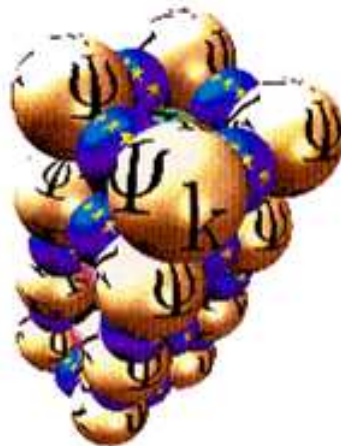


AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 97

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Contents

1 Editorial	4
2 Psi-k2010 Conference	5
2.1 Psi-k Volker Heine Young Investigator Award	5
3 Psi-k Activities	7
3.1 Reports on the Workshops supported by Psi-k	7
3.1.1 Report on Workshop Computational Physics and Chemistry of Graphene	7
3.1.2 Report on YRM2009	15
3.1.3 Report on Summer School	27
3.1.4 Report on 4th International TDDFT Workshop and School	47
3.1.5 Report on the Workshop "CATALYSIS FROM FIRST PRINCIPLES" . .	58
4 General Job Announcements	60
5 Abstracts	67
6 Presenting Other Initiatives	78
6.1 PEtot: A planewave pseudopotential DFT code for large system calculations . .	78
7 SCIENTIFIC HIGHLIGHT OF THE MONTH: "Recent Developments in KKR Theory"	79
7.1 Introduction	79
7.2 Basic idea of the KKR-GF method	80
7.3 The single-site problem	82
7.4 Multiple scattering	83
7.5 The single electron Green's function and Dyson's equation	85
7.6 Embedding of atoms clusters in a perfect host system	88
7.7 Treatment of chemical disorder	90
7.7.1 Magnetic Anisotropy and Exchange interaction	95
7.7.2 Magnetic response functions	98
7.7.3 Transport properties	99

7.7.4	Electron Spectroscopy	102
7.8	Concluding remarks	105

1 Editorial

First of all a very happy and successful year to all!

This first Psi-k Newsletter of 2010, No. 97, we start with reprinting after the Psi-k web pages the details on the "Psi-k Volker Heine Young Investigator Award" to be given at the forthcoming Psi-k2010 Conference in Berlin, in September 2010.

The newsletter is dominated by reports on the recent schools and workshops organized with support of the Psi-k Network. The reports are followed by a few position announcements and abstracts of newly submitted or recently published papers. After the abstracts we have a short information on a new plane wave pseudopotential code PEtot, for large system calculations, developed in the Lawrence Berkeley Laboratory.

This issue's scientific highlight is by Hubert Ebert (LMU Munich) and collaborators on "Recent Developments in KKR Theory", exposing its usefulness, flexibility, and numerous applications to complex systems of current interest.

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

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

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

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

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

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2 Psi-k2010 Conference

12-16 September, 2010

2.1 Psi-k Volker Heine Young Investigator Award

For excellence of research in all fields involving electronic structure calculations

Young computational science researchers are invited to put themselves forward for the Psi-k Volker Heine Young Investigator Award 2010. Finalists will compete at a special oral session of the big Psi-k Conference, Psi-k-2010.

Purpose:

The purpose of the Psi-k Volker Heine Young Investigator Award is to recognize an individual for her or his outstanding research in computer simulation of any type of material or in nano science or other condensed matter science using calculations of the electronic structure. In 2010 there will be one award of 2500 Euro and four runner-up prizes of 500 Euro each.

Regulations and Procedure:

- 1) Applicants may be of any nationality working anywhere in the world.
- 2) The applicant's PhD certificate must not be dated more than 5 years before the first day of the Psi-k-2010 conference (12 September 2010), and those who have not yet completed a PhD can also apply (up to 8 years after the first university degree).
- 3) Young investigators who wish to compete for the Psi-k Volker Heine Young Investigator Award 2010 must submit:
 - an abstract (in the format of the poster-submission abstract for the conference) a two-page description making the case for her/his outstanding scientific contribution
 - an extended CV (incl. list of publications and talks/posters) evidence of satisfying the conditions of regulation (2) above.

These items must be submitted by email, as a pdf attachment, to the chairperson of Psi-k.org whose address is given below. It must be received not later than 2 weeks before the official abstract submission deadline of the Psi-k Conference, i.e. before 17 April 2010. The abstract must also be submitted as a regular contribution to the Psi-k Conference following the standard procedure.

- 4) The candidate must arrange for two confidential support letters to be sent directly by the writers to the Psi-k chairperson (see below). These letters (sent by email) need to be received before 17 April 2010. One of the letters must certify that the candidate meets the requirements of regulations (2) above.

5) The award committee will select five finalists who will get an invitation to present their work at the Psi-k Conference (25 min. talk + 5 min. discussion). After these presentations, the award committee will select the award winner.

6) The award winner will receive her or his award of 2500 Euro and the four runner-up their prizes of 500 Euro each, together with a certificate, at a presentation before the end of the conference.

Prize Committee:

The prize committee will consist of:

- Volker Heine
- Three Trustees of Psi-k.org
- Three well recognized international members of the computational science community (limited to one term) as determined by the Psi-k.org board of trustees.

Chairperson of Psi-k:

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3 Psi-k Activities

”Towards Atomistic Materials Design”

3.1 Reports on the Workshops supported by Psi-k

3.1.1 Report on Workshop Computational Physics and Chemistry of Graphene

Lausanne, Switzerland

October 14–16, 2009

Sponsors: CECAM, Psi-k, QuantumWise A/S

Organizers: Oleg YAZYEV (UC Berkeley, USA), Mikhail KATSNELSON (Radboud University Nijmegen, NL), Annalisa FASOLINO (Radboud University Nijmegen, NL)

<http://www.cecama.org/workshop-302.html>

<http://civet.berkeley.edu/~yazyev/Graphene2009>

Summary

Graphene is a two-dimensional hexagonal allotrope of carbon. Since its isolation in 2004, this seemingly simple material has revealed a number of intriguing physical properties. Immediately, this series of discoveries ignited an ever-growing interest among researchers coming from various disciplines of basic and applied science. This workshop was the first attempt to bring together computational scientists working on various aspects of graphene physics and chemistry under the roof of CECAM. The workshop aimed at a broad coverage of computational methods applied to study graphene and its properties. The challenges posed by graphene for theory and computation are related with the following issues:

- Identification of the main factors limiting electron mobility in graphene and search for ways to increase it further. This requires taking into account not only the electronic structure of pristine graphene but also its structural properties, like ripples, defects, edges. For computation this implies either very large samples or strong approximations.
- Modification of electronic structure meant to open a gap that is needed for development of graphene transistors and other applications in electronics. This can be done either by size quantization in graphene quantum dots and nanoribbons or by chemical functionalization. The importance of computational methods in this respect is demonstrated by the discovery of graphane (a fully hydrogenated graphene) which was first predicted theoretically and then synthesized, showing the predicted insulating behavior.

- Search for procedures of mass production of graphene. This aspect requires a detailed description of its chemistry and interactions with different solvents, substrates, intercalation processes, etc.
- Graphene-based spintronics related with the very weak spin-orbit coupling and small concentration of nuclear spins which allows expecting very long-lived spin-polarized states, governed by electric current.
- Possible ferromagnetism with high Curie temperature in carbon-based materials.
- Peculiarities of electronic properties and possible applications of systems made of a few layers of graphene. These systems pose important, not yet fully solved, problems for computations within the Density Functional approach because of the dipolar interlayer interactions.

For all these questions, one can benefit from studying also other carbon systems, like nanotubes and fullerenes as well as hexagonal BN and bulk graphite.

To address these problems the workshop was divided into sessions devoted to the following topics:

- Electronic structure and transport properties of graphene
- Magnetism, spintronics and quantum computing
- Optical properties of graphene
- Structure, defects and edges
- Interaction with substrates and adsorbates
- Chemical functionalization and reactivity

The workshop took place at the new location of CECAM headquarters in Lausanne, Switzerland. The program consisted of three full days of intensive talks and a poster session. The total number of registered participants was 45, including 3 organizers, 20 invited speakers and 1 representative of a sponsoring organization (QuantumWise A/S, Denmark). In fact, the number of applications for participating the workshop was significantly larger than the established limit of 50 participants. This illustrates very well the growing interest to graphene in the community of computational researchers. Geography of the workshop participants covers most of the countries in western and central Europe, USA, Singapore and South Korea.

