thermal and photomagnetic transport will be performed, on the basis of ab initio calculations. The research will be conducted together with experimental groups in Europe within a multidisciplinary EU-funded research collaboration.

The candidate is expected to have an excellent background in theoretical or computational physics. Experience with large scale ab initio calculations is desirable, as is also the ability to collaborate in a multidisciplinary environment.

At the Physics Department of Uppsala University a strong research environment exists in computational material science and condensed matter theory, which provides an excellent scientific working place for the postdoc.

To apply, please send a CV, list of publications, and names of two reference persons, before September 15, 2006, to Peter Oppeneer, at the address given below.

Peter Oppeneer,
Assoc. Prof., Dept. of Physics,
Uppsala University, Box 530
S-751 21 Uppsala, Sweden
peter.oppeneer@fysik.uu.se

Ph. D. Studentship : ”Application of electronic-structure calculations to the description of technological materials at the nanoscale”

Donostia International Physics Center (DIPC) Paseo Manuel de Lardizabal, 4 PO BOX 1072 20018 San Sebastian/Donostia, SPAIN

The Donostia International Physics Center (DIPC) is a world-leading laboratory in the theoretical description of processes at the nanoscale using electronic structure methods. DIPC is looking for a highly qualified research student with good command of English, interested in pursuing research studies leading to the Ph. D. degree. A full studentship is available for suitable candidates interested in starting research studies as soon as possible after April 1, 2006 and not later than September 30, 2006. The studentship provides 15,000 euros per annum after taxes (at current rates).

The studentship is part of an ETORTEK research grant from the Basque Government, awarded to a 3-years research project entitled ”Nanomaterials for multidisciplinar applications”. Our contribution to the project concerns computer simulations and modelling in the field of atomic scale manipulation and characterization of nanostructures related to problems in cements and nanocomposites based on carbon nanotubes. The simulations and modelling will primarily be based on density functional theory. The proposed work will be carried out in close collaboration with experimental groups in technological centers.

The student will work under the supervision of Dr. D. Sanchez-Portal and Dr A. Ayuela.

Candidates should have (or be about to receive) a Masters degree or equivalent in physics or chemistry and should be highly qualified. Experience of computational physics/chemistry is essential. Candidates should be able to demonstrate good command of English and good understanding of condensed matter, sound mathematical background and aptitude for fundamental research topics that are of industrial relevance. Applications should be made to Dr. A. Ayuela via e-mail: swxayfea@sw.ehu.es ¡mailto:swxayfea@sw.ehu.es¿ or by phone 943-01-5421. Please mention that you are interested in this studentship in your application. Applicants should send their CV with a few references.

Further information about DIPC can be found at

http://dipc.ehu.es.

Closing Date: September 1, 2006 and continues until post is filled

Postdoctoral Position
University of Maryland

A postdoctoral position is available starting September 2006 to work with D. Kosov at the University of Maryland. The research projects focus on the applications of ab initio calculations for the investigation of charge transport and photoexcitations at interfaces. Much of our research is done in close collaboration with experimentalists.

We are interesting in somebody who can help us with the following projects:

(1) Development of Hartree-Fock/Non-equilibrium Green's function based transport code to compute current-voltage characteristics of nanostructures

(2) DFT/Non-equilibrium Green's function calculations of molecular conductivity for particular systems

(3) DFT calculations of molecules chemisorbed on surfaces

Profound knowledge of electronic structure methods and programming experience are required. Familiarity with modern electron transport theory (non-equilibrium Green's functions) and standard codes (CPMD, SIESTA, Trans-SIESTA) are desired. Postdoctoral position is available for a year with a possibility of extension.

Interested applicants should contact D. Kosov (dkosov@umd.edu)

Daniel Kosov, Assistant Professor
Department of Chemistry and Biochemistry
University of Maryland
College Park, MD 20742-2021
Phone: 301-405-1384
Fax: 301-314-912
http://www.chem.umd.edu/groups/kosov/
E-mail: dkosov@umd.edu

Two Postdoctoral Positions in Computational Materials Science

University of Nebraska

Two postdoctoral positions in computational materials science are immediately available to work with Kirill Belashchenko and Renat Sabirianov at University of Nebraska's Lincoln and Omaha campuses. The research work will be in the studies of electronic structure and transport in magnetic materials and nanostructures with applications in spintronics, particularly at finite temperatures. Powerful computing resources are available. We are seeking highly motivated applicants with experience in computational materials science, especially involving electronic structure calculations. The initial appointment will be for one year, with a possible extension for a second year upon mutual agreement and funding availability. Candidates must have a doctoral degree in a field closely related to computational materials science. Competitive annual salary will depend on qualifications and experience. Interested candidates should complete an initial online application at http://employment.unl.edu (Requisition #060460) and then send an application letter, CV, list of publications, and contact information for at least two references to Kirill Belashchenko by email or regular mail.

Review of applications will begin July 10, 2006, and will continue until suitable candidates are found. UNL is committed to a pluralistic campus community through AA/EO. We assure reasonable accommodation under the ADA; contact Kirill Belashchenko at (402)472-2770 for assistance.

Kirill Belashchenko, Assistant Professor
Department of Physics and Astronomy
University of Nebraska-Lincoln, Lincoln, NE 68588-0111
Phone: (402)472-2396
Fax: (402)472-2879
Email: kdbel@unlserve.unl.edu

Team Member

Ab Initio High Throughput Computing and Computational Materials Science

Computational Modeling Consultants, MIT

Computational Modeling Consultants, a company started by two MIT researchers is looking for a qualified individual to work with a team on the largest computational materials design project ever initiated.

With modern ab initio methods it is now possible to construct virtual materials testing environments and evaluate the properties of materials without the need to synthesize them. CMC is looking for a team member interested in the application of modern computational quantum mechanics (Density Functional Theory) to design materials for corporate clients.

An ideal candidate for this position is self-motivated, can work well in a team, and is good at formal thinking and problem solving. Recommended qualifications include coding and scripting on Linux clusters (especially Java or equivalent is desirable). Knowledge of typical Density Functional Theory codes is a plus, as is any knowledge of materials science.

Position is for approximately 1 year (full-time or part-time considered). Available immediately.

For more information contact Kristin Persson phone: 617-252-1507 or email:cmchire@lanai.mit.edu.

POSTDOCTORAL POSITION

Strategic Research Centre for Materials Science for Nanoscale Surface Engineering at Linköping University, Sweden

A postdoctoral position in theoretical condensed matter physics is available starting October 1, 2006 at the Department of Physics, Chemistry and Biology, Linköping University, Sweden.

This project is part of the newly established Strategic Research Centre for Materials Science for Nanoscale Surface Engineering MS2E supported by the Swedish Foundation for Strategic Research, and belongs to a Competence Platform "Computational Tools for Materials Science; Multiscale Simulations". The goal for the project is to integrate theory and experiments in all projects within MS2E, to develop further our competence in atomistic simulations at the nanoscale, and to transfer the competence to experimental groups within the Centre. The objectives are to expand our Competence Platform with an ability of an expert evaluation of the proper theoretical tools to be used for the studies of materials and phenomena relevant for MS2E activities, e.g. hard thin film coatings, multilayer systems relevant for X-ray mirrors, alloy wide-gap nitrides, etc. The theory group will also participate in the development of the user-friendly simulation packages for the electronic structure calculations, molecular dynamics and statistical mechanics simulations of the phase stabilities of materials, fitted to the particular tasks of the MS2E.

We are looking for a strong candidate with Ph. D. in physics and substantial experience in Density Functional calculations and/or statistical mechanics/molecular dynamics simulations. Demonstrated ability of programming in Fortran and /or C++ are requested. Interested candidates should submit their CV, including names of at least two references and the list of publication, before August 31, 2006 to

Prof. Igor A. Abrikosov,
Department of Physics, Chemistry and Biology (IFM),
Linköpings University,
SE-581 83 Linköping, Sweden,
e-mail: igor.abrikosov@ifm.liu.se,
`http://www.ifm.liu.se/~abrikos/`

Postdoctoral Position

"Computational Spintronics Group" in the School of Physics at Trinity College Dublin (IRELAND)

One postdoctoral position is available in the "Computational Spintronics Group" in the School of Physics at Trinity College Dublin (IRELAND). The project is part of a EU-funded network on Molecular Spintronics, whose main focus is to investigate spin-transport through molecules, including magnetic molecules. The network comprises both experimental and theoretical groups at Trinity College Dublin (Ireland), the National Nanotechnology Laboratory (Italy), the University of Hamburg (Germany) and the Nijmegen Institute for Molecules and Materials (The Netherlands).

The project involves the theoretical investigation of spin-transport through various molecules and it will provide theoretical insights into the experimental activity of the network. Quantitative calculations of the I-V characteristics of molecular junctions will be obtained with the code Smeagol (www.smeagol.tcd.ie), which combines density functional theory with transport theory. Some development aspects of the Smeagol code will be also part of the project and in particular an extension of the present capabilities to multi-terminal geometries is planned. Finally properties of novel molecules synthesized within the network will be investigated with quantum chemistry methods (the TURBOMOLE code).

The successful candidate will be based in Dublin, working with Dr.Sanvito, and she/he will frequently visit the various partners in the network, in particular the group of Dr. della Sala at the National Nanotechnology Laboratory. The position is tenable up to two years and eventually renewable for a third one, with starting date in October 2006 or at a mutually agreed convenient date.

Applications are accepted until the position will be filled. We are seeking for strongly motivated researchers with previous experience in electronic structure methods including quantum chemistry and/or transport theory. Candidates are invited to send a CV together with the full address of two potential referees (including e-mail) by post or e-mail to Dr.Sanvito at the address below.

Dr. Stefano Sanvito
Director of Graduate Studies School of Physics
School of Physics
Trinity College Dublin
Dublin 2, IRELAND
Ph. : +353-1-608306
Mob.: +353-87-414678
Fax.: +353-1-6711759

http://www.tcd.ie/Physics/People/Stefano.Sanvito/

Ph. D. Studentship

”Computational Spintronics Group” in the School of Physics at Trinity College Dublin (IRELAND)

One Ph. D. studentship is available in the ”Computational Spintronics Group” in the School of Physics at Trinity College Dublin (IRELAND). The project is part of a EU-funded network on Molecular Spintronics, whose main focus is to investigate spin-transport through molecules, including magnetic molecules. The network comprises both experimental and theoretical groups at Trinity College Dublin (Ireland), the National Nanotechnology Laboratory (Italy), the University of Hamburg (Germany) and the Nijmegen Institute for Molecules and Materials (The Netherlands).

The project involves the theoretical investigation of spin-transport through various molecules and it will provide theoretical insights into the experimental activity of the network. Quantitative calculations of the I-V characteristics of molecular junctions will be obtained with the code Smeagol (www.smeagol.tcd.ie), which combines density functional theory with transport theory. Some development aspects of the Smeagol code will be also part of the project. Finally properties of novel molecules synthesized within the network will be investigated with quantum chemistry methods (the TURBOMOLE code).

The successful candidate will be based in Dublin, working with Dr. Sanvito, and she/he will frequently visit the various partners in the network, in particular the group of Dr. della Sala at the National Nanotechnology Laboratory. The position will start in October 2006 or at a mutually agreed convenient date. Applications are accepted until the position will be filled. We are seeking for strongly motivated students with solid theoretical background and passion for research work. The knowledge of electronic structure methods including quantum chemistry and/or transport theory will be considered as an advantage. Candidates are invited to send a CV together with the full address of two potential referees (including e-mail) by post or e-mail to Dr. Sanvito at the address indicated below.

Dr. Stefano Sanvito
Director of Graduate Studies School of Physics
School of Physics
Trinity College Dublin
Dublin 2, IRELAND
Ph. : +353-1-608306
Mob.: +353-87-414678
Fax.: +353-1-6711759

http://www.tcd.ie/Physics/People/Stefano.Sanvito/

M.Sc. in High-Performance Computing
School of Mathematics, Trinity College, Dublin

The School of Mathematics of Trinity College, Dublin offers a one-year full-time, taught postgraduate course in High-Performance Computing. The course provides practical training in this rapidly emerging sector. The programme is taught in close collaboration with the Trinity Centre for High-Performance Computing (http://www.tchpc.tcd.ie) and the Schools of Physics and Chemistry and has close links to the IITAC interdisciplinary research project in computational science.

The M.Sc. provides practical training in the use of the large-scale computing resources used to carry out advanced simulations of complex systems found in many areas of science, applied mathematics and finance. Topics covered include hardware and software technology, software optimisation, parallel computer architectures and programming methods. Along with these skills, students will learn the necessary advanced mathematical skills to work on large simulations through a number of optional modules. Students will have access to the large parallel computing resources managed by the Trinity Centre for High-Performance Computing as well as a dedicated computing laboratory. The course includes substantial practical work and involes successful completion of a large project.

The successful student will have career opportunities in advanced mathematical modelling, simulation and forecasting and large-scale computing resource management. Technical computing methods are widely used in research and simulation in mathematics, physics, chemistry, engineering and finance providing a wide range of career options.

A primary degree at the I or II.i level (or equivalent) in a scientific or financial mathematics field is normally required. The closing date for applications is 31st July. Application information may be obtained from the Graduate Studies Office of Trinity College.

For enquiries, please contact the course co-ordinator:

Dr. Michael Peardon
School of Mathematics
Trinity College
Dublin 2
Ireland

mjp@maths.tcd.ie

For further details see the course web-pages at:

http://www.maths.tcd.ie/hpcmsc

Ph. D. Position

University of Antwerp, Belgium

A Ph. D. position is available in the condensed matter theory (CMT) group for 4 years starting from October 2006. The aim of the project is to study the electronic properties of new transparent conducting oxides by means of ab initio electronic structure calculations. The CMT group is specialized in the computational study of the electronic and structural properties of materials e.g. semiconductor nanostructures, amorphous carbon, etc., and has several high performance computer clusters to its disposal.

The candidate should have a master's degree in (applied) physics, chemistry, engineering or materials sciences and a solid background in computational techniques and condensed matter physics. The position also involves teaching duties within the physics department, therefore the candidate should have sufficient knowledge of the Dutch language.

For more information on the project, contact Prof. F. Peeters (Francois.Peeters@ua.ac.be), Prof. B. Partoens (Bart.Partoens@ua.ac.be), or Prof. D. Lamoen (Dirk.Lamoen@ua.ac.be).

Application forms can be downloaded from http://www.ua.ac.be/vacatures.

Postdoctoral Position

Theory and modelling of potential high-gravimetric density hydrogen storage materials

Departments of Materials and Chemistry, University of Oxford, U. K.

An 18 month postdoctoral position is available in the Departments of Materials and Chemistry at the University of Oxford to work with Professor David Pettifor, Professor Peter Edwards, Dr. Martin Owen Jones and Dr. Ralf Drautz on the 'Theory and modelling of potential high-gravimetric density hydrogen storage materials'. This is part of an EPSRC-DTI Technology project on 'High throughput synthesis and screening of novel hydrogen storage materials', involving researchers from the Inorganic Chemistry Laboratory and the Materials Modelling Laboratory at Oxford University, the CCLRC's Rutherford Appleton Laboratory, and the spin-out company Ilika Ltd.

Please follow this link for a detailed project description and information on how to apply:

http://www.materials.ox.ac.uk/vacancies

Further information on the project partners may be found at:

Oxford Materials: http://www.materials.ox.ac.uk/
Oxford Chemistry: http://www.chem.ox.ac.uk/
CCLRC: http://www.cclrc.ac.uk/
Ilika Ltd.: http://www.ilika.com/

Dr Ralf Drautz
Department of Materials
University of Oxford
Parks Road
Oxford OX1 3PH

Tel +44 1865 273731
Fax +44 1865 273789

Ph. D. Research Position

Netherlands Institute for Metals Research (NIMR)
Delft, 2628 CD, (Zuid-Holland)

Job description: Ph. D. Researcher MC5.05239

Carbides form a great variety of crystal structures in steel and alloying elements can strongly affect their occurrence, structure type and morphology. This in turn has far-reaching effects on the properties of alloyed steel. Using state-of-the-art tools in computational materials science (alloy theory) based on electronic density functional theory and statistical thermodynamics the effects of alloying elements on the relative thermodynamic stability and the competition between carbide structures are elucidated.

The ultimate objective is to advance the modeling of the microstructure and physical properties of steels during processing and during actual use.

The Ph. D. researcher will carry out density functional calculations on a wide variety of carbides and determine how alloying elements affects the thermodynamic and structural parameters. He/she will implement these results in a thermodynamic model that predicts which carbides are present in steel as a function of composition, temperature and processing conditions. Furthermore, results will be analyzed so that a deeper understanding of tendencies and trends can be extracted.

Modeling tools will be developed in cooperation with a steel producing company and will be used industrially for optimization of compositions and treatment procedures of TRIP and other advanced steels. The Ph. D. researcher will cooperate closely with the Industrial partner and will undergo a one-month traineeship at the Industrial partner.

Requirements

The Ph. D. candidate must have:

- A Master degree in Materials Science, Physics, Chemistry or equivalent with graduate level quantum mechanics, thermodynamics and elementary solid state physics or metallurgy
- Interest in computational research, scientific curiosity and be comfortable in a unix/linux environment
- Good English language skills (speaking, reading and writing)
- Good communicative abilities

We are looking for a Ph. D. candidate that feels comfortable working with and interacting with academic and industrial collaborators.

The vacancy is located at the Delft University of Technology (TUD) and the Ph. D. Researcher will obtain a doctorate degree awarded by the TUD.

All applicants are asked to submit a list of grades of their Master's study and a statement of purpose.

Please note that the deadline to apply for this vacancy is 7 August 2006.

Organization: Netherlands Institute for Metals Research NIMR

Conditions of employment

Employment basis: Temporary for specified period
Duration of the contract: 4 years
Maximum hours per week: 40

Additional conditions of employment:

When fulfilling a Ph. D. position at the NIMR, you will be given the status of Ph. D. Researcher. You will have employee status and will be eligible for all the employee benefits offered by the NIMR. The contract is for 4 years. Gross salary for the first year is EUR 2,120 gross per month. This amount increases to EUR 2,447 gross per month in the fourth year. Your thesis should be completed at the end of your four year term with the NIMR. A training programme is part of the agreement. You and your supervisor will draw up a plan for any additional training and supervision you specifically need.

Additional Information

Or additional information can be obtained through one of the following link: http://www.nimr.nl/

Application

You can apply for this job before 07-08-2006 by sending your application to:

E-mail address: hrm@nimr.nl

Only applicants who submitted their cv, statement of purpose and their Master's grading list, will be taken into consideration.

When applying for this job always mention the vacancy number AT/MC5.05239.

Graduate and Postdoctoral Positions at Imperial College, Oxford and Cambridge

Five postdoctoral- and four Ph. D. positions are being filled within the project 'Alloys by Design: application to nickel-based superalloy turbine blades'. The EPSRC-funded project is a collaboration between Imperial College, Oxford and Cambridge with the full support of Rolls Royce and Siemens. State-of-the-art multi-scale materials modelling will be used to guide the design of a new Ni-based superalloy suitable for application in future aircraft engines. Members of the consortium are Roger Reed (coordinator), David Pettifor, Mike Finnis, Peter Lee, Cathie Rae, Fionn Dunne, David Dye and Ralf Drautz.

The following three projects are currently being advertised. Please follow the links for a detailed project description and information on how to apply, or contact Ralf Drautz (ralf.drautz@materials.ox.ac.uk) for further information.

3 and a half- years Postdoc (Oxford):
MML PDRA for the atomistic simulation of novel Ni-based superalloys for gas turbine blades

`http://www.materials.ox.ac.uk/vacancies/index.htm#Post-doctoralResearchers`

3 years PostDoc (Cambridge):
Modelling dislocation/precipitate interactions under creep conditions

`http://www.jobs.ac.uk/jobfiles/RF049.html`

DPhil project (Oxford):
Modelling topologically close-packed (TCP) phases in nickel-based superalloys

`http://www.materials.ox.ac.uk/postgraduate/newprojects.html#funded10`

Dr Ralf Drautz
Department of Materials
University of Oxford
Parks Road
Oxford OX1 3PH

Tel +44 1865 273731
Fax +44 1865 273789

Ph. D. Position

Max Planck Institute for Polymer Research (MPIP), Mainz, Germany

A Ph. D. position is available at the theory group of the Max Planck Institute for Polymer Research (MPIP), Mainz, Germany (www.mpip-mainz.mpg.de) to participate in the project

”Morphology and structure formation in multicomponent macromolecular systems supported by inorganic substrates”

The position is a part of a broad collaboration program between Germany and Korea related to electronic structure/charge transport of organic macromolecules. Successful participation in the study and student exchange programs (between Mainz and Seoul) is required. PhD program usually takes 2.5 years including first 6 months of probation period.

We welcome applications of highly qualified graduates with a Diploma, a Master's degree or comparable qualification in Physics, Chemistry, Materials Science, and adjacent fields. A strong interest for multidisciplinary research is required. Good knowledge of the English language, both spoken and written, is essential. Due to the international character of the project, international students are especially encouraged to apply.

The position is available starting from November 1st, 2006.

Your application should contain the following documents:

* cover letter outlining the background of the application
* resume / CV
* certificates and references of completed course work
* certificate of scientific degree

Letters of recommendation and a publication list are appreciated.

Please send your documents electronically to Prof. Kurt Kremer (Email: kremer@mpip-mainz.mpg.de).

After receipt and evaluation of the documents, applicants will be notified wether they are considered for an interview and presentation of their recent scientific work.

MPIP is seeking to increase the fraction of female staff in academia. Qualified women are therefore especially encouraged to apply.

Fellowships, Isfahan University of Technology, Iran

Fellowships are available in Isfahan University of Technology. 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 three years. Following such a mission, the ICTP and IUT have agreed to support the below mentioned fellowships for the year 2006:

a). 6 Fellowship to young researchers (possess a PhD degree or at the final stage of getting it) from the Regional countries to come and work in the Centre as medium term visitors (10-12 weeks).

b). 2 Fellowship to young researchers from former Soviet Union countries to come and work in the Centre as medium term visitors (10-12 weeks).

c). 3 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, 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 +98-311-3913711 (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 to 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. Investigation of the surfaces of Co2MnSi Heusler alloys as a novel material for spintronic applications and also the study of its interface with GaAs substrate.
2. Theoretical study of the structural and electronic properties of Co2Cr0.5Fe0.5Al alloy and its interface with GaAs.
3. Theoretical study of CO absorption on Pt surface.

Postdoctoral Position

LENS/FOTON Laboratory, UMR6082 CNRS, INSA de Rennes, France

A postdoctoral position is opened in our laboratory for one year (2006/2007). It could be also converted into a Ph. D. position for two years (2006/2007, 2007/2008) jointly directed in collaboration with another lab. Here you can find a summary of the subject.

Subject:

"Ab initio studies for the fundamental understanding of semiconductor quantum dots properties"

LENS/FOTON Laboratory is dedicated to the study of the growth and the optoelectronic applications of semiconductor nanostructures on InP substrate

http://www.insa-rennes.fr/foton/

(and references below).

The aim of the study is to obtain a deep understanding of mechanical and electronical properties either for the InAs/InP quantum dots already used in our laboratory or for nanostructures studied in our new research projects. This study will be performed in the framework of the Sandie European Network of Excellence

`https://www.uni-leipzig.de/~sandie/`.

Candidates for the post-doc position must have a Ph. D. in computational condensed matter physics or theoretical chemistry (experiences on abinit, siesta, matlab, linux softwares will be appreciated and a detailed curriculum vitae should be sent to jacky.even@insa-rennes.fr. Candidates for the joint Ph. D. position must be supported by another laboratory. Please contact jacky.even@insa-rennes.fr.

J. Even
Professor, LENS/FOTON laboratory, UMR6082 CNRS, INSA de Rennes, France

References :

InAs/InP quantum dots :

C. Cornet, A. Schliwa, J. Even, F. Dor, C. Celebi, A. Ltoublon, E. Mac, C. Paranthon, A. Simon, P. M. Koenraad, N. Bertru, D. Bimberg and S. Loualiche,
"Theory of electronic and optical properties of InAs quantum dots on (100) and (311) InP substrates",
Phys. Rev. B., in press (July 2006).

C. Cornet, C. Platz, P. Caroff, J. Even, C. Labbe, H. Folliot, A. Le-Corre et S. Loualiche,
"Approach to wetting-layer-assisted lateral coupling of InAs/InP quantum dots",
Physical Review B : Condensed Matter and Materials Physics, 2005, vol. 72 (3), p. 35342.