The oral presentations were given by invited speakers. However, during a dedicated session all contributing participants were invited to give short talks summarizing their poster presentations. Many contributing participants used this opportunity to expose their research. In addition to the researchers working in various fields of computational science, three talks were given by the leading experimentalists. In particular, Irina Grigorieva (University of Manchester, UK) spoke on the recent studies of the magnetic properties of graphene performed in the group of Andre Geim, where graphene has been isolated for the first time. Andrea Ferrari (University of

Cambridge, UK) gave a talk on the optical properties of graphene with a particular emphasis on the applications of this material in optoelectronics. An extensive overview of epitaxial graphene grown on a variety of metal surfaces was presented by Thomas Greber (University of Zurich, Switzerland).

Anders Blom (QuantumWise A/S, Denmark) offered a tutorial talk on the methodological aspects of Atomistix ToolKit, a software package for modeling electronic transport in nanostructures developed by QuantumWise A/S. Specific examples of the applications to graphene nanostructures have been shown.

The other invited speakers reported their latest progress in studying graphene *in silico*. The organizers did not constrain the speakers in choosing the subjects of their talks. However, all major trends in the current computational research of graphene have been covered in the final program. Electronic transport of graphene still receives particular attention (M. Lazzeri, E. Molinari, P. Ordejon, J.C. Charlier). Several speakers covered the related field of spintronics and magnetic properties of graphene nanostructures (J. Fernandez-Rossier, E. Kaxiras, P. Kelly). A very novel and promising subject is the engineering of electronic structure by use of strain. This topic was discussed by F. Guinea and Y.W. Son. Another emerging topic is related to the chemical properties of graphene. Various aspects of graphene chemistry have been covered, in particular, graphene/substrate interactions and relation to SiC and BN (L. Magaud, Y.W. Son, T. Greber), tuning the properties of graphene by adsorbates (T. Wehling, A. Lichtenstein), chemical functionalization (B. Sanyal). Modelling defects in graphene and related carbon nanostructures was another major focus of computational research covered at the workshop (D. Tomanek, A. Krasheninnikov). Topological defects such as grain boundaries and dislocations are now gaining increasing attention (O. V. Yazyev, J. Carlsson). The effect of edges was discussed in several talks (in particular D. Gunlycke, J.C. Charlier, B. Sanyal)

The workshop was sponsored by the Centre Européen de Calcul Atomique et Moléculaire (CE-CAM), the Psi-k Network, and QuantumWise A/S. The organizers and participants of the workshop thank these organizations for their generous support for the workshop.

We are pleased to conclude that the workshop was highly successful. The feedback from the workshop participants was very positive.

Programme

Day 1 – October, 14th 2009

08:30 to 09:00 – Welcome

09:00 to 09:40 – Michele Lazzeri

Transport properties of graphene in the high-current limit

09:40 to 10:20 – Elisa Molinari

Illuminating graphene nanostructures: nanoribbons and dots vs. nanotubes

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – Alexander Lichtenstein

Impurity states and electron scattering in graphene

11:30 to 12:10 – Irina Grigorieva

Magnetism in graphene-based systems: experiment

12:10 to 14:00 – Lunch Break

14:00 to 14:40 – Oleg Yazyev

Imperfect graphene: point defects, edges, dislocations and grain boundaries

14:40 to 15:20 – Joaquin Fernandez-Rossier

Spintronics and magnetism in graphene nanostructures

15:20 to 15:50 – Coffee Break

15:50 to 16:30 – Efthimios Kaxiras

Graphene nano-flakes with large spin as structural elements for all-carbon spintronics devices

16:30 to 18:00 – Poster highlights

18:00 to 19:30 – Poster Session

Day 2 – October, 15th 2009

09:00 to 09:40 – Tim Oliver Wehling

Adsorbates and inhomogeneities on graphene: first principles studies

09:40 to 10:20 – Biplab Sanyal

Chemical functionalisation of graphene, experiment and theory

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – Pablo Ordejon

Transport properties of Carbon Nanotube links connecting Graphene layers

11:30 to 12:10 – Anders Blom

Modeling of graphene nanotransistors

12:10 to 14:00 – Lunch Break

14:00 to 14:40 – Francisco Guinea

Strains and electronic transport in graphene

14:40 to 15:20 – Jean-Christophe Charlier

Electronic Quantum Transport in Graphene Nanoribbons

15:20 to 15:50 – Coffee Break

15:50 to 16:30 – Thomas Greber

Corrugated and Chiral Graphene and Boron Nitride single layers on transition metals

16:30 to 17:10 – Andrea Ferrari

Strain and Photoluminescence in Graphene

17:10 to 17:50 – David Tomanek

Probing and changing graphene with electric current and light

20:00 to 23:00 – Dinner

Day 3 – October, 16th 2009

09:00 to 09:40 – Laurence Magaud

Atomic and electronic structure of graphene on SiC

09:40 to 10:20 – Young-Woo Son

Electronic properties of graphene under external perturbations

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – Paul Kelly

The ultimate HYPE: materials for Highly Planar Electronics

11:30 to 12:10 – Johan Carlsson

Structural and Electronic Properties of Grain Boundaries in Graphene

12:10 to 14:00 – Lunch Break

14:00 to 14:40 – Arkady Krasheninnikov

Ion and electron irradiation of graphene

14:40 to 15:20 – Daniel Gunlycke

The effects of edges on the electronic and transport properties of graphene nanoribbons

15:20 to 16:20 – Closing word

List of poster presentations

P1 – Angela Acocella

Coronene XPS spectrum: electron dynamics simulations

P2 – Nicolae Atodiresei

Control of magnetization direction in molecules formed by π -ligands and 4f-metals

P3 – Soumya Bera

Structural properties and elasticity of graphene flakes: density functional study

P4 – Manuel Cobian Gonzalez

Electron transport simulations through organic adlayers on metal surfaces

P5 – Martin Gradhand

Spin relaxation time in graphene induced by impurities

- P6 – Petr Khomyakov
Nonlinear screening of charges induced by metal contacts in graphene
- P7 – Jani Kotakoski
Simulations of electron beam damage on graphene
- P8 – Alexey Kuzmenko
Infrared observation of the bandgap and phonon anomalies in gated bilayer graphene
- P9 – Predrag Lazic
Graphene on Ir(111) surface: From van der Waals to strong chemical bonding
- P10 – Ortwin Leenaerts
Hydrogenation of bilayer graphene
- P11 – Tony Low
Ballistic-Ohmic quantum Hall plateau transition in graphene p-n junction
- P12 – Georgo Metalidis
Disorder-induced pseudodiffusive transport in graphene nanoribbons
- P13 – Marcel Mohr
Exploring the two-dimensional Brillouin zone of the electronic and the vibrational band structure of uniaxially strained graphene
- P14 – Branislav K. Nikolić
Nonequilibrium phase transitions and shot noise as all-electrical probes of magnetism in zigzag graphene nanoribbons
- P15 – Ivan Oleynik
Computational Nanomechanics of Graphene
- P16 – Julien Ruppen
Ab-Initio Study of the Graphene/SiC Interface
- P17 – Jiatao Sun
Linearly doped graphene by charge transfer complex
- P18 – Manfred Taut
Co dimers on graphene proposed as magnetic storage bits
- P19 – Michiel van Setten
Band structure engineering in graphene Ribbons by edge chemistry
- P20 – Marco Vanin
Graphene on metals
- P21 – Wei Wang
Graphene nanostructures and their fabrication

List of participants

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Mikhail KATSNELSON (*Radboud University Nijmegen, NL*)

Oleg YAZYEV (*University of California at Berkeley, USA*)

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Anders BLOM (*QuantumWise A/S, DK*)

Johan CARLSSON (*Fritz-Haber-Institut and Accelys GmbH, DE*)