C. Platz, C. Paranthoen, P. Caroff, N. Bertru, C. Labbe, J. Even, O. Dehaese, H. Folliot, A. Le-Corre, S. Loualiche, G. Moreau, J. C. Simon et A. Ramdane,
"Comparison of InAs quantum dot lasers emitting at 1.55 mu m under optical and electrical injection",
Semiconductor Science and Technology, 2005, vol. 20 (5), p. 459-63.

New materials and new quantum dots :

F. Dor, C. Cornet, A. Schliwa, A. Ballestar, J. Even, N. Bertru, O. Dehaese, I. Alghoraibi, H. Folliot, R. Piron, A. Le Corre et S. Loualiche,
"InAs(Sb)/InP(100) quantum dots for mid-infrared emitters : observation of 2.35 μm photoluminescence",
Physica status solidi(c), 2006, vol. 3, p. 524.

C. Cornet, F. Dore, A. Ballestar, J. Even, N. Bertru, A. Le-Corre et S. Loualiche,
"InAsSb/InP quantum dots for midwave infrared emitters: a theoretical study",
Journal of Applied Physics, 2005, vol. 98 (12), p. 126105-1-3.

N. Chimot, J. Even, H. Folliot et S. Loualiche,
"Structural and electronic properties of BAs and BGaAs/BInAs alloys",
Physica B : Condensed Matter, 2005, vol. 364 (1-4), p. 263-72.

5 Abstracts

A Periodic Genetic Algorithm with Real-Space Representation for Crystal Structure and Polymorph Prediction

N. L. Abraham and M. I. J. Probert
Department of Physics, University of York,
Heslington, York, YO10 5DD, United Kingdom

Abstract

A novel Genetic Algorithm is described that is suitable for determining the global minimum energy configurations of crystal structures and which can also be used as a polymorph search technique. This algorithm requires no prior assumptions about unit cell size, shape or symmetry, nor about the ionic configuration within the unit cell. This therefore enables true *ab initio* crystal structure and polymorph prediction. Our new algorithm uses a real-space representation of the population members, and makes use of a novel periodic cut for the crossover operation. Results on large Lennard-Jones systems with FCC- and HCP-commensurate cells show robust convergence to the bulk structure from a random initial assignment and an ability to successfully discriminate between competing low enthalpy configurations. Results from an *ab initio* carbon polymorph search show the spontaneous emergence of both Lonsdaleite and graphite like structures.

(Accepted for publication in Phys. Rev. B, cond-mat/0605066)
Contact person: Luke Abraham (nla101@york.ac.uk)

Giant anisotropy in x-ray magnetic linear dichroism from (Ga,Mn)As

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School of Physics and Astronomy, University of Nottingham,
Nottingham NG7 2RD, UK
G. van der Laan
CCLRC Daresbury Laboratory, Warrington WA4 4AD, UK
N.R.S. Farley
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E. Arenholz
Advanced Light Source, Lawrence Berkeley National Laboratory,
Berkeley, California 94720, USA
R.P. Campion, C.T. Foxon, and B.L. Gallagher
School of Physics and Astronomy, University of Nottingham,
Nottingham NG7 2RD, UK

Abstract

Hugely anisotropic Mn $L_{2,3}$ x-ray magnetic linear dichroism (XMLD) is reported for the ferromagnetic semiconductor (Ga,Mn)As. The sign, magnitude, and line shape of the dichroism changes with azimuthal rotation of the samples between the in-plane $\langle 110 \rangle$ and $\langle 100 \rangle$ directions. The strong anisotropy is confirmed by multiplet calculations for a Mn $3d^5$ configuration where charge anisotropy and magnetocrystalline anisotropy are absent. This allows a precise determination of the Mn $3d$ crystal-field splitting, and establishes the anisotropy in the XMLD as a general feature for localized moment systems with crystal-field symmetry.

Accepted for publication in Physical Review B **73**, 233303 (2006).
Contact person: g.vanderlaan@dl.ac.uk

Evidence for in-plane spin-flop orientation at the MnPt/Fe(100) interface revealed by x-ray magnetic linear dichroism

J. Fujii, F. Borgatti and G. Panaccione
TASC-INFM CNR Laboratory, Basovizza, Trieste, Italy
M. Hochstrasser
Laboratorium für Festkřperphysik, ETH Hönggerberg,
CH-8093 Zürich, Switzerland
F. Maccherozzi and G. Rossi
TASC-INFM CNR Laboratory, Basovizza, Trieste, Italy
G. van der Laan
Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

Abstract

X-ray magnetic linear and circular dichroism at the Mn $L_{2,3}$ edges are used to determine the magnetic properties of epitaxial MnPt films on Fe(100). The good agreement between experimental linear dichroism and multiplet calculations reveals that the Mn spins are aligned in plane but perpendicularly to the underlying in-plane Fe spins. The absence of magnetic circular dichroism rules out the presence of uncompensated Mn spins at the interface.

Accepted for publication in Physical Review B **73**, 214444 (2006).
Contact person: g.vanderlaan@dl.ac.uk

Thermal collapse of spin-polarization in half-metallic ferromagnets

M. Ležaić, Ph. Mavropoulos, J. Enkovaara, G. Bihlmayer, and S. Blügel
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Abstract

We propose two novel approaches to study the temperature dependence of the magnetization and of the spin polarization at the Fermi level in magnetic compounds, and apply them to half-metallic ferromagnets. We reveal a new mechanism, where the hybridization of states forming the half-metallic gap depends on thermal spin fluctuations and the polarization can drop abruptly at temperatures much lower than the Curie point. We verify this for NiMnSb by *ab initio* calculations. The thermal properties are studied by mapping *ab initio* results to an *extended Heisenberg model* which includes longitudinal fluctuations and is solved by a Monte Carlo method.

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Hitchhiker's Guide to Multiplet Calculations

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Abstract

Core level spectra from localized magnetic systems, such as $3d$ transition metal compounds or rare earths, obtained with high resolution synchrotron radiation can be simulated theoretically by calculating the transitions from the ground state to the allowed final states, e.g. $3d^n \rightarrow 2p^5 3d^{n+1}$. Presented here is the angular momentum coupling theory, Racah-Wigner algebra, point group theory and multipole moment expansion behind such calculations for the dichroic spectra of x-ray absorption, photoemission and x-ray resonant magnetic scattering. The first part of this chapter reviews the standard results of multiplet theory and surveys the Cowan-Butler-Thole approach. The last part presents some more advanced topics, such as the x-ray optical activity, which is induced by interference between different electric and magnetic multipole fields, and the method of statistical moment analysis, which relates the moment distribution of the dichroic spectra to effective operators.

1. Introduction,
2. Spin-orbit interaction versus Coulomb interaction,
3. Multiplet Structure,
4. Reduced Matrix Elements,
5. Selection Rules for Electric-Dipole Transitions,
6. Angular Momentum Coupling,
7. Coefficients of Fractional Parentage,
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21. Statistical Moment Analysis,
22. Spectral Moments for Ground State Tensors,
23. Conclusions and Outlook,
References

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Magnetic Metastability in Tetrahedrally Bonded Magnetic III-Nitride Semiconductors

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Abstract

Results of density-functional calculations for isolated transition metal (TM=V, Cr, Mn, Fe, Co, Ni on cation sites) doped GaN demonstrate a novel magnetic metastability in dilute magnetic semiconductors. Besides the expected high spin (HS) ground states (4 μ_B/Mn and 5 μ_B/Fe), there are also metastable low spin (LS) states (0 μ_B/Mn and 1 μ_B/Fe) — a phenomenon that can be explained in simple terms on the basis of ligand field theory. The transition between the HS and LS states corresponds to an intra-ionic transfer of two electrons between the t_2 and e orbitals, accompanied by a spin-flip process. The results suggest that TM-doped wide-band semiconductors (such as GaN and AlN) may present a new type of light-induced spin-crossover material.

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Dielectric anisotropy in the GW space-time method

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Abstract

Excited-state calculations, notably for quasiparticle band structures, are nowadays routinely performed within the GW approximation for the electronic self-energy. Nevertheless, certain numerical approximations and simplifications are still employed in practice to make the computations feasible. An important aspect for periodic systems is the proper treatment of the singularity of the screened Coulomb interaction in reciprocal space, which results from the slow $1/r$ decay in real space. This must be done without introducing artificial interactions between the quasiparticles and their periodic images in repeated cells, which occur when integrals of the screened Coulomb interaction are discretised in reciprocal space. An adequate treatment of both aspects is crucial for a numerically stable computation of the self-energy. In this article we build on existing schemes for isotropic screening and present an extension for anisotropic systems. We also show how the contributions to the dielectric function arising from the non-local part of the pseudopotentials can be computed efficiently. These improvements are crucial for obtaining a fast convergence with respect to the number of points used for the Brillouin zone integration and prove to be essential to make GW calculations for strongly anisotropic systems, such as slabs or multilayers, efficient.

(submitted to: Computer Physics Communications)
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Band gap and band parameters of InN and GaN from quasiparticle energy calculations based on exact-exchange density-functional theory

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Abstract

We have studied the electronic structure of InN and GaN employing G_0W_0 calculations based on exact-exchange density-functional theory. For InN our approach predicts a gap of 0.7 eV. Taking the Burnstein-Moss effect into account, the increase of the apparent quasiparticle gap with increasing electron concentration is in good agreement with the observed blue shift of the experimental optical absorption edge. Moreover, the concentration dependence of the effective mass, which results from the non-parabolicity of the conduction band, agrees well with recent experimental findings. Based on the quasiparticle band structure the parameter set for a 4×4 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian has been derived.

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Density-functional theory investigation of oxygen adsorption at Pd(11N)(N=3,5,7) vicinal surfaces

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Abstract

We present a density-functional theory study addressing the on-surface adsorption of oxygen at the Pd(11N) ($N = 3, 5, 7$) vicinal surfaces, which exhibit (111)steps and (100) terraces of increasing width. We find the binding to be predominantly governed by the local coordination at the adsorption site. This leads to very similar bonding properties at the threefold step sites of all three vicinalsurfaces, while the binding at the central fourfold hollow site in the four atomic row terrace of Pd(117) is already very little disturbed by the presence of the neighboring steps.

(submitted to: Phys. Rev. B.)
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Lifshitz transitions and elastic properties of Osmium under pressure

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Abstract

Topological changes of the Fermi surface under pressure may cause anomalies in the low-temperature elastic properties. Our density functional calculations for elemental Osmium evidence that this metal undergoes three such Lifshitz transitions in the pressure range between 70 GPa and 130 GPa. The related elastic anomalies are, however, invisibly weak. The critical pressures considerably exceed the values for recently measured and calculated anomalies in the pressure (P) dependence of the hexagonal c/a lattice parameter ratio close to 25 GPa. We demonstrate that the latter anomalies are statistically not significant and that $(c/a)(P)$ can be fitted equally well by a smooth dependence.

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Independent particle descriptions of tunneling from the many-body quantum transport approach

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Abstract

Currents across thin insulators are commonly taken as single electrons moving across classically forbidden regions; this independent particle picture is well-known to describe most tunneling phenomena. Examining quantum transport from a different perspective, i.e., by explicit treatment of electron-electron interactions, we evaluate different single particle approximations with specific application to tunneling in metal-molecule-metal junctions. We find maximizing the overlap of a Slater determinant composed of single particle states to the many-body current-carrying state is more important than energy minimization for defining single particle approximations in a system with open boundary conditions. Thus the most suitable single particle effective potential is not one commonly in use by electronic structure methods, such as the Hartree-Fock or Kohn-Sham approximations.

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Facility for combined in situ magnetron sputtering and soft x-ray magnetic circular dichroism

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Abstract

An ultrahigh vacuum chamber that enables the in situ growth of thin films and multilayers by magnetron sputtering techniques is described. Following film preparation, x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) measurements are performed by utilizing an in vacuum electromagnet. XMCD measurements on sputtered thin films of Fe and Co yield spin and orbital moments that are consistent with those obtained previously on films measured in transmission geometry and grown in situ by evaporation methods. Thin films of FeN prepared by reactive sputtering are also examined and reveal an apparent enhancement in the orbital moment for low N content samples. The advantages of producing samples for in situ XAS and XMCD studies by magnetron sputtering are discussed.