Jean-Christophe CHARLIER (*University of Louvain, BE*)

Joaquin FERNANDEZ-ROSSIER (*University of Alicante, ES*)

Andrea FERRARI (*University of Cambridge, UK*)

Thomas GREBER (*University of Zurich, CH*)

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Paul KELLY (*University of Twente, NL*)

Arkady KRASHENINNIKOV (*University of Helsinki, FI*)

Michele LAZZERI (*Université Pierre et Marie Curie, FR*)

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Elisa MOLINARI (*Università di Modena, IT*)

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3.1.2 Report on YRM2009

Sixth International Young Researchers Nanoquanta-ETSF Meeting (YRM2009)

Berlin, June 2nd-6th, 2009

Sponsors: DFG, Psi-k, ETSF, Free University Berlin

Organizers: Ali Abedi, Tim Baldsiefen, Christophe Bersier, Alberto Castro, Kay Dewhurst, Florian Eich, Frank Essenberg, Andrea Floris, Henning Glawe, Elham Khosravi, Kevin Krieger, Andreas Linscheid, Danilo Nitsche, Stefano Pittalis, Antonio Sanna, Sangeeta Sharma and Angelica Zacarias

Web Page: <http://www.nanoquanta.de/yrm2009/open/index.xhtml>

Short Report:

The Organizing Committee of the Sixth International Young Researchers Nanoquanta-ETSF Meeting (YRM2009) was composed of members of the ETSF-FUB Node located at the Theoretical Physics Department of the Free University Berlin. The full list of the organizing committee can be found on the conference web site: <http://www.nanoquanta.de/yrm2009>

This meeting was funded mainly through the “Deutsche Forschungsgemeinschaft” and the Ψ_k Network. The program included 8 hour-long Keynote talks and 29 short talks. There were 28 posters and a total of 89 participants, 35 of which were Bachelor and PhD students.

The YRM2009 brought together young researchers, comprising PhD students and postdocs working on applications and code development in diverse fields of theoretical physics. The scientific program covered areas from spectroscopy to electron correlation systems, molecular transport and nanostructural properties and some aspects of superconducting systems.

This meeting offered a unique opportunity for the attendees to have an open exchange of ideas and gain a better understanding of the theoretical and computational aspects of spectroscopy. Participants in their initial stage of research have the opportunity to discuss in more detail their project challenges, and the forum enables them to establish contact with other young researchers working in fields of mutual interest, as well as allowing them to build scientific relations with more experienced members of the community.

New developments in the study of the transport properties of molecular devices were presented, as well as some aspects of the transport properties of carbon nanotubes. The key concepts

in the comprehension of the phenomenon of superconductivity were described, with particular emphasis on the recently developed superconducting DFT and its application to real materials.

State-of-the-art methods for treating electron correlations were covered. Recent advances in theoretical approaches to spectroscopic studies for diverse materials were exposed during the conference talks. The application of theoretical tools, including codes developed within the ETSF community, like ELK, Abinit, Octopus, DP, EXC, etc., to the study of nanostructures and biological systems provided an overview of the state-of-the-art tools available to aid in the understanding of electronic and spectroscopic properties of diverse molecular and solid state systems (i.e. dynamics of chemical and physical reactivity of molecular and biological systems, cubic ice and time-dependent studies of silicon).

The conference program also offered interaction with industrial and experimental participants, highlighting from one side the practical aspects of the gathered experiences in a theoretical research group during graduate studies and from another side the current collaborations between experimental and theoretical groups. Additionally, there was an opportunity for the participants to learn some aspects of gender and social issues that might hinder or facilitate research in different work environments.

We are pleased to report that the feedback from the participants was encouragingly positive.

Program

	Tuesday 2	Wednesday 3	Thursday 4	Friday 5
		Welcome		
9:00		Keynote 1	Keynote 3	C. Meisenbichler
9:20		Transport	Spectroscopy	J. Wang
9:40		Frank Ortmann	Eleonora Luppi	Keynote 5
10:00		J. Hashemi	H. Huebener	Electron Correlat.
10:20		A. Lherbier	S. Sagmeister	Daniel Rohr
10:40		Coffee break	Coffee break	Coffee break
11:00		P. Myohanen	L. Espinosa Leal	P. Buczek
11:20		H. Ness	J. Vidal	F. Essenbergler
11:40		D. Nitsche	V. Garbuio	M. Guzzo
12:00		Lunch break	Lunch break	Lunch break
		(12:00-13:30)	(12:00-13:30)	(12:00-13:30)
13:40		Keynote 2	Keynote 4	A. Miglio
14:00		Superconductivity	Nanostruc. & Bio	C. Panse
14:20		Gianni Profeta	Daniele Varsano	G. Pegolotti

14:40		E. Cannuccia	X. Declerck	R. Requist
15:00		P. Cudazzo	K. Krieger	Coffee break
15:20		Coffee break	Coffee break	Gender &
15:40		H. Glawe	A. Mosca Conte	social issues
16:00		M. Monni	N. Spallanzani	Kerstin Palm
16:20	Arrival	Experimental talk	Industry talk	
16:40		Karsten Heyne	Jan Werschnik	
17:00				
17:20		ETSF G. Bruant	Poster Session	
17:40		ETSF Software		
18:00	Welcome			
18:20	reception			
19:00				Social dinner

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3.1.3 Report on Summer School

”Simulation Approaches to Problems in Molecular and Cellular Biology”

Miramar Palace, San Sebastián (Spain)

31 August-4 September 2009

School directors:

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Michele Parrinello (ETH Zürich and Appl. Biosciences Lugano, Switzerland)

Ursula Röthlisberger (EPFL, Lausanne, Switzerland)

Local organizers:

Daniel Sánchez-Portal (CSIC-UPV/EHU and DIPC, San Sebastián, Spain)

Angel Rubio (UPV/EHU and DIPC, San Sebastián, Spain)

Sponsors: Psi_k, CECAM, ESF and DIPC

Web sites:

<http://www.sissa.it/sbp/SSSAPMCB/index.htm>

<http://www.cecama.org/workshop-0-340.html>

http://dipc.ehu.es/ws_presentacion.php?id=46

The Summer School on *Simulation Approaches to Problems in Molecular and Cellular Biology* was held in the Miramar Palace, San Sebastián, Spain from August 31 to September 4, 2009. The main goal of the School was to present the latest developments and applications of biomolecular simulation approaches aimed at predicting structure, dynamics and energetics of biomolecules. Aspects of bioinformatics-based structural prediction algorithms were also discussed.

The topics treated included:

- Simulation of rare events
- Prediction from first principles of spectroscopic and redox
- Protein and nucleic acid structure prediction
- Critical analysis of the force fields used for biomolecular simulation
- Molecular simulation of cellular events

Table 1: Nationalities of the students attending the Summer School

Country	Number of Students
Australia	1
Belgium	2
Bulgaria	1
China	2
Egypt	1
France	6
Germany	4
Greece	2
India	3
Island	1
Italy	14
Korea	2
Luxembourg	1
Malaysia	1
Mexico	1
Poland	2
Russia	5
Spain	15
Switzerland	3
Thailand	1
Turkey	1
USA	1
Vietnam	2

- Simulation in molecular medicine

During the Summer School some of the most important experts in the field presented the latest developments in the theory, methodology and applications of molecular dynamics simulations applied to the biological problems described in more detail below.

There was a total of 92 assistants:

- 72 students (25 females and 47 males)
- 20 invited speakers and organizers (4 females and 16 males)

The students of the School came from 23 different countries (see Table 1 and the List of Participants below) working in Institutions from 16 different countries. The invited speakers and the organizers work in 8 different countries (see the List of Participants below).

40 of the students (55%) have received support for traveling (the average amount of this financial aid has been 478.70 euros).

Scope of the School

Cellular functions - like growth, (programmed) cell death, metabolism, etc. - ultimately depend of interactions between macromolecules encoded by DNA. Proteins and RNA directly control the cell and regulate its functions through the reactions they perform, by allosteric changes driven by endogeneous and exogeneous factors and by their mutual interactions.

All of these processes involve molecular recognition, i.e. the process by which two or more biological molecules interact to form a specific complex. Molecular recognition is dominated by short-range, often transient, interactions at the contact surface of the interacting molecules. Even conformational changes and assembly of very large macromolecular aggregates, which can be propagated through long distances (tens of Angstroms), are the sum of local interactions between small molecules (like messengers) or macromolecules with their cellular targets.

Ultimately, therefore, even the understanding of the integration of biological complexes into cellular pathways (the so called 'systems biology') requires mechanistic understanding of the physical basis of molecular recognition. A quantitative description of cellular pathways in molecular terms is still mostly missing, although it would strongly impact on pharmaceutical sciences, as drugs target (and mutations affect) pathways, rather than single biomolecules. Such information is also crucial in nanobiotechnology, e.g. to design artificial sensing devices, which in Nature involve entire cascades of events and not only a single protein.

Molecular simulation constitute a key field to contribute to this issue. It can predict structure, dynamics, energetics, reactivity and spectroscopic properties of the cellular components (i.e. large macromolecular aggregates) involved in these pathways.

Tremendous challenges have to be taken before this ambitious goal can be reached. First, the systems are very complex and so are the interactions involved. In addition, ligand-protein processes involve small changes of free energies (less than 1 eV for non-covalent protein-protein interactions), and they are often entropy-driven. Next, the environment is very complex: cell membranes are far from being a simple lipid bilayer whilst the cytoplasm is far from being a simple aqueous solution. Finally, most often experimental structural information is partially or totally lacking. These issues and challenges have been discussed in detail in the Summer School on *Simulation Approaches to Problems in Molecular and Cellular Biology*.

Programme of the School

Monday, 31st August 2009

Chairperson: Gregory A. Voth

09:00 - 09:40 J. Hutter/ University of Zurich, Switzerland

Progress in large scale density functional calculations

09:40 - 10:20 J. Hutter/ University of Zurich, Switzerland

Calculation of NMR and EPR parameters for proteins in solution

10:20 - 10:50 — Coffee Break —

10:50 - 11:30 F. Alber/ UCLA, Los Angeles, USA

Determining the structures of macromolecular assemblies - Part 1

11:30 - 12:10 F. Alber/ UCLA, Los Angeles, USA

Determining the structures of macromolecular assemblies - Part 2

12:10 - 14:00 — Lunch Break —

Chairperson: Angel Rubio

14:00 - 14:40 G. A. Voth/ University of Utah, Salt Lake City, USA

Rigorous coarse-graining of condensed phase and biomolecular systems

14:40 - 15:20 G. A. Voth/ University of Utah, Salt Lake City, USA

Multiscale modeling of proteins and membranes: from the molecular to the mesoscale

15:20 - 16:00 — Coffee Break —

16:00 - 16:40 M. Cascella/ UNIBE, Bern, Switzerland

Development of unbiased coarse grained potentials for simulations of proteins

16:40 - 17:20 M. Dal Peraro/ EPFL Lausanne, Switzerland

Coarse-grained electrostatics in multiscale simulations of proteins

Tuesday, 1st September 2009

Chairperson: Michele Parrinello

09:00 - 09:40 R. Lavery/ Institut de Biologie et Chimie des Proteines, Lyon, France
DNA dynamics and recognition

09:40 - 10:20 R. Lavery/ Institut de Biologie et Chimie des Proteines, Lyon, France
Coarse-grain models of protein mechanics

10:20 - 10:50 — Coffee Break —

10:50 - 11:30 M. Orozco/ Institute for Research in Biomedicine, Barcelona, Spain
Pushing the boundary of MD simulations. Proteome scale atomistic simulations

11:30 - 12:10 M. Orozco/ Institute for Research in Biomedicine, Barcelona, Spain
Coarse grained dynamics simulations of proteins and nucleic acids

12:10 - 14:00 — Lunch Break —

Chairperson: Mike Klein

14:00 - 14:40 M. Sulpizi/ University of Cambridge, Cambridge, UK
Redox properties in metalloproteins

14:40 - 15:20 M. Sulpizi/ University of Cambridge, Cambridge, UK
Pka calculations from DFT-based MD simulations

15:20 - 16:00 — Coffee Break —

16:00 - 16:40 M. Dal Peraro/ EPFL Lausanne, Switzerland
Proton conduction and drug binding in the M2 channel from Influenza A virus

16:40 - 17:20 M. Cascella/ UNIBE, Bern, Switzerland
Electronic structure/function relationship in copper-bound redox proteins

Wednesday, 2nd September 2009

Chairperson: Ursula Rothlisberger

09:00 - 09:40 F. Gervasio/ Fundacion CNIO - Carlos III, Madrid, Spain

Quantitative structure-activity relationship with Metadynamics and Path-collective variables: ligand binding

09:40 - 10:20 F. Gervasio/ Fundacion CNIO - Carlos III, Madrid, Spain

Quantitative structure-activity relationship with Metadynamics and Path-collective variables: conformational selection and induced fold effects

10:20 - 10:50 — Coffee Break —

10:50 - 11:30 S. Piana/ D.E. Shaw Research, New York, USA

The precision and accuracy problems in MD simulations

11:30 - 12:10 S. Piana/ D.E. Shaw Research, New York, USA

Improving force fields for MD simulations

12:10 - 14:40 — Lunch Break —

Chairperson: Juerg Hutter

14:40 - 14:40 A. Rubio/ ETSF, Donostia-San Sebastian, Spain

First principles description of the optical properties of biochromophores

15:20 - 16:00 — Coffee Break —

16:00 - 16:40 I. Tavernelli/ EPFL, Lausanne, Switzerland

TDDFT as a tool in chemistry and biology

16:40 - 17:20 I. Tavernelli/ EPFL, Lausanne, Switzerland

Light driven reactions in biological systems

Thursday, 3rd September 2009

Chairperson: Paolo Carloni

09:00 - 09:40 C. Rovira/ ICREA, Barcelona, Spain

Substrate conformational changes in glycoside hydrolase catalysis

09:40 - 10:20 C. Rovira/ ICREA, Barcelona, Spain

The reaction mechanisms of heme peroxidases by QM/MM simulations

10:20 - 10:50 — Coffee Break —

10:50 - 11:30 H. Grubmüller/ MPI, Gottingen, Germany

Conformational motions of biological macromolecules

11:30 - 12:10 H. Grubmüller/ MPI, Gottingen, Germany

Molecular dynamics simulations of biological nanomachines: may the force be with you

12:10 - 14:00 — Lunch Break —

14:00 - 18:00 Poster Session

Friday, 4th September 2009

Chairperson: Helmut Grubmüller

09:00 - 09:40 S. Raugei/ SISSA and INFM-DEMOCRITOS, Trieste, Italy

Computational vibrational spectroscopy for biomolecules: basics

09:40 - 10:20 S. Raugei/ SISSA and INFM-DEMOCRITOS, Trieste, Italy

Computational vibrational spectroscopy for biomolecules: an application to the bacterial resistance to antibiotics

10:20 - 10:50 — Coffee Break —

10:50 - 11:30 L. Guidoni/ Universit degli Studi dell'Aquila, L'Aquila, Italy

Computing vibrational spectra of biomolecules by Quantum Mechanics / Molecular Mechanics simulations

11:30 - 12:10 L. Guidoni/ Universit degli Studi dell'Aquila, L'Aquila, Italy

First principles calculations of photoreceptors

12:10 - 16:00 Poster Session with Buffet

Chairperson: Paolo Carloni

Participant talks

16:00 - 16:20 Brunk Elizabeth / EPFL, Lausanne, Switzerland

16:20 - 16:40 Zhu Lihze / University of Amsterdam, Amsterdam, The Netherlands

16:40 - 17:00 Losasso Valeria/ SISSA, Trieste, Italy

17:00 - 17:20 — Coffee Break —

17:20 - 17:40 Tipmanee Varomyalin / University of Cambridge, Cambridge, UK

17:40 - 18:00 Deplazes Evelyne / University of Western Australia, Crawley, Australia