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Magneto-elastic lattice collapse in YCo_5

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Abstract

The isomorphic collapse of crystalline lattices under pressure is a rare and intriguing phenomenon – the most famous examples being samarium sulphide and cerium metal. Both lattices are cubic under ambient conditions and collapse isomorphically under pressure, remaining cubic with $\sim 15\%$ volume reduction[1−3]. In SmS the transition results from a change of the $4f$ chemical valence. The collapse in Ce is connected with the altering contributions of the $4f$ electrons to the chemical bonding, the details of which are currently much debated[4,5]. In contrast, YCo_5 is a hexagonal metallic compound with a stable valence and no $4f$ electrons. Here, we present a combination of high-pressure X-ray diffraction measurements and density functional electronic-structure calculations to demonstrate an entirely different type of isomorphic transition under hydrostatic pressure of 19 GPa. Our results suggest that the lattice collapse is driven by magnetic interactions and can be characterized as a first-order Lifshitz transition, where the Fermi surface changes topologically. These studies support the existence of a bistable bonding state due to the magneto-elastic interaction.

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6 SCIENTIFIC HIGHLIGHT OF THE MONTH: ”Density functional theory for superconductors”

Density functional theory for superconductors

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Abstract

In this highlight we review density functional theory for superconductors. This formally exact theory is a generalisation of normal-state density functional theory, which also includes the superconducting order parameter and the diagonal of the nuclear density matrix as additional densities. We outline the formal framework and the construction of approximate exchange-correlation functionals. Several aspects of the theory are demonstrated by some examples: a first application to simple metals shows that weakly and strongly coupled superconductors are equally well described. Calculations for MgB_2 with its two gap superconductivity demonstrate the capability to go beyond simple BCS superconductivity. Finally the formalism is applied to aluminium, lithium and potassium under high pressure, describing correctly the experimental behaviour of Al and Li, and predicting fcc-K to become superconducting at high pressures.

1 Introduction

More than one century after the discovery of superconductivity, the prediction of critical temperatures from first principles remains one of the grand challenges of modern solid state physics. It had taken nearly 50 years until Bardeen, Cooper and Schrieffer (BCS) [1] developed their theory of superconductivity, identifying the mechanism of conventional superconductors as a phonon-mediated pairing of electrons and a condensation into the so-called BCS wave function. This theory, however, only allows for the calculation of universal quantities, such as the ratio of the critical temperature and the gap at zero temperature, and not for material specific properties. The first major step beyond this limitation was Eliashberg theory [2–7], based on many-body perturbation theory in the superconducting state. The difference to normal state calculations is that in the superconducting state also expectation values of two electronic creation or two destruction operators remain finite. They give rise to the anomalous Green's functions which, when evaluated for equal times, result in the superconducting order parameter, introduced already in the BCS theory. In principle, Eliashberg theory is a complete theory of the superconducting state, taking proper account of the electron-phonon (e-ph) interaction and the electron-electron repulsion. In practise, however, the Coulomb repulsion is very difficult to treat and is normally included through the pseudopotential μ^*, whose value is typically fitted to obtain the experimental critical temperature of the material. Therefore Eliashberg theory, in its common practical implementation, cannot be considered a truly ab initio theory either.

The standard tool for material specific first principles calculations of normal-state properties, such as the geometrical or magnetic structure, is density functional theory (DFT). This theory is based on the Hohenberg-Kohn (HK) theorem [8] that guarantees that all physical observables of a system, in particular the total energy, are functionals of the ground-state density. The HK theorem was employed by Kohn and Sham [9] to introduce an auxiliary non-interacting system, subject to an effective potential, constructed such that the non-interacting system reproduces the ground-state density of the fully interacting system. To this end, the total energy functional was rewritten in terms of a part corresponding to this non-interacting system and the remainder, the so-called exchange-correlation (xc) energy functional, which includes all our ignorance about the interacting system. Good approximations to this unknown functional, such as the local (spin) density approximation [L(S)DA], are the key to successful applications of DFT. The LSDA and also the generalised gradient approximation (GGA) have so far triggered a broad variety of accurate applications of DFT, ranging from atomic and molecular systems to solids. It can be said that DFT is the main working horse for virtually all computational material science. For reviews of DFT see, for example, Refs. [10–14].

In this highlight we review how density functional theory can be generalised to superconducting systems [15–17], yielding a theory that overcomes the above mentioned problems and has the potential to become a standard tool for the calculation of superconducting properties.

2 Formal framework

Before turning to the problem of superconductivity, it is instructive to reconsider how magnetic systems are usually treated. The HK theorem states that all observables, in particular also the magnetisation, are functionals of the electronic density *alone*. This, however, assumes the knowledge of the magnetisation as a functional of the density. To approximate this functional is extremely hard and, in practise, one chooses a different approach. The task can be vastly simplified by treating the magnetisation density $\mathbf{m}(\mathbf{r})$, i.e., the order parameter of the magnetic state, as an additional fundamental density in the density functional framework. An auxiliary field – here a magnetic field $\mathbf{B}_{\mathrm{ext}}(\mathbf{r})$ – is introduced, which couples to $\mathbf{m}(\mathbf{r})$ and breaks the corresponding (rotational) symmetry of the Hamiltonian. In other words, it drives the system into the ordered state. The resulting magnetisation then leads to a finite value of the effective magnetic field. If the system wants to be magnetic, the order parameter will survive even if the auxiliary perturbation is switched off again. In this way, the ground-state magnetisation density is determined by minimising the total energy functional (free energy functional for finite temperature calculations) with respect to both the normal density and the magnetisation density. Much simpler approximations to the xc functional (now a functional of two densities) can lead to satisfactory results. This idea forms the basis of the local spin density approximation and, likewise, of current density functional theory [18,19].

The same idea is also at the heart of density functional theory for superconductors, as formulated by Oliveira, Gross and Kohn [15]. Here the order parameter is the so-called anomalous density,

$$\chi(\mathbf{r},\mathbf{r}') = \langle \hat{\Psi}_{\uparrow}(\mathbf{r})\hat{\Psi}_{\downarrow}(\mathbf{r}')\rangle\,, \tag{1}$$

and the corresponding potential is the non-local pairing potential $\Delta(\mathbf{r},\mathbf{r}')$. It can be interpreted as an external pairing field, induced by an adjacent superconductor via the proximity effect. Again, this external field only acts to break the symmetry (here the gauge symmetry) of the system, and is set to zero at the end of the calculation. As in the case of magnetism, the order parameter will be sustained by the self-consistent effective pairing field, if the system wants to be superconducting. The formalism outlined so far captures, in principle, all electronic degrees of freedom. To describe conventional, phonon-mediated, superconductors, also the electron-phonon interaction has to be taken into account. In the weak coupling limit, this phonon-mediated interaction can be added as an additional BCS-type interaction. However, in order to treat also strong electron-phonon coupling, the electronic and the nuclear degrees of freedom have to be treated on equal footing. This can be achieved by a multi-component DFT, based on both the electronic density and the nuclear density [20]. The starting point is the full electron-ion Hamiltonian

$$\hat{H} = \hat{T}^{\mathrm{e}} + \hat{U}^{\mathrm{ee}} + \hat{T}^{\mathrm{n}} + \hat{U}^{\mathrm{nn}} + \hat{U}^{\mathrm{en}}\,, \tag{2}$$

where $\hat{T}^{\mathrm{e}}$ represents the electronic kinetic energy, $\hat{U}^{\mathrm{ee}}$ the electron-electron interaction, $\hat{T}^{\mathrm{n}}$ the nuclear kinetic energy, and $\hat{U}^{\mathrm{nn}}$ the Coulomb repulsion between the nuclei. The interaction between the electrons and the nuclei is described by the term

$$\hat{U}^{\mathrm{en}} = -\sum_{\sigma}\int \mathrm{d}^3r \int \mathrm{d}^3R\, \hat{\Psi}^{\dagger}_{\sigma}(\mathbf{r})\hat{\Phi}^{\dagger}(\mathbf{R})\frac{Z}{|\mathbf{r}-\mathbf{R}|}\hat{\Phi}(\mathbf{R})\hat{\Psi}_{\sigma}(\mathbf{r})\,, \tag{3}$$

where $\hat{\Psi}_{\sigma}(\mathbf{r})$ and $\hat{\Phi}(\mathbf{R})$ are respectively electron and nuclear field operators. (For simplicity we assume the nuclei to be identical, and we neglect the nuclear spin degrees of freedom. The extension of this framework to a more general case is straightforward.) Note that there is no external potential in the Hamiltonian. In addition to the normal and anomalous electronic densities, we also include the diagonal of the nuclear density matrix [1]

$$\Gamma(\underline{\mathbf{R}}) = \langle \hat{\Phi}^{\dagger}(\mathbf{R}_1)\ldots\hat{\Phi}^{\dagger}(\mathbf{R}_N)\hat{\Phi}(\mathbf{R}_N)\ldots\hat{\Phi}(\mathbf{R}_1)\rangle \tag{4}$$

---

[1] Taking only the nuclear density would lead to a system of strictly non-interacting nuclei which obviously would give rise to non-dispersive, hence unrealistic, phonons.

In order to formulate a Hohenberg-Kohn theorem for this system, we introduce a set of three potentials, which couple to the three densities described above. Since the electron-nuclear interaction, which in normal DFT constitutes the external potential, is treated explicitly in this formalism, it is *not* part of the external potential. The nuclear Coulomb interaction $\hat{U}^{\mathrm{nn}}$ already has the form of an external many-body potential, coupling to $\Gamma(\underline{\mathbf{R}})$, and for the sake of the Hohenberg-Kohn theorem, this potential will be allowed to take the form of an arbitrary N-body potential. All three external potentials are merely mathematical devices, required to formulate a Hohenberg-Kohn theorem. At the end of the derivation they will be set to zero (in case of the external electronic and pairing potentials) and to the nuclear Coulomb interaction (for the external nuclear many-body potential).

As usual, the Hohenberg-Kohn theorem guarantees a one-to-one mapping between the set of the densities $\{n(\mathbf{r}), \chi(\mathbf{r},\mathbf{r}'), \Gamma(\underline{\mathbf{R}})\}$ in thermal equilibrium and the set of their conjugate potentials $\{v^{\mathrm{e}}_{\mathrm{ext}}(\mathbf{r}) - \mu, \Delta_{\mathrm{ext}}(\mathbf{r},\mathbf{r}'), v^{\mathrm{n}}_{\mathrm{ext}}(\underline{\mathbf{R}})\}$. As a consequence, all the observables are functionals of the set of densities. Finally, it assures that the grand canonical potential,

$$\begin{aligned}\Omega[n,\chi,\Gamma] = F[n,\chi,\Gamma] &+ \int \mathrm{d}^3 r\, n(\mathbf{r})[v^{\mathrm{e}}_{\mathrm{ext}}(\mathbf{r}) - \mu] \\ &- \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \,\left[\chi(\mathbf{r},\mathbf{r}')\Delta^*_{\mathrm{ext}}(\mathbf{r},\mathbf{r}') + \mathrm{h.c.}\right] + \int \mathrm{d}^3 \underline{R}\;\Gamma(\underline{\mathbf{R}}) v^{\mathrm{n}}_{\mathrm{ext}}(\underline{\mathbf{R}})\,, \end{aligned} \tag{5}$$

is minimised by the equilibrium densities. We use the notation $A[f]$ to denote that A is a functional of f. The functional $F[n,\chi,\Gamma]$ is universal, in the sense that it does not depend on the external potentials, and is defined by

$$F[n,\chi,\Gamma] = T^{\mathrm{e}}[n,\chi,\Gamma] + T^{\mathrm{n}}[n,\chi,\Gamma] + U^{\mathrm{en}}[n,\chi,\Gamma] + U^{\mathrm{ee}}[n,\chi,\Gamma] - \frac{1}{\beta} S[n,\chi,\Gamma]\,, \tag{6}$$

where S is the entropy of the system,

$$S[n,\chi,\Gamma] = -\mathrm{Tr}\{\hat{\rho}_0[n,\chi,\Gamma]\ln(\hat{\rho}_0[n,\chi,\Gamma])\}\,. \tag{7}$$

The proof of the theorem follows closely the proof of the Hohenberg-Kohn theorem at finite temperatures [21].