18:00 - 18:20 Delemotte Lucie / Universit Henri Poincar, Nancy, France

18:20 - 18:40 Concluding Remarks

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3.1.4 Report on 4th International TDDFT Workshop and School

TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY: PROSPECTS AND APPLICATIONS

4th International Workshop and School

Benasque (Spain), January 2 – 15, 2010

A. Rubio (Univ. País Vasco and ETSF, Spain),
E. K. U. Gross (MPI Halle, Germany),
M. A. L. Marques (LPMCN, Universit Lyon I, France),
F. Nogueira (CFC, Univ. de Coimbra, Portugal)

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SPONSORED BY:

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ESF SimBioMa Programme
ESF IntelBioMat Programme
CECAM
Spanish Ministry of Science and Technology
Benasque Center for Science
Universities of the Basque Country and Coimbra

The fourth school and workshop was hosted, as the previous ones, by the Benasque Center for Science. The aim of the school was to introduce theoretical, practical, and numerical aspects of time-dependent-density functional theory (TDDFT) to young graduate students and post-docs interested in the tool in itself or planning to use it for their own research. The physical conditions offered by the new Benasque Center for Science (<http://www.benasque.org/>) allow for a very fruitful and informal contact between the students and the teachers, that we strongly encouraged.

All the pedagogical documents of the school are made available to the everybody through the webpage of the meeting (<http://www.benasque.org/2009tddft/>). Also, as in previous editions we provided all the students with the book "Time-Dependent Density-Functional Theory", edited by M.A.L. Marques, C. Ullrich, F. Nogueira, A. Rubio, and E.K.U. Gross, *Lecture Notes in*

Physics (Springer: Berlin, 2006), as it has all the basic material to be discussed in the lectures. We plan to have a new edition of the book (completely revised based on the input of the students in the last schools) by the next event (5th school to be held in Benasque also in winter, January, 2012).

In order to allow for the students to better discuss their research projects among themselves and with the teachers of the school, we asked them to present posters describing their current work and/or planned research project. Two of these posters were then selected as oral contributions to the international workshop and were granted the second Pedro Pascual Prize for the best posters of the school. As in previous editions of this event, the number of applications (above 180, the largest of all the events organised till now) surpassed all expectations and, of course, also the limit of 48 places that we had to satisfy in order for the students to get the maximum benefit from the school, and also due to space and computer resource limitations. The participants in the school were distributed in the following way:

Sex	PhD students	Post-docs	Total
Female	9	2	11
Male	25	12	37

All the students participated also in the workshop held just after the 8 days of school. The total number of participants was 101, with 31 different nationalities from 5 continents. There were 21 female participants, six of them being invited speakers/lecturers. The distribution between countries, experience and gender is provided in the following table:

	School	Teachers	Invited	Workshop	Total
Argentina	1				1
Australia	1		1		2
Austria	1		1		2
Belgium	1	1			2
Canada			1		1
Chile		1			1
China	1				1
Colombia	1			1	2
Czech Republic	1				1
France	1		1	1	3
Germany	5	4	5	4	18
India	4				4
Iran	1			1	2
Ireland		1			1
Israel			2	1	3
Italy	7	6	2	2	17
Japan			1	1	2
Korea	1				1
Mexico	1				1
Morocco	1				1
New Zealand		1			1
Portugal	1	3	1		5
Romania	1				1
Russia	2	1	2		5
Spain	6	3	1	1	11
Sweden	1				1
Switzerland		1	1		2
Turkey	1				1
UK	4				4
Ukraine	1				1
USA	3				3
Male PhD	25	2		5	32
Female PhD	9			1	10
PhD	34	2		6	42
Male Post-doc	12	17	16	3	48
Female Post-doc	2	3	3	3	11
Post-doc	14	20	19	6	59
Male	37	19	16	8	80
Female	11	3	3	4	21
# Participants	48	22	19	12	101

The aim of the Workshop was to assess the present status of TDDFT approaches to the study of

spectroscopic properties of real materials, and explore their capability for applications in further systems with technological and biological interest. The recent developments of TDDFT covered during the workshop include TDDFT versus current-DFT, van der Waals interactions, applications to biological systems, new functionals, transport phenomena, optical spectra of solids, etc. Due to the different methods used to tackle this problem (Many-Body Theory, Density Functional Theory, Configuration Interaction, semi-empirical approaches), this Workshop was intended as a way to promote links among scientists coming from different communities working or interested in electron excited states. Also it was intended as a follow-up event for the students attending the school as it was a good opportunity for them to see the real implications of the school lectures and get the new theoretical advances in the the development of exchange-correlation functionals as well as applications to complex systems (nanostructures, bio-molecules, interstellar molecular analysis, solids, etc.) Our goal was to bring together scientists working on foundations and different applications of TDDFT and many-body theory, trying to assess the capability of current approximations to be applied to real systems of increasing complexity. The invited and contributed talks covered:

- I) Fundamental topics on TDDFT, Many-Body Theory, and electron transport theory.
- II) New approximations and techniques.
- III) Ab-initio calculations of spectroscopic properties of large scale systems.
- IV) Materials Science, Nanoscience, Biology and Chemical applications.

As a consequence, there was a broad variety of participants which helped to get an interdisciplinary vision of the field. Thus, although some of the more specific topics were far from the research interest of many participants, the meeting was an excellent opportunity to see how the same techniques are used by members of other communities

School Program

Day	Hour	Title	T/P
1 (3/1)	8h30 – 9h15	TDDFT I (EG)	T
	9h30 – 10h15	TDDFT II (EG)	T
	10h30 – 11h15	Overview of spectroscopies I (FH)	T
	11h30 – 12h15	Many-Body: GW I (MV)	T
	15h00 – 17h30	Introduction to the practical classes	T/P
	18h00 – 21h00	Quantum Dots I	P
2 (4/1)	8h30 – 9h15	TDDFT III (EG)	T
	9h30 – 10h15	Overview of spectroscopies II (FH)	T
	10h30 – 11h15	Theoretical spectroscopy (SB)	T
	11h30 – 12h15	TDDFT IV (EG)	T
	15h00 – 17h30	Discussion groups	T/P
	18h00 – 21h00	Quantum Dots II	P
3 (5/1)	8h30 – 16h30	Discussion groups	T/P
	16h30 – 17h15	Many-Body: GW II (MV)	T
	17h30 – 18h15	Linear response theory (SB)	T
	18h30 – 19h15	Overview of spectroscopies III (FH)	T
	19h30 – 20h15	Propagation schemes (AC)	T
4 (6/1)	8h30 – 9h15	TDDFT in chemistry and biochemistry I (BC)	T
	9h30 – 10h15	Spectroscopy of surfaces (EO)	T
	10h30 – 11h15	Overview of spectroscopies IV (FH)	T
	11h30 – 12h15	Models for time-dependent phenomena I (ML)	T
	15h00 – 18h00	Quantum Dots III	P
	18h30 – 20h30	Poster session	T
5 (7/1)	8h30 – 9h15	Models for time-dependent phenomena II (ML)	T
	9h30 – 10h15	TDDFT in chemistry and biochemistry II (BC)	T
	10h30 – 11h15	TD Current DFT I (CU)	T
	11h30 – 12h15	Many-Body: BSE I (MG)	T
	15h00 – 18h00	OCTOPUS I	P
	18h30 – 20h30	Poster session	T
6 (8/1)	8h30 – 15h00	Discussion groups	T/P
	15h00 – 15h45	Advanced TDDFT I (NM)	T
	15h45 – 16h30	Optimal control theory (AC)	T
	16h45 – 17h30	Models for time-dependent phenomena III (ML)	T
	17h30 – 18h15	TD Current DFT II (CU)	T
	18h15 – 21h15	OCTOPUS II	P
7 (9/1)	8h30 – 9h15	Models for time-dependent phenomena IV (ML)	T
	9h30 – 10h15	Advanced TDDFT II (NM)	T
	10h30 – 11h15	Many-Body: BSE II (MG)	T
	11h30 – 12h15	TDDFT in chemistry and biochemistry III (DR)	T
	15h30 – 20h30	YAMBO	P
8 (10/1)	8h30 – 16h30	Discussion groups	T/P
	16h30 – 17h15	TDDFT versus Many-Body (MG/AR)	T
	17h30 – 18h15	TDDFT in chemistry and biochemistry IV (DR)	T
	18h30 – 19h15	TD Current DFT III (CU)	T
	19h30 – 20h15	Advanced TDDFT III (NM)	T
	20h15 – 20h45	Closing session / Pedro Pascual Prize 2010 (organisers: AR, MM, FN, EG)	

School Lecturers

Lecturers for the theoretical classes

- AC** A. Castro (Zaragoza, Spain)
Propagation schemes + Optimal control theory
- AR** A. Rubio (Donostia/San Sebastian, Spain)
TDDFT vs. Many-Body
- BC** B. Curchod (Lausanne, Switzerland)
TDDFT in chemistry and biochemistry
- CU** C. Ullrich (Missouri, USA)
TD Current DFT
- DR** D. Rappoport (Harvard, USA)
TDDFT in chemistry and biochemistry
- EG** E. K. U. Gross (MPI Halle, Germany)
TDDFT
- EO** E. Ortega (Donostia/San Sebastian, Spain)
Spectroscopy of surfaces
- FH** F. Himpsel (Madison, USA)
Overview of spectroscopies
- MG** M. Gatti (Paris, France)
Many-Body: BSE + TDDFT vs. Many-Body
- ML** M. Lein (MPI Heidelberg, Germany)
Models for time-dependent phenomena
- MV** M. Verstraete (Lige, Belgium)
Many-Body: GW
- NM** N. Maitra (New York, USA)
Advanced TDDFT
- SB** S. Botti (Paris, France)
Linear Response Theory + Theoretical spectroscopy

Teachers for Quantum Dots and octopus

- AC** Alberto Castro (Zaragoza, Spain)
- AR** Angel Rubio (San Sebastian, Spain)
- FN** Fernando Nogueira (Coimbra, Portugal)
- MM** Miguel Marques (Lyon, France)
- MO** Micael Oliveira (Lyon, France)
- XA** Xavier Andrade (San Sebastian, Spain)

Teachers for YAMBO

- AM** Andrea Marini (Rome, Italy)

CO Conor Hogan (Rome, Italy)
DV Daniele Varsano (Modena, Italy)
PG Claudio Attaccalite (San Sebastian, Spain)
MG Myrta Grüning (Coimbra, Portugal)

Workshop Program

Day I: Monday 11th		
Chairperson: Angel Rubio		
09h20 - 09h30	A. Rubio	Opening remarks
09h30 - 10h20	S. Kuemmel	Excitations in finite systems: pragmatic improvements of DFT and fundamental
10h20 - 11h10	C. Cardoso	Long-range correction effects on the evaluation of first hyperpolarizability of high intrinsic hyperpolarizability molecules
11h10 - 11h30 Caffeine break		
Chairperson: Angel Rubio		
11h30 - 12h20	C. Ullrich	Time-dependent density-functional theory for weakly disordered systems: application to dilute magnetic semiconductors
12h20 - 13h10	O. Gritsenko	Time-dependent density matrix functional theory: an interacting alternative to TDDFT
13h10 - 17h20 Discussion groups		
Chairperson: Fernando Nogueira		
17h20 - 18h10	M. Gatti	Sodium under pressure: a charge-transfer insulator
18h10 - 19h00	S. Botti	Electronic properties of materials for thin-film solar cells: Which ab-initio approaches can we trust?
19h00 - 19h20 Beer break		
Chairperson: Fernando Nogueira		
19h20 - 20h10	J. Dobson	Applications of RPA, TDDFT and related response functions to correlation energies
20h10 - 21h00	E. Suraud	TDDFT description of irradiation and the Self Interaction Problem
Day II: Tuesday 12th		
08h30 - 17h00 Mini-workshops		
Chairperson: Mark Casida		
17h00 - 17h50	T. Seideman	Why Time-Dependent Density Functional Theory?
17h50 - 18h40	N. Maitra	Phase-Space Density Dynamics
18h40 - 19h00 Beer break		
Chairperson: Mark Casida		
19h00 - 19h50	R. Baer	Pragmatic and Dogmatic Spirits in Time-Dependent Density Functional Theory
19h50 - 20h40	I. Tokatly	Time-dependent deformation functional theory: From basic theorems to first applications

Day III: Wednesday 13th		
Chairperson: Miguel Marques		
08h30 - 09h20	M. Sprik	Electronic energy levels in liquids and near liquid-solid interfaces: An electrochemical perspective
09h20 - 10h10	I. Tavernelli	Non-adiabatic molecular dynamics with external fields
10h10 - 10h30	Caffeine break	
Chairperson: Miguel Marques		
10h30 - 11h20	H. Appel	Stochastic Quantum Molecular Dynamics: a functional theory for electrons and nuclei dynamically coupled to an environment
11h20 - 12h10	R. D'Agosta	Stochastic time dependent (current) density functional theory: fundamentals and applications
12h10 - 13h00	O. Sugino	Non-adiabatic molecular simulations
13h00 - 17h00	Discussion groups	
17h00 - 18h30	Poster session	
Chairperson: John Dobson		
18h30 - 19h20	M. Casida	The Multifaceted Problem of Double- and Higher-Excitations in TDDFT
19h20 - 20h10	A. Goerling	New Developments in Density-Functional Response Methods and new Correlation Functionals
20h10 - 21h00	T. Niehaus	Inverse quantum confinement in luminescent Silicon quantum dots
Day IV: Thursday 14th		
Chairperson: Carsten Ullrich		
16h00 - 16h50	F. Martin	Kinematically complete theoretical description of molecular ionization by synchrotron radiation and ultrashort pulses
16h50 - 17h40	C. Ambrosch-Draxl	Q-dependent TDDFT spectra from metals
17h40 - 18h10	D. Strubbe	Non-linear optics and local-field factors in liquid chloroform: A time-dependent density-functional theory study <i>Winner of the school poster session</i>
18h10 - 18h30	Beer break	
Chairperson: Stephan Kuemmel		
18h30 - 19h00	G. Avendaño-Franco	Time-Dependent Density Functional Theory study of transfer of charge by atomic impact, a case study with C ₄ H ₂₀ + Au <i>Winner of the school poster session</i>
19h00 - 19h50	P. Umari	GW quasi-particle spectra from occupied states only
19h50 - 20h00	A. Rubio	Closing remarks
21h00 -	Workshop dinner	

List of Students

Péter ÁGOSTON	Technical University Darmstadt
Joseba ALBERDI	EHU/UPV and ETSF
Guillermo AVENDAÑO FRANCO	Université Catholique de Louvain
Fulvio BERARDI	EHU/UPV and ETSF
Robertson BURGESS	The University of Newcastle
Pablo CAMPOMANES RAMOS	Ecole Polytechnique Federale Lausanne (EPFL)
Elena CANNUCCIA	Università di Roma Tor Vergata
Vince CHO	Norhtwestern University
Pierluigi CUDAZZO	UPV/EHU
Ingo DREISSIGACKER	Leibniz Universität Hannover
Luiza EPURE	Technical University "Gh.Asachi"
Corina ETZ	MPI for Microstructure Physics Halle
James FINN	King's College London
Johanna FUKS	Universidad del Pais Vasco
Pablo GARCIA	Universidad de Zaragoza
Tahereh GHANE	Natl. Center S3 INFM-CNR
Prasenjit GHOSH	The Abdus Salam ICTP
Marco GOVONI	University of Modena and Reggio Emilia
Prokop HAPALA	Inst. of Phys. of the Academy of Sc. of Czech Republic
S. M. Javad HASHEMI	Helsinki University of Technology
Miquel HUIX-ROTLLANT	Université Joseph Fourier (Grenoble I)
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Federico IORI	Ecole Polytechnique
Olexandr ISAYEV	Case Western Reserve University
Dominik JOCHYM	STFC Rutherford Appleton Laboratory
Deniz KECIK	Paul Scherrer Institute
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Aritz LEONARDO LICERANZU	University of Missouri
Pablo LOPEZ TARIFA	Universidad Autónoma de Madrid
Sergio Alberto LOSILLA FERNÁNDEZ	University of Helsinki
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James RAMSDEN	The University of York
Laurids SCHIMKA	University of Vienna
Estelina Lora SILVA	University of Aveiro
John SNYDER	University of California
David STRUBBE	University of California
David TEMPEL	Harvard University
Gilberto TEOBALDI	University College London
Omar VALSSON	University of Twente
Alejandra VARGAS CALDERÓN	CINVESTAV Querétaro
Feng WANG	Institute of Modern Physics