3 Kohn-Sham system

In standard DFT one normally defines a Kohn-Sham system, i.e., a non-interacting system chosen such that it has the same ground-state density as the interacting one. In our formalism, the Kohn-Sham system consists of non-interacting (superconducting) electrons, and *interacting* nuclei. It is described by the thermodynamic potential [cf. Eq. (5)]

$$\begin{aligned}\Omega_{\mathrm{s}}[n,\chi,\Gamma] = F_{\mathrm{s}}[n,\chi,\Gamma] &+ \int \mathrm{d}^3 r\, n(\mathbf{r})[v^{\mathrm{e}}_{\mathrm{s}}(\mathbf{r}) - \mu_{\mathrm{s}}] \\ &- \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \,\left[\chi(\mathbf{r},\mathbf{r}')\Delta^*_{\mathrm{s}}(\mathbf{r},\mathbf{r}') + h.c.\right] + \int \mathrm{d}^3 \underline{R}\;\Gamma(\underline{\mathbf{R}}) v^{\mathrm{n}}_{\mathrm{s}}(\underline{\mathbf{R}})\,, \end{aligned} \tag{8}$$

where F_{s} if the counterpart of (6) for the Kohn-Sham system, i.e.,

$$F_{\mathrm{s}}[n,\chi,\Gamma] = T^{\mathrm{e}}_{\mathrm{s}}[n,\chi,\Gamma] + T^{\mathrm{n}}_{\mathrm{s}}[n,\chi,\Gamma] - \frac{1}{\beta} S_{\mathrm{s}}[n,\chi,\Gamma]\,. \tag{9}$$

Here $T_{\rm s}^{\rm e}[n,\chi,\Gamma]$, $T_{\rm s}^{\rm n}[n,\chi,\Gamma]$, and $S_{\rm s}[n,\chi,\Gamma]$ are the electronic and nuclear kinetic energies and the entropy of the Kohn-Sham system, respectively. From Eq. (8) it is clear that the Kohn-Sham nuclei interact with each other through the N-body potential $v_{\rm s}^{\rm n}(\underline{\mathbf{R}})$, while they do not interact with the electrons.

The Kohn-Sham potentials, which are derived in analogy to normal DFT, include the external fields, Hartree, and exchange-correlation terms. The latter account for all many-body effects of the electron-electron and electron-nuclear interactions and are, as usual, given by the respective functional derivatives of the xc energy functional defined through

$$F[n,\chi,\Gamma] = F_{\rm s}[n,\chi,\Gamma] + F_{\rm xc}[n,\chi,\Gamma] + E_{\rm H}^{\rm ee}[n,\chi] + E_{\rm H}^{\rm en}[n,\Gamma]\,. \tag{10}$$

There are two contributions to $E_{\rm H}^{\rm ee}$, one originating from the electronic Hartree potential, and the other from the anomalous Hartree potential

$$E_{\rm H}^{\rm ee}[n,\chi] = \frac{1}{2}\int {\rm d}^3r \int {\rm d}^3r'\,\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \int {\rm d}^3r \int {\rm d}^3r'\,\frac{|\chi(\mathbf{r},\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|}\,. \tag{11}$$

Finally, $E_{\rm H}^{\rm en}$ denotes the electron-nuclear Hartree energy

$$E_{\rm H}^{\rm en}[n,\Gamma] = -Z\sum_{\alpha}\int {\rm d}^3r \int {\rm d}^3\underline{R}\,\frac{n(\mathbf{r})\Gamma(\underline{\mathbf{R}})}{|\mathbf{r}-\mathbf{R}_\alpha|}\,. \tag{12}$$

The problem of minimising the Kohn-Sham grand canonical potential (8) can be transformed into a set of three differential equations that have to be solved self-consistently: One equation for the nuclei, which resembles the familiar nuclear Born-Oppenheimer equation, and two coupled equations which describe the electronic degrees of freedom and have the algebraic structure of the Bogoliubov-de Gennes [22] equations.

The Kohn-Sham equation for the nuclei has the form

$$\left[-\sum_{\alpha}\frac{\nabla_\alpha^2}{2M} + v_{\rm s}^{\rm n}(\underline{\mathbf{R}})\right]\Phi_l(\underline{\mathbf{R}}) = \mathcal{E}_l\Phi_l(\underline{\mathbf{R}})\,. \tag{13}$$

We emphasise that the Kohn-Sham equation (13) does not rely on any approximation and is, in principle, exact. In practise, however, the unknown effective potential for the nuclei is approximated by the Born-Oppenheimer surface. As already mentioned, we are interested in solids at relatively low temperature, where the nuclei perform small amplitude oscillations around their equilibrium positions. In this case, we can expand $v_{\rm s}^{\rm n}[n,\chi,\Gamma]$ in a Taylor series around the equilibrium positions, and transform the nuclear degrees of freedom into collective (phonon) coordinates. In harmonic order, the nuclear Kohn-Sham Hamiltonian then reads

$$\hat{H}_{\rm s}^{\rm ph} = \sum_{\lambda,\mathbf{q}}\Omega_{\lambda,\mathbf{q}}\left[\hat{b}^{\dagger}_{\lambda,\mathbf{q}}\hat{b}\dagger_{\lambda,\mathbf{q}} + \frac{1}{2}\right]\,, \tag{14}$$

where $\Omega_{\lambda,\mathbf{q}}$ are the phonon eigenfrequencies, and $\hat{b}^{\dagger}_{\lambda,\mathbf{q}}$ creates a phonon of branch λ and wave-vector $\mathbf{q}$. Note that the phonon eigenfrequencies are functionals of the set of densities $\{n,\chi,\Gamma\}$, and can therefore be affected by the superconducting order parameter.

The Kohn-Sham Bogoliubov-de Gennes (KS-BdG) equations read

$$\left[-\frac{\nabla^2}{2}+v^{\mathrm{e}}_{\mathrm{s}}(\mathbf{r})-\mu\right]u_{n\mathbf{k}}(\mathbf{r})+\int\mathrm{d}^3r'\,\Delta_{\mathrm{s}}(\mathbf{r},\mathbf{r}')v_{n\mathbf{k}}(\mathbf{r}')=\tilde{E}_{n\mathbf{k}}\,u_{n\mathbf{k}}(\mathbf{r})\,, \tag{15a}$$

$$-\left[-\frac{\nabla^2}{2}+v^{\mathrm{e}}_{\mathrm{s}}(\mathbf{r})-\mu\right]v_{n\mathbf{k}}(\mathbf{r})+\int\mathrm{d}^3r'\,\Delta^*_{\mathrm{s}}(\mathbf{r},\mathbf{r}')u_{n\mathbf{k}}(\mathbf{r}')=\tilde{E}_{n\mathbf{k}}\,v_{n\mathbf{k}}(\mathbf{r})\,, \tag{15b}$$

where $u_{n\mathbf{k}}(\mathbf{r})$ and $v_{n\mathbf{k}}(\mathbf{r})$ are the particle and hole amplitudes. This equation is very similar to the Kohn-Sham equations in the OGK formalism [15]. However, in the present formulation the lattice potential is not considered an external potential but enters via the electron-ion Hartree term. Furthermore, our exchange-correlation potentials depend on the nuclear density matrix, and therefore on the phonons. Although equations (13) and (15) have the structure of static mean-field equations, they contain, in principle, all correlation and retardation effects through the exchange-correlation potentials.

These KS-BdG equations can be simplified by the so-called decoupling approximation [16, 23], which corresponds to the following ansatz for the particle and hole amplitudes:

$$u_{n\mathbf{k}}(\mathbf{r})\approx u_{n\mathbf{k}}\varphi_{n\mathbf{k}}(\mathbf{r})\,;\quad v_{n\mathbf{k}}(\mathbf{r})\approx v_{n\mathbf{k}}\varphi_{n\mathbf{k}}(\mathbf{r})\,, \tag{16}$$

where the wave functions $\varphi_{n\mathbf{k}}(\mathbf{r})$ are the solutions of the normal Schrödinger equation. In this way the eigenvalues in Eq. (15) become $\tilde{E}_{n\mathbf{k}}=\pm E_{n\mathbf{k}}$, where

$$E_{n\mathbf{k}}=\sqrt{\xi^2_{n\mathbf{k}}+|\Delta_{n\mathbf{k}}|^2}\,, \tag{17}$$

and $\xi_{n\mathbf{k}}=\epsilon_{n\mathbf{k}}-\mu$. This form of the eigenenergies allows us to interpret the pair potential $\Delta_{n\mathbf{k}}$ as the gap function of the superconductor. Furthermore, the coefficients $u_{n\mathbf{k}}$ and $v_{n\mathbf{k}}$ are given by simple expressions within this approximation

$$u_{n\mathbf{k}}=\frac{1}{\sqrt{2}}\mathrm{sgn}(\tilde{E}_{n\mathbf{k}})\mathrm{e}^{\mathrm{i}\phi_{n\mathbf{k}}}\sqrt{1+\frac{\xi_{n\mathbf{k}}}{\tilde{E}_{n\mathbf{k}}}}\,, \tag{18a}$$

$$v_{n\mathbf{k}}=\frac{1}{\sqrt{2}}\sqrt{1-\frac{\xi_{n\mathbf{k}}}{\tilde{E}_{n\mathbf{k}}}}\,. \tag{18b}$$

Finally, the matrix elements $\Delta_{n\mathbf{k}}$ are defined as

$$\Delta_{n\mathbf{k}}=\int\mathrm{d}^3r\int\mathrm{d}^3r'\,\varphi^*_{n\mathbf{k}}(\mathbf{r})\Delta_{\mathrm{s}}(\mathbf{r},\mathbf{r}')\varphi_{n\mathbf{k}}(\mathbf{r}')\,, \tag{19}$$

and $\phi_{n\mathbf{k}}$ is the phase $\mathrm{e}^{\mathrm{i}\phi_{n\mathbf{k}}}=\Delta_{n\mathbf{k}}/|\Delta_{n\mathbf{k}}|$. The normal and the anomalous densities can then be easily obtained from:

$$n(\mathbf{r})=\sum_{n\mathbf{k}}\left[1-\frac{\xi_{n\mathbf{k}}}{E_{n\mathbf{k}}}\tanh\left(\frac{\beta}{2}E_{n\mathbf{k}}\right)\right]|\varphi_{n\mathbf{k}}(\mathbf{r})|^2 \tag{20a}$$

$$\chi(\mathbf{r},\mathbf{r}')=\frac{1}{2}\sum_{n\mathbf{k}}\frac{\Delta_{n\mathbf{k}}}{E_{n\mathbf{k}}}\tanh\left(\frac{\beta}{2}E_{n\mathbf{k}}\right)\varphi_{n\mathbf{k}}(\mathbf{r})\varphi^*_{n\mathbf{k}}(\mathbf{r}')\,. \tag{20b}$$

Within the decoupling approximation outlined above, a major part of the calculation is to self-consistently determine the effective pairing potential. As will be seen in the next sections, the actual approximations for the xc functionals are not explicit functionals of the densities, but rather functionals of the potentials, still being implicit functionals of the density. Therefore the task of calculating the effective pair potential is to solve the non-linear functional equation

$$\Delta_{\mathrm{s},n\mathbf{k}} = \Delta_{\mathrm{xc},n\mathbf{k}}[\mu, \Delta_{\mathrm{s}}]. \tag{21}$$

In the vicinity of the critical temperature, where the order parameter and hence the pairing potential vanishes, this equation can be linearised, giving rise to a BCS-like gap equation:

$$\breve{\Delta}_{n\mathbf{k}} = -\frac{1}{2}\sum_{n'\mathbf{k}'} \mathcal{F}_{\mathrm{Hxc}\;n\mathbf{k},n'\mathbf{k}'}[\mu] \frac{\tanh\left(\frac{\beta}{2}\xi_{n'\mathbf{k}'}\right)}{\xi_{n'\mathbf{k}'}} \breve{\Delta}_{n'\mathbf{k}'}\,, \tag{22}$$

where the anomalous Hartree exchange-correlation kernel of the homogeneous integral equation reads

$$\mathcal{F}_{\mathrm{Hxc}\;n\mathbf{k},n'\mathbf{k}'}[\mu] = -\left.\frac{\delta\Delta_{\mathrm{Hxc}\,n\mathbf{k}}}{\delta\chi_{n'\mathbf{k}'}}\right|_{\chi=0} = \left.\frac{\delta^2(E_{\mathrm{H}}^{\mathrm{ee}} + F_{\mathrm{xc}})}{\delta\chi^*_{n\mathbf{k}}\delta\chi_{n'\mathbf{k}'}}\right|_{\chi=0}\,. \tag{23}$$

Although this linearised gap equation is strictly valid only in the vicinity of the transition temperature, we use the same kernel $\mathcal{F}_{\mathrm{Hxc}}$ in a partially linearised equation, that has the same structure but contains the energies $E_{n\mathbf{k}}$ in place of the $\xi_{n\mathbf{k}}$, also at lower temperatures. Furthermore, we split the kernel into a purely diagonal part $\mathcal{Z}$ and a truly off-diagonal part $\mathcal{K}$,

$$\Delta_{n\mathbf{k}} = -\mathcal{Z}_{n\mathbf{k}}\Delta_{n\mathbf{k}} - \frac{1}{2}\sum_{n'\mathbf{k}'} \mathcal{K}_{n\mathbf{k},n'\mathbf{k}'} \frac{\tanh\left(\frac{\beta}{2}E_{n'\mathbf{k}'}\right)}{E_{n'\mathbf{k}'}} \Delta_{n'\mathbf{k}'}\,. \tag{24}$$

Explicit expressions for $\mathcal{Z}_{n\mathbf{k}}$ and $\mathcal{K}_{n\mathbf{k},n'\mathbf{k}'}$ will be given below.