List of School Teachers

Xavier Iago ANDRADE VALENCIA	Universidad del Pais Vasco
Claudio ATTACCALITE	Universidad del Pais Vasco
Silvana BOTTI	LSI-Laboratoire des Solides Irradis
Alberto CASTRO	Free University of Berlin / BIFI
Hogan CONOR	Università di Roma Tor Vergata
Basile CURCHOD	École Polytechnique Fédérale
Matteo GATTI	ETSF and UPV - Universidad del Pais Basco
E. K. U. GROSS	FU Berlin
Myrta GRÜNING	Universidade de Coimbra
Franz HIMPSEL	University of Wisconsin Madison
Manfred LEIN	Universität Hannover
Neepa MAITRA	Hunter College of the City University of New York
Andrea MARINI	Università di Roma Tor Vergata
Miguel MARQUES	LPMCN - Université Lyon I
Fernando NOGUEIRA	Universidade de Coimbra
Micael OLIVEIRA	LPMCN - Université Lyon I
Enrique ORTEGA	UPV - Universidad del Pais Basco
Dmitrij RAPPOPORT	Harvard University
Angel RUBIO	UPV - Universidad del Pais Vasco
Carsten ULLRICH	University of Missouri
Daniele VARSANO	National Center CNR-INFN S3
Matthieu VERSTRAETE	Universidad del Pais Vasco

List of Workshop Participants

(besides the students and teachers from the school)

Akbari ALI	Universidad del País Vasco
Claudia AMBROSCH-DRAXL	University of Leoben
Heiko APPEL	University of California
Roi BAER	The Hebrew University of Jerusalem
Leonardo BERNASCONI	STFC Rutherford Appleton Laboratory
Cláudia CARDOSO	Universidade de Coimbra
Mark CASIDA	Université Joseph Fourier (Grenoble I)
Roberto D'AGOSTA	EHU/UPV and ETSF
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Oleg GRITSENKO	Free University Amsterdam
Nicole HELBIG	EHU/UPV and ETSF
Hirotooshi HIRAI	University of Tokyo
Stephan KUMMEL	University of Bayreuth
Stefan KURTH	Free University of Berlin
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Fernando MARTIN	Universidad Autonoma de Madrid
Thomas NIEHAUS	Universität Bremen
Yann POUILLON	Universidad del Pais Vasco
Tamar SEIDEMAN	Northwestern University
Michiel SPRIK	University of Cambridge
Tamar STEIN	The Hebrew University of Jerusalem
Osamu SUGINO	ISSP
Eric SURAUD	Université Paul Sabatier
Ivano TAVERNELLI	Ecole Poly. Fédérale de Lausanne (EPFL)
Ilya TOKATLY	Universidad del Pais Vasco UPV/EHU and ETSF
Paolo UMARI	INFN crs Democritos
Jessica WALKENHORST	Universität Kassel
Marius WANKO	University of Bremen
Zeila ZANOLLI	Université catholique de Louvain

3.1.5 Report on the Workshop "CATALYSIS FROM FIRST PRINCIPLES"

Erwin Schrödinger Institute (ESI) for Mathematical Physics

Wien, May 25-28, 2009

The Working Group "Catalysis and Surface Science" of the Ψ_k -Network organizes a biannual series devoted to the discussion of recent progress and methodological advances in first-principles methods applied to catalysis, co-organized by Jürgen Hafner (Universität Wien), Jens Norskov (Technical University of Denmark) and Matthias Scheffler (Fritz-Haber Institute of the Max-Planck Gesellschaft). The sixth workshop in this series was held from May 25 to May 28, 2009 at the Erwin Schrödinger Institute (ESI) for Mathematical Physics in Wien. The workshop was sponsored by the Ψ_k -Network, the ESI, the Center for Computational Materials Science and the institutions of the organizers.

Topical sessions were devoted to the discussion of

- (A) Recent progress in density functional theory of solids - and beyond (invited speakers J.P. Perdew, B. Lundqvist, S. Grimme, G. Kresse, M. Fuchs)
- (B) Ab-initio calculations of free-energy barriers and reaction rates (C. Dellago, M. Parrinello, H. Metiu, T. Bucko, T. Bligaard)
- (C) Materials design (D. Morgan, F. Studt)
- (D) Catalysis by metals and metal-support interactions (G. Pacchioni, S. Piccinin, R. Grybos, P. Raybaud, A. Michaelides, A. Gross)
- (E) Electrocatalysis (M. Koper, J. Rossmeisl, S. Sugino)
- (F) Acid-based catalysis in zeolites and related materials (J. Sauer, L. Benco, R. Catlow, S. Bordiga)
- (G) Catalysis by oxides (R. Schlögl, F. Mittendorfer, C. Noguera, J. van Bokhoven, K. Reuter)

Abstracts of all invited presentations and of all contributed poster presentations can be found on the Psi-k Portal.

Sessions A and B described recent progress in the methodology. Session A concentrated on the development of improved exchange-correlation functionals and on attempts to push the level of theory beyond density-functional methods, with the aim to achieve an improved description of weak "non-bonding" interactions (van-der-Waals forces, hydrogen bonds) by accounting for dynamical many-electron correlations. The presentations in Session B described current attempts to push the theoretical description of chemical reactions beyond the level of harmonic transition-state theory, using concepts such as Monte-Carlo based transition-path sampling and free-energy integrations using molecular dynamics simulations based on collective reaction-path variables.

The contributions to Sessions C to G described the state of the art in key areas of catalysis research, from catalysis on metals and oxides over electrocatalysis to nanoporous systems (zeolites and metal-organic frameworks) and included a discussion of multi-scale simulation methods designed to bridge the gaps in the time-, pressure- and temperature-gaps between atomistic simulations and real-world experiments.

Jürgen Hafner
Faculty of Physics, Universität Wien
and Center for Computational Materials Science

4 General Job Announcements

Post-Doctoral Position in Lyon: "Theoretical heterogeneous catalysis"

École Normale Supérieure de Lyon (ENS-Lyon, France)

The position is now open, and funded for 12 months from starting date. The net salary will be between 2300 and 2500 EUR net/month depending on the candidate's experience.

The successful candidate will develop and test methods to realize hybrid quantum method/classical force fields (QM/MM) or quantum method high level/quantum method lower level (QM/QM') calculations. This project is focused on calculations in heterogeneous catalysis. Ab initio methods will be coupled to standard quantum chemistry packages as well as molecular dynamic codes. Besides simple test reactions, applications will include realistic models of complex systems used in heterogeneous catalysis.

Applicants should hold a PhD in theoretical chemistry or theoretical solid state physics, or other related areas with a competitive track record, preferably applied to catalysis. Candidates are required to have experience in numerical scientific computing, with either VASP or CPMD knowledge. Fluency in a high-level programming language, such as FORTRAN90 or/and C/C++ is a requirement. Experience with parallel computing libraries, such as MPI, and extensive experience in a unix/linux environment is a definite advantage.

Scientific meetings and stays in Saudi Arabia at KAUST will take place. The aim of KAUST is to become one of the top leading world class university within 10 years (see www.kaust.edu.sa). To reach this objective, world class scientists and research institutes (among which ENS-Lyon) are associated with the education and research buildup of KAUST. Several challenging scientific problems have been identified and human and material resources have been gathered to solve them.

Motivated candidates are invited to send their CV, including a short motivation for carrying out this project, list of publications, abstract of research results (1 page) and two recommendation letters by e-mail (preferred format pdf or plain text) to

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Postdoctoral Position(s) in Jena, Germany

Position 1: From Januar 2010 until December 2010 there is a postdoc position in the framework of the European Theoretical Spectroscopy Facility (ETSF) (<http://www.etsf.eu>). The payment follows the regulations of the German Public Service. The research topic is free within the ETSF framework.