4 Functionals

So far, only the formal framework of the theory was presented. But, like for any DFT, its success strongly depends on the availability of reliable approximations to the xc functional. For normal-state calculations, a variety of such functionals is available, ranging from the local density approximation (LDA), based on highly accurate Quantum Monte Carlo calculations of the homogeneous electron gas, and generalised gradient approximations (GGA), to orbital functionals such as exact exchange, and combinations thereof.

Recently, some first approximations to the xc energy functional for superconductors have been presented. In contrast to the normal-state functionals, here the functional also depends on the anomalous density. Furthermore, in order to describe conventional superconductors, it must contain the electron-phonon interaction, as well as the electronic Coulomb correlations.

The proposed functional is based on many-body perturbation theory in the superconducting state, and is guided by parallels to the Eliashberg theory. The building blocks of many-body perturbation theory are the electronic propagators (including the so-called anomalous propagators in the superconducting state), the phonon propagator and the electron-electron as well as the electron-phonon interaction. It can be seen from quite general arguments that all diagrams can be classified into purely electronic ones and diagrams including the phonon propagator. This classification warrants that these two contributions can be treated in a different way, because they describe different mechanisms.

For the electronic terms, we construct a local density approximation, in other words, we approximate the xc energy density of a homogeneous but superconducting electron gas [24]. Since the anomalous density is a non-local quantity, the xc energy remains a functional – rather than a function – even in the homogeneous electron gas. This, unfortunately, makes the construction of approximations much more complicated, and, at present, rules out full fledged Quantum Monte Carlo calculations, as available for the normal state. Instead, functionals based on the RPA [24] and its static limit [17] have been proposed. The latter is quite easy to implement and was used (with slight variations, described in Ref. [17]) for the calculations presented below.

For the electron-phonon contributions an LDA-type functional is not meaningful, because the homogeneous electron gas does not posses phonons. Instead, the e-ph contribution to the xc energy is directly calculated from many-body perturbation theory by evaluating the two lowest order diagrams, shown in Figure 1. The expressions for the xc energies can be found in Ref. [16].

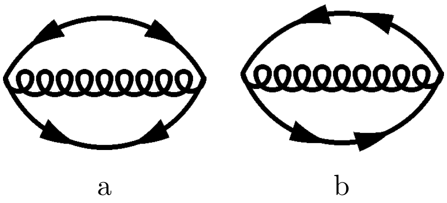

Figure 1: Lowest order phononic (a, b) contributions to F_{xc}. The two types of electron propagators correspond to the normal and anomalous Green's functions.

Besides the Coulomb repulsion and the electron-phonon coupling, spin-fluctuations constitute another important mechanism. Ferromagnetic spin-fluctuations are known to lower the critical temperature in materials such as vanadium and even to suppress superconductivity in palladium, while antiferromagnetic spin-fluctuations are amongst the candidates for the mechanism of the high-T_c superconductors. Spin fluctuations can be treated in a similar way to the electron-phonon term by replacing the phonon-propagator in the diagrams by the spin-fluctuation propagator. This has been proposed in the context of the Eliashberg theory [25, 26] and recently a first approximation in the context of DFT for superconductors was constructed [27].

5 Potentials and kernels

The functionals described above are only implicit functionals of the densities. The desired functional derivatives can nevertheless be evaluated by applying the chain rule of functional derivatives, similar to the procedure used in the optimised effective potential method [28, 29]. The xc energy is an explicit functional of the pairing potential and the chemical potential, and therefore we can write

$$\Delta_{\mathrm{xc}\,n\mathbf{k}} = -\frac{\delta F_{\mathrm{xc}}}{\delta \mu}\frac{\delta \mu}{\delta \chi^*_{n\mathbf{k}}} - \sum_{n'\mathbf{k}'}\left[\frac{\delta F_{\mathrm{xc}}}{\delta|\Delta_{n'\mathbf{k}'}|^2}\frac{\delta|\Delta_{n'\mathbf{k}'}|^2}{\delta \chi^*_{n\mathbf{k}}} + \frac{\delta F_{\mathrm{xc}}}{\delta(\phi_{n'\mathbf{k}'})}\frac{\delta(\phi_{n'\mathbf{k}'})}{\delta \chi^*_{n\mathbf{k}}}\right] . \qquad (25)$$

The partial derivatives of F_{xc} can be calculated directly. The remaining functional derivatives are somewhat harder to obtain, but can be derived from the definitions of the densities, Eqs. (20),

Table 1: Critical temperature (left panel) and superconducting gap at Fermi level and $T = 0.01\,\mathrm{K}$ (right panel), compared with experiment [30]. We also show the total electron-phonon coupling constant λ [31, 32]. While TF-ME represents an approximation with the full matrix elements, TF-SK and TF-FE correspond to simplified expressions. For details see Ref. [17].

	T_c [K]				
	TF-ME	TF-SK	TF-FE	exp	λ
Mo	—	0.33	0.54	0.92	0.42
Al	0.90	0.90	1.0	1.18	0.44
Ta	3.7	2.7	4.8	4.48	0.84
Pb	6.9	7.2	6.8	7.2	1.62
Nb	9.5	8.4	9.4	9.3	1.18

	Δ_0 [meV]				
	TF-ME	TF-SK	TF-FE	exp	λ
Mo	—	0.049	0.099	—	0.42
Al	0.14	0.15	0.15	0.179	0.44
Ta	0.63	0.53	0.76	0.694	0.84
Pb	1.34	1.40	1.31	1.33	1.62
Nb	1.74	1.54	1.79	1.55	1.18

and from the fact that the particle density and the anomalous density are independent variables, leading to the condition

$$\frac{\delta n(\mathbf{x})}{\delta \chi^*(\mathbf{r}, \mathbf{r}')} = 0\,. \tag{26}$$

After a number of further approximations (see [16, 17]), the final expressions for the functionals $\mathcal{Z}_{n\mathbf{k}}$ and $\mathcal{K}_{n\mathbf{k},n'\mathbf{k}'}$ in the gap equation (24) read as follows. There are two contributions stemming from the electron-phonon interaction: i) The non-diagonal one is:

$$\begin{aligned}\mathcal{K}^{\mathrm{ph}}_{n\mathbf{k},n'\mathbf{k}'} = & \frac{2}{\tanh\left(\frac{\beta}{2}\xi_{n\mathbf{k}}\right)\tanh\left(\frac{\beta}{2}\xi_{n'\mathbf{k}'}\right)} \\ & \times \sum_{\lambda,\mathbf{q}} \left| g^{n\mathbf{k},n'\mathbf{k}'}_{\lambda,\mathbf{q}} \right|^2 \left[I(\xi_{n\mathbf{k}}, \xi_{n'\mathbf{k}'}, \Omega_{\lambda,\mathbf{q}}) - I(\xi_{n\mathbf{k}}, -\xi_{n'\mathbf{k}'}, \Omega_{\lambda,\mathbf{q}}) \right] ,\end{aligned} \tag{27}$$

where $g^{n\mathbf{k},n'\mathbf{k}'}_{\lambda,\mathbf{q}}$ are the electron-phonon coupling constants and the function I is defined as

$$I(\xi, \xi', \Omega) = f_\beta(\xi)\, f_\beta(\xi')\, n_\beta(\Omega) \left[\frac{\mathrm{e}^{\beta\xi} - \mathrm{e}^{\beta(\xi'+\Omega)}}{\xi - \xi' - \Omega} - \frac{\mathrm{e}^{\beta\xi'} - \mathrm{e}^{\beta(\xi+\Omega)}}{\xi - \xi' + \Omega} \right] . \tag{28}$$

In the previous expression f_β and n_β are the Fermi-Dirac and Bose-Einstein distributions; ii) The second contribution is diagonal in $n\mathbf{k}$ and reads

$$\mathcal{Z}^{\mathrm{ph}}_{n\mathbf{k}} = \frac{1}{\tanh\left(\frac{\beta}{2}\xi_{n\mathbf{k}}\right)} \sum_{n'\mathbf{k}'} \sum_{\lambda,\mathbf{q}} \left| g^{n\mathbf{k},n'\mathbf{k}'}_{\lambda,\mathbf{q}} \right|^2 \left[J(\xi_{n\mathbf{k}}, \xi_{n'\mathbf{k}'}, \Omega_{\lambda,\mathbf{q}}) + J(\xi_{n\mathbf{k}}, -\xi_{n'\mathbf{k}'}, \Omega_{\lambda,\mathbf{q}}) \right] , \tag{29}$$

where the function J is defined by

$$J(\xi, \xi', \Omega) = \tilde{J}(\xi, \xi', \Omega) - \tilde{J}(\xi, \xi', -\Omega)\,, \tag{30}$$

and we have

$$\tilde{J}(\xi, \xi', \Omega) = -\frac{f_\beta(\xi) + n_\beta(\Omega)}{\xi - \xi' - \Omega} \left[\frac{f_\beta(\xi') - f_\beta(\xi - \Omega)}{\xi - \xi' - \Omega} - \beta f_\beta(\xi - \Omega) f_\beta(-\xi' + \Omega) \right] . \tag{31}$$

On the other hand, the Coulomb interaction leads to the term

$$\mathcal{K}^{\text{TF-ME}}_{n\mathbf{k},n'\mathbf{k}'} = v^{\mathrm{TF}}_{n\mathbf{k},n'\mathbf{k}'}\,, \tag{32}$$

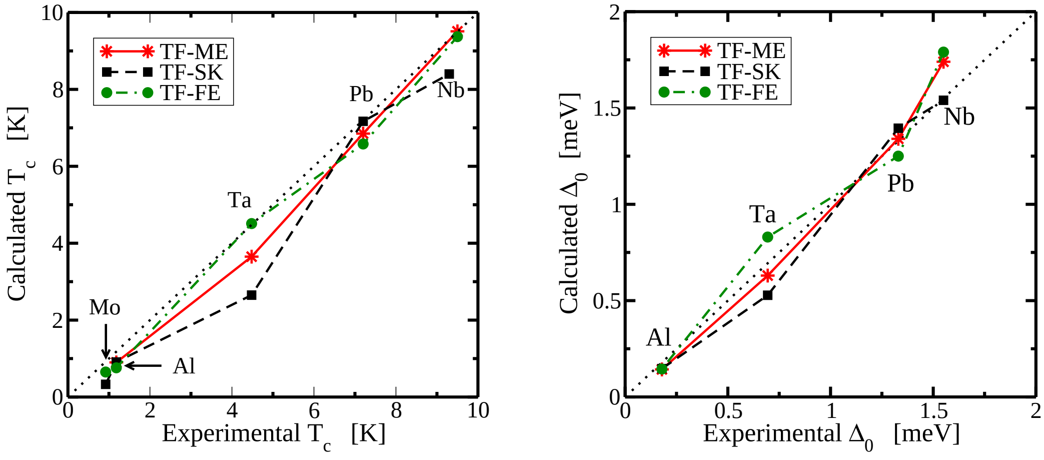

Figure 2: The critical temperature and superconducting gap at Fermi level and $T = 0.01\,\mathrm{K}$, compared with experiment. The numerical values can be found in Table 1.

with the definition

$$v^{\mathrm{TF}}_{n\mathbf{k},n'\mathbf{k}'} = \int \mathrm{d}^3r \int \mathrm{d}^3r' \, v^{\mathrm{TF}}(\mathbf{r}-\mathbf{r}')\varphi^*_{n\mathbf{k}}(\mathbf{r})\varphi_{n\mathbf{k}}(\mathbf{r}')\varphi_{n'\mathbf{k}'}(\mathbf{r})\varphi^*_{n'\mathbf{k}'}(\mathbf{r}') \tag{33}$$

and

$$v^{\mathrm{TF}}(\mathbf{r}-\mathbf{r}') = \frac{e^{-k_{\mathrm{TF}}|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\,, \tag{34}$$

with the Thomas-Fermi screening length, $k^2_{\mathrm{TF}} = 4\pi N(0)$. Finally, $N(0)$ denotes the total density of states at the Fermi level.

It should be noted here that these approximations, such as the partial linearisation, are used for all systems studied below, and hence the constructed exchange and correlation functionals remain truly universal.

6 Results

In order to assess the accuracy of the method and the functionals described above, we calculated the gaps and transition temperatures for a set of simple metals, including typical weak coupling systems, such as Al and Mo, but also the strong coupling metals Pb and Nb. Table 1 and Fig. 2 summarise the results and compare the theoretical values for the transition temperature and the gap at zero temperature with experimental values. The different theoretical results correspond to slightly different approximations to the electronic part of the xc pairing potential, which are described in reference [17]. The results demonstrate that the method works equally well for the weak coupling superconductors Al and Mo, as well as for intermediate (Ta) and strong coupling superconductors, such as Pb and Nb. It should be noted that we also applied the method to Cu, which does not show superconductivity in experiments, and we were not able to find a non-trivial solution of the gap equation, showing clearly that the theory is reliable.

Figure 3 shows the pair potential Δ_k plotted against the single particle energies $\epsilon_k - \mu$. The plots reveal how the retardation effects work in this formalism. As already pointed out by Morel and

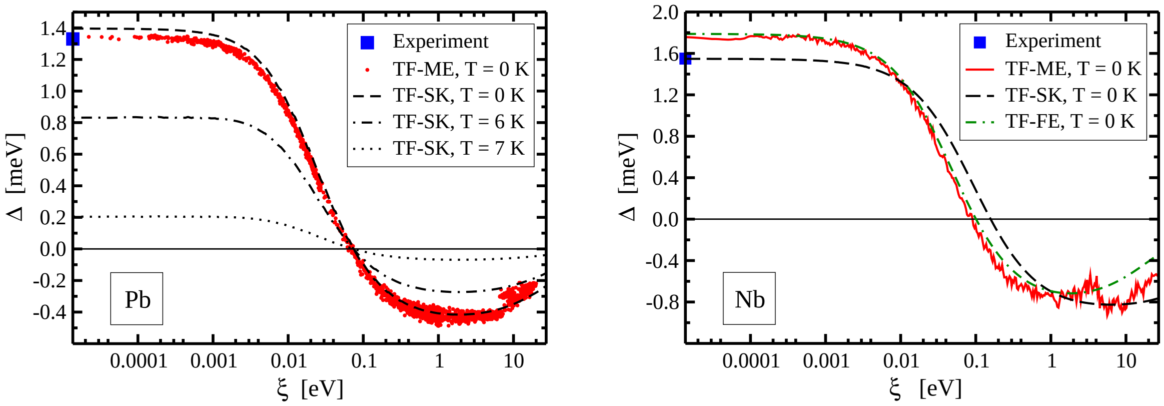

Figure 3: The function $\Delta(\xi_{n\mathbf{k}}, T)$ for lead (left panel) and niobium (right panel).

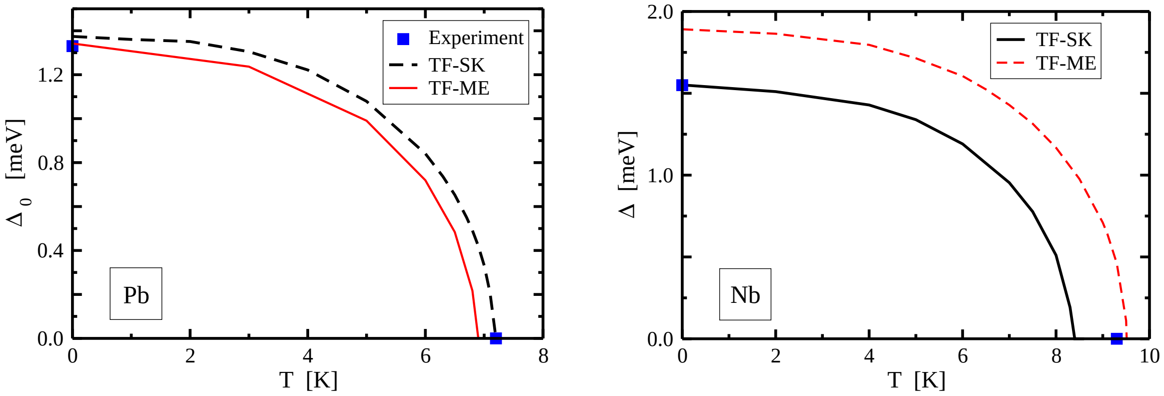

Figure 4: The gap function at the Fermi surface Δ_0 for Pb and Nb as a function of temperature.

Anderson [33], the system can benefit from the repulsive Coulomb interaction by changing sign of the pair potential away from the Fermi surface. In fact, our gap equation does not converge to a superconducting solution unless all electronic states in a large energy window are included. This is also the mechanism which in the Eliashberg theory gives rise to the renormalised Coulomb pseudopotential μ^*. It should be pointed out that no such pseudo-potential was used here. It is the full (screened) Coulomb interaction, that enters the corresponding term of the gap equation. The renormalisation is a result of our calculation. Finally, Figure 4 shows the temperature dependence of the gap.

The very satisfactory results for simple metals gave us confidence to apply the formalism also to non-trivial systems. A material that has raised much interest over the last years is $\mathrm{MgB_2}$. Although the material has been known and well-studied for a long time, its superconductivity with the critical temperature of 39.5 K (the highest among phonon-mediated superconductors) was discovered only recently. Its two-gap nature, observed experimentally, classifies this superconductor as a non-BCS superconductor, which makes it a very interesting and important test case.

The normal state of $\mathrm{MgB_2}$ is characterised by a Fermi-surface with several sheets of different orbital character (see e.g. Ref. [34]). In particular, the tubular structures with σ character are

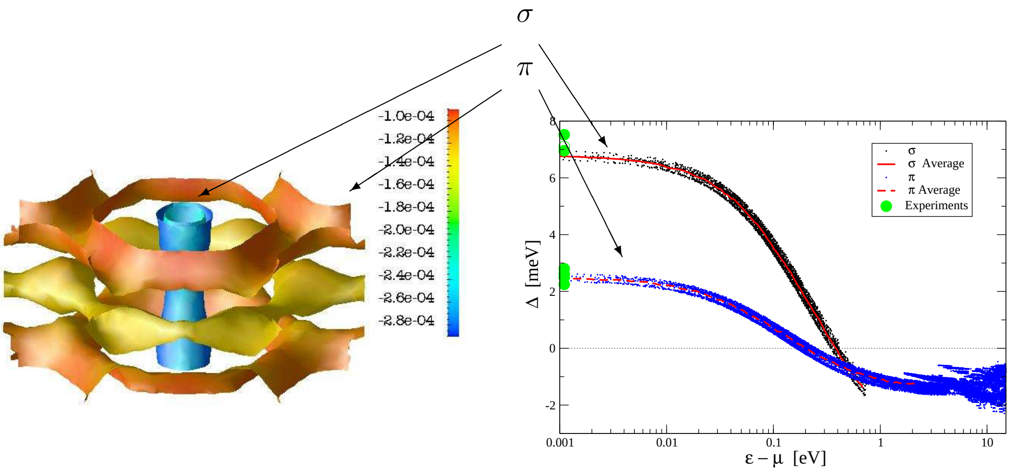

Figure 5: Calculated superconducting gap of $\mathrm{MgB_2}$ as a function of energy ($T = 0\,\mathrm{K}$). The two values correspond to the two sheets of the Fermi-surface, depicted in the left panel.

very strongly coupled to the E_{2g} phonon mode, that corresponds to a B-B bond-stretching in the boron planes [34–36]. $\mathrm{MgB_2}$ also has three-dimensional π bands, that give rise to a complicated Fermi surface. Without holes in the σ bands, the compound would not be superconducting, like $\mathrm{AlB_2}$. The π bands are coupled much less efficiently to phonons, but are nevertheless crucial to superconductivity.

In our density functional calculations we used the four, band resolved, Eliashberg functions, $(\alpha^2F_{n,n'}(\Omega); n, n' = \sigma, \pi)$, previously employed within a two-band Eliashberg scheme by Golubov *et al.* [37]. Our procedure keeps the fundamental distinction between σ and π gaps, analogously to the Eliashberg calculations reported to date. Further details of the calculation can be found in Ref. [38].

In Fig. 5 we plot the energy gap as a function of (positive) energy distance from the Fermi energy (the gap function exhibits particle-hole symmetry to a good extent). We can see that the two gaps of the material, Δ_σ and Δ_π, arise naturally from our calculations. The σ gap is defined only up to the energy of the top of the σ band. Both Δ_σ and Δ_π are anisotropic. This results from the anisotropy of the Coulomb potential matrix elements – roughly 0.4 meV, $\approx 6\%$ of Δ_σ at the FS – and gets much larger at high energy, where there are many bands with different character. The averages of Δ_σ and Δ_π at the Fermi level (6.8 meV and 2.45 meV respectively) are in excellent agreement with experiment.

In Fig. 6 (panel (**a**)), the superconducting gaps are plotted versus temperature, together with a few experimental results. The agreement is striking: the values of T_c (34.1 K) and of Δ_σ and Δ_π at $T = 0\,\mathrm{K}$ are very close to the experimental data. Moreover, the temperature behaviour of both gaps, along with their strongly non-BCS behaviour, are very well reproduced. Obviously, unlike calculations performed using the Eliashberg theory, we do not reproduce exactly the experimental critical temperature, as our calculations are not fitted to match any experimental quantity.

We also calculated the Kohn-Sham entropy as a function of temperature and, from its temperature derivative, the specific heat. In Fig. 6 (panel (**b**)), we plot our calculated versus the

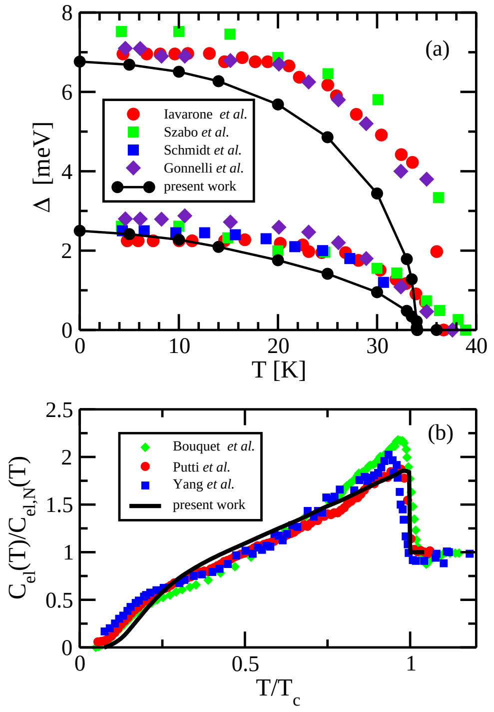

Figure 6: Superconducting gaps at the FS and specific heat of MgB_2. Panel (**a**): Comparison between theoretical and experimental gap at the FS plotted as a function of temperature. The calculated gaps and T_c (34.1 K) are obtained without the use of any adjustable parameter. Panel (**b**): Experimental and calculated electronic specific heat, as a function of T/T_c.

experimental (see Refs. [39–41]) reduced specific heat as a function of temperature, normalised to T_c. For T_c, we used the corresponding calculated and experimental values. Both the shape of the curve as well as the discontinuity at T_c are almost perfectly reproduced by the calculation. We recall that the shoulder of this curve at low temperature comes from the presence of the smaller π gap and that our Δ_σ/Δ_π is slightly different from the experimental ratio.

Another interesting application of the theory is the study of metals under high pressure. Within the class of phonon mediated superconductors, the effect of high pressure has been the subject of many investigations. These studies have revealed new peculiarities such as the strong material dependence of the onset of superconductivity at extreme densities: applied pressure suppresses superconductivity in some materials while favouring it in others [42]. Even for simple metals, the physics underlying pressure effects on the superconducting properties can be very complicated. For example, Li [42–49] and Al [50–52], despite behaving in many respects like nearly free electron gases, exhibit very different behaviours, still only partially understood within Eliashberg theory. At ambient pressure, Al is a superconductor with $T_c = 1.18\,\mathrm{K}$ [50]. Application of hydrostatic pressure rapidly reduces the critical temperature bringing it down to 0.075 K at 6.2 GPa [50]. Li, on the other hand, is a rather complex material, despite the popular belief that it behaves just like a simple metal. Below 77 K and zero pressure, it shows a martensitic transition to energetically competing closed packed structures [53]. From 7.5 to 70 GPa it undergoes several structural transitions [43] which may suggest the presence of strong e-ph interactions. No sign of a transition to a superconducting state was found up to ≈ 20 GPa. However, at higher pressures,

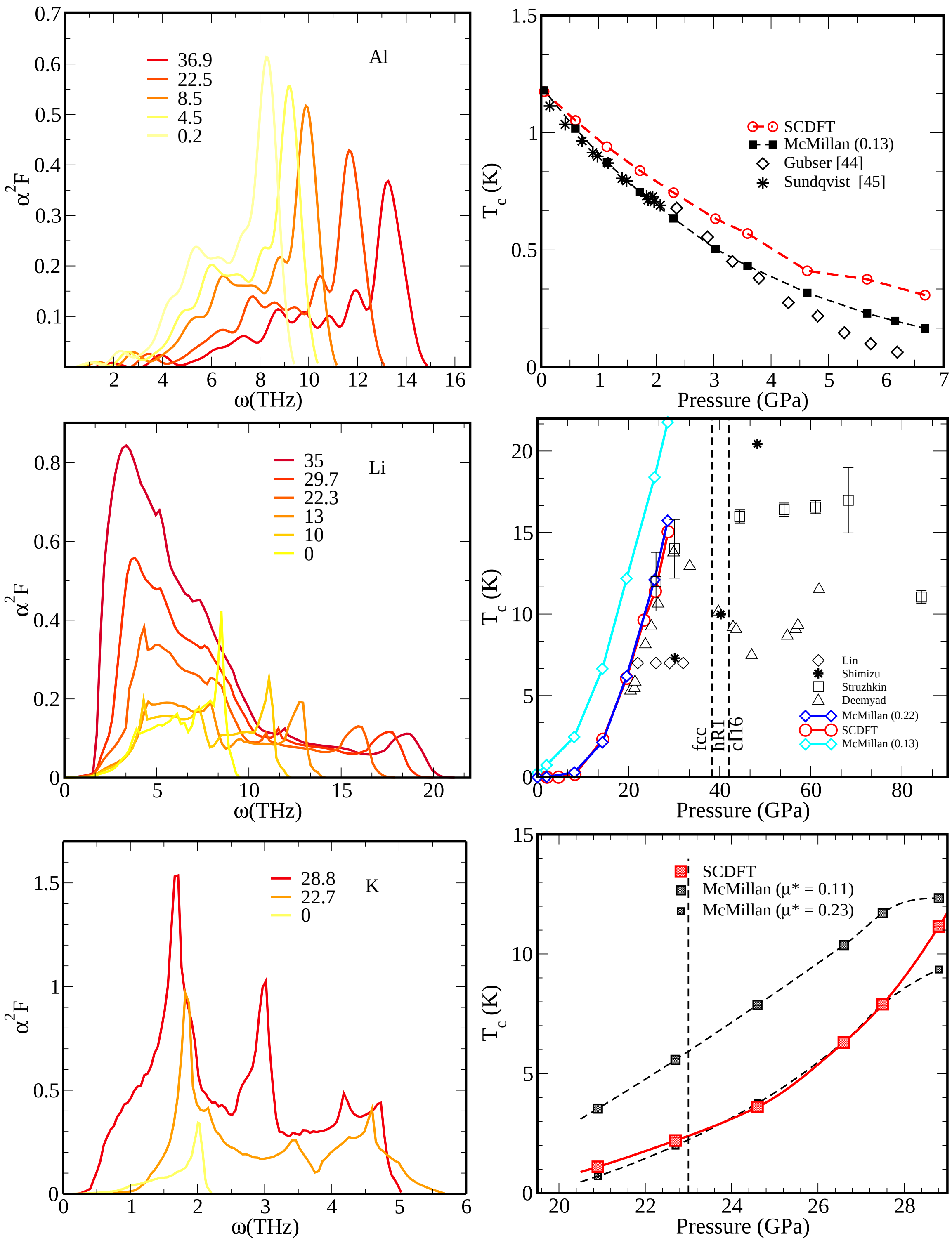

Figure 7: Left Column: Calculated $\alpha^2F(\omega)$ for Al (top), Li (middle) and K (down) at different pressures (inset in each graph). Right column: Calculated and experimental (for Al and Li) T$_c$ for fcc-Al (upper panel), fcc-Li (middle panel) and fcc-K (lower panel) as a function of pressure. Vertical dashed lines indicate the pressure values where structural transitions occur (see text). In the present work only the fcc phase was considered; therefore for Li at pressures larger than $\approx 39\,$GPa, where the fcc phase becomes unstable, our estimates cannot be compared to the experimental values.

Li becomes a superconductor [44–47]. In the range 20-38.3 GPa, where Li crystalizes in an fcc structure, experiments by Shimizu [45], Struzhkin [46], and Deemyad [47] found that T_c increases rapidly with pressure, reaching values around 12–17 K (one of the highest T_c observed so far in any elemental superconductor). However, experiments report different behaviours and quite large deviations.

In Fig. 7 we show the calculated pressure dependence of T_c for Al (upper panel), Li (middle panel), and K (lower panel), compared with experimental results. (Details about the calculations can be found in Refs. [54,55].) For Al, the calculated zero pressure T_c =1.18 K matches exactly the experimental value.[2] Upon compression, the calculation reproduces quite well the rapid decrease of T_c. A reduction by a factor of 10 with respect to the zero-pressure value is obtained at a pressure ($\simeq$ 8.5 GPa) slightly higher than experiment (6.2 GPa). Similar theoretical results are obtained within the standard McMillan formula [56] (open circles in Fig. 7) using μ^*=0.13 in agreement with previous calculations [52]. The small values of T_c in this pressure range make it quite difficult to extract a good estimate, from both experiments and theory. Nevertheless, the calculations show the asymptotic saturation of T_c rather than the linear decay suggested by experimental data. This discrepancy (with the only experiment available) calls for further experimental investigations in this pressure range.

In the middle panel of Fig. 7 we report the available experiments for Li compared with our calculated values. In the pressure range from 20 to 35 GPa, where the newer experiments [46,47] are in agreement and show a clear increase of T_c with increasing pressure, our calculated results reproduce the experimental trend of T_c and sit close to the experimental values. The calculated pressure which determines the onset of the superconducting state is about 10 GPa, where we predict $T_c \approx 0.2$ K. This finding agrees with Deemyad and Schilling [47], who claim that no superconducting transition above 4 K exists below 20 GPa. Our result is in good agreement with the highest measured T_c, 14 K [47], 16 K [46] and 17 K [45], and improves significantly upon the theoretical estimates by Christensen *et al.* [48], who discussed a paramagnon (i.e., spin fluctuations) dependent T_c varying between 45 and 75 K.

Due to the first principles nature of the method, it is feasible to make predictions on unknown superconductors: we apply the method to find a possible superconducting instability in potassium under pressure. Fcc-K shows a behaviour quite similar to Li: beyond a pressure threshold (20 GPa) T_c rises rapidly. In the range where phonons were found to be stable, it reaches $\sim$ 11 K; the experimentally observed instability of the fcc phase, however, limits this value to $\sim$ 2 K.

We relate the appearance of superconductivity in Li and K to an incipient phase transition, which gives rise to phonon softening and very strong electron-phonon coupling, that then leads to the unusually high transition temperatures. In addition, our calculations for Li and K confirm that a full treatment of electronic and phononic energy scales is required, which is in agreement with previous arguments by Richardson and Ashcroft [57].

The different behaviour of Al on one side and Li and K on the other can be understood by analysing the Eliashberg function as a function of pressure (see Fig. 7). In Al, the phonon

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[2] This value is slightly different from the ones reported in Table 1, where the e-ph λ included was taken from Ref. [32]. More details are given in Ref. [54].

frequencies increase as the pressure rises, corresponding to the normal stiffening of phonons with increasing pressure. In addition, the height of the peaks in the Eliashberg spectral function $\alpha^2F(\Omega)$ decreases with increasing pressure. These factors contribute to a decrease of the overall coupling constant λ and, consequently, of the critical temperature T_c.

For alkali metals the situation is completely different: due to the incipient phase transitions, a phonon softening at low frequencies increases the value of λ in both materials. However, the different topology of the Fermi surfaces and the different range of the phonon frequencies sets the critical temperature much higher in lithium with respect to potassium. For more details see Ref. [54, 55]

7 Conclusion

We have developed a truly ab-initio approach to superconductivity without any adjustable parameters. The key feature is that the electron-phonon interaction and the Coulombic electron-electron repulsion are treated on the same footing. This is achieved within a density-functional framework, based on three "densities": the ordinary electronic density, the superconducting order parameter, and the diagonal of the nuclear N-body density matrix. The formalism leads to a set of Kohn-Sham equations for the electrons and the nuclei. The electronic Kohn-Sham equations have the structure of Bogoliubov-de Gennes equations but, in contrast to the latter, they incorporate normal and anomalous xc potentials. Likewise, the Kohn-Sham equation describing the nuclear motion contains, besides the bare nuclear Coulomb repulsion, an exchange-correlation interaction.

The exchange-correlation potentials are functional derivatives of a universal functional $F_{\mathrm{xc}}[n, \chi, \Gamma]$ that represents the exchange-correlation part of the free energy. Approximations for this functional were then derived by many-body perturbation theory. To this end, the effective nuclear interaction was expanded to second order in the displacements from the nuclear equilibrium positions. By introducing the usual collective (phonon) coordinates, the nuclear Kohn-Sham equation is then transformed into a set of harmonic oscillator equations describing independent phonons. These non-interacting phonons, together with non-interacting but superconducting (Kohn-Sham) electrons serve as unperturbed system for a Görling-Levy-type perturbative expansion [58] of F_{xc}. The electron-phonon interaction and the bare electronic Coulomb repulsion, as well as some residual exchange-correlation potentials, are treated as the perturbation. In this way, both Coulombic and electron-phonon couplings are fully incorporated.

The solution of the KS-Bogoliubov-de Gennes equation (or the KS gap equation together with the normal-state Schrödinger equation) fully determines the Kohn-Sham system. Therefore, within the usual approximation to calculate observables from the Kohn-Sham system, one can apply the full variety of expressions for physical quantities, known from phenomenological Bogoliubov-de Gennes theory, also in the present framework.

Superconducting properties of simple conventional superconductors have been computed without any experimental input. In this way, we were able to test the theory and to assess the quality of the functionals proposed. The most important result is that the calculated transition temperatures and superconducting gaps are in good agreement with experimental values. The largest deviations from the experimental results are found for the elements in the weak coupling limit with Mo being the most pronounced example. We also calculated the isotope effect for Mo and Pb (see Ref. [17]), achieving again rather good agreement with experiment. These results clearly show that retardation effects are correctly described by the theory.

For MgB_2 we obtained the value of T_c, the two gaps, as well as the specific heat as a function of temperature in very good agreement with experiment. We stress the predictive power of the approach presented: Being, by its very nature, a fully ab-initio approach, it does not require semi-phenomenological parameters, such as μ^*. Nevertheless, it is able to reproduce with good accuracy superconducting properties, previously out of reach of first-principles calculations.

Finally, we also calculated the superconducting transition temperature of Al, K and Li under high pressure from first principles. The results obtained for Al and Li are in very good agreement with experiment, and account for the opposite behaviour of these two metals under pressure. Furthermore, the increase of T_c with pressure in Li is explained in terms of the strong e-ph coupling, which is due to changes in the topology of the Fermi surface, and is responsible for the observed structural instability. Finally, our results for fcc-K provide predictions interesting enough to suggest experimental work on this system.

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