Position 2: In addition we offer a 12-month postdoc position (second level researcher) within the EU Initial Training Network RAINBOW (<http://rainbow.ensicaen.fr>). The salary follows the rules of the Marie Curie Programme of EU. The research topic is related to the theoretical description of properties of In-rich InGaN alloys, their surfaces and nanostructures.

The two positions can be combined to an almost two-year stay in our group. They can also be used for the parallel one-year stay of two young colleagues, e.g. a couple. The hiring procedure may start now. It should be finished not too late in 2010. Please, recommend applications. All interested colleagues should contact me. In a first step we need a curriculum vitae, a copy of the PhD certificate, and a list of publications.

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Position at Illinois

University of Illinois, Urbana-Champaign, Department of Materials Science and Engineering, and Department of Physics

I have a post-doctoral position at Illinois starting immediately. Interest parties should send CV and names of Three References to:

Duane Johnson, Ivan Racheff Professor of Materials Science and Engineering (email: duanej@illinois.edu).

Applicants background should included electronic-structure methods with experience with Fortran and C++, and scripting languages as well as MPI and MPICH are a plus.

Candidate will spend part of the time developing multiple-scattering application code for large-scale parallel applications, on the "BlueWaters" petascale supercomputer at NCSA/Illinois.

Applications will be on warm, dense matter, and large-scale defected materials in collaboration with two National Laboratories, as well as using other relevant methods to address nanoscale material stability and catalysis. There is a strong research community at Illinois that may stir a variety of interactions also.

Duane D. Johnson, Ph.D, and Ivan Racheff Professor Materials Science & Engineering University of Illinois Urbana-Champaign

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Nanoscale Device Modelling Research Positions

IBM India Semiconductor Research and Development Center, Bangalore, India

The IBM India Semiconductor Research and Development Center invites applications from outstanding scientists/engineers for multiple positions in the area of nano science and technology at IBM, Bangalore, India. The candidates are expected to contribute to the design, theory, and modelling of next generation semiconductor nanodevices. The research and development work involves atomistic modeling and Technology-CAD of nano devices.

Atomistic/Quantum Effects in Nanodevices :

This work involves theoretical understanding of quantum effects in 22 nm scale devices; these include carrier transport, geometry and material dependent bandstructure calculations, role of metal and high-k material interfaces, role of high-k on bandstructure and related phenomena to enable development of 22 nm scale devices.

Candidates to be considered for this area are required to have a strong understanding of semiconductor physics and quantum effects in nanodevices. The candidates are also expected to have a strong background in devices physics, electronic structure methods, numerical programming, hands on experience with ab-initio modelling tools, and computer programming in mixed language environment.

Technology-CAD :

This work involves the improvement and development of an IBM proprietary tool for the simulation of leading edge semiconductor devices. In particular, physical and numerical models for carrier transport influenced by e.g., channel materials, strain, high-k materials, and crystallographic orientation on device performance will be developed and implemented.

A comprehensive knowledge of modern device physics is essential to this position, including both FET and BJT device operation, as well as bulk and SOI device structures. Also, a good background and understanding of quantum phenomenon relevant to semiconductor nanodevices is essential.

Computer/Software Skills :

Demonstrated proficiency with C++, C, and Tcl are required, and experience with team-based large scale software design is desired. Familiarity with concepts related to numerical solution of PDEs, and the ability to realize robust numerical implementations of semiconductor-related physical models in discretized form, are highly desired. Experience with scientific computation on massively parallel computer architectures is a plus. Familiarity with the Linux and/or AIX operating systems, as well as the AFS file system, would be an added plus.

Qualifications :

Interested applicants for the above regular research positions should have a Ph.D/MS in Physics, Electrical Engineering, Applied Physics, Computer Science, or Theoretical Materials Science. Please send your resume to,

kotamurali@in.ibm.com

About IBM Semiconductor Research and Development Center :

IBM's Semiconductor Research and Development Center is responsible for the definition and development of industry leading technologies such as Copper Interconnect, Silicon on Insulator (SOI), High-Performance Logic-Based Embedded DRAM technologies, and SiGe for RF and analog applications, and high-k material technologies. SRDC is also the leading organization in defining the most advanced technologies for the 45 nm and 22 nm nodes, including research in various aspects of Lithography, strained silicon, and Magnetic RAM (MRAM). IBM SRDC develops all of IBM's semiconductor technologies including SOI, Bulk CMOS, RFCMOS, HV CMOS, SiGe HBT BiCMOS, and nanodevice technologies. For more information about leadership semiconductor technologies at IBM, please visit www.ibm.com/chips.

Ph. D. Position on the Modelling of the Properties of High Dielectric Response Nanocomposite Materials

**Research and Development, Electricite de France (EDF)
and Université de Pauy et des Pays de l'Adour (UPPA)**

The development of new devices for the production and transport of electricity (such as batteries, capacitors, fuel cells, thermoelectricity, photovoltaic, etc.) faces new one of the principal challenges. The principal one is to find innovative processes to the energy storage. In this framework, materials with high dielectric permittivities are interesting for the development of devices such as hyper-capacitors. This project will be devoted to the study of the dielectric response of some nanocomposites based on perovskites. In the context of a research in EDF R&D, the goal of this PhD position is to understand the microscopic and nanometric properties of these materials and connect them with microscopic high capacities.

The Ph. D. student will have to use first-principles modelling (Hartree-Fock, Density Functional Theory, etc.) to understand the structural and electronic properties of these materials and their influence on the dielectric responses. The work will be focussed on three topics: a) study of various defects in different perovskites; b) study of the surfaces and interfaces properties of these materials and c) influence of the temperature, pressure, ..., on the properties. The work has both an applied and a theoretical aspect. This is why the Ph. D. will be co-supervised by EDF R&D and the Université de Pauy et des Pays de l'Adour (UPPA), represented by Philippe Baranek and Professor Michel Rérat, respectively. Most of the time the PhD will take place at the department of Materials and Mechanics of Components (MMC) of EDF R&D (in Moret-sur-Loing, near Fontainebleau, south of Paris, France) and supervised by Philippe Baranek. The programming part will take place at the UPPA and in the Group of Theoretical Chemistry of Turin, supervised by Professors Michel Rérat and Roberto Dovesi.

The expected starting date is : the 1st of October 2010

The candidate must have a formation background in nano-materials and nano-objects sciences, and, a skill for programming. A knowledge of the first-principles methods and/or molecular modelling is recommended.

The interested candidate must send us a curriculum vitae with a cover letter and a list of two contacts for references.

Contacts:

Philippe Baranek (philippe.baranek@edf.fr)
EDF R&D

Professor Michel Rérat (michel.rerat@univ-pau.fr)
IPREM-UPPA

Professor Roberto Dovesi (roberto.dovesi@unito.it)
Università di Torino and NIS

5 Abstracts

Quantum nature of the proton in water-hydroxyl overlayers on metal surfaces

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Abstract

Using *ab initio* path integral molecular dynamics we show that water-hydroxyl overlayers on transition metal surfaces exhibit surprisingly pronounced quantum nuclear effects. The metal substrates serve to reduce the classical proton transfer barriers within the overlayers and, in analogy to ice under high pressure, to shorten the corresponding intermolecular hydrogen bonds. Depending on the substrate and the intermolecular separations it imposes, the traditional distinction between covalent and hydrogen bonds is lost partially (e.g. on Pt(111) and Ru(0001)) or almost entirely (e.g. on Ni(111)). We suggest that these systems provide an excellent platform on which to systematically explore the magnitude of quantum nuclear effects in hydrogen bonds.

(To appear in Physical Review Letters in February 2010)

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Chemical accuracy for the van der Waals density functional

Jiří Klimeš

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Abstract

The non-local van der Waals density functional (vdW-DF) of Dion *et al.* [Phys. Rev. Lett. **92**, 246401 (2004)] is a very promising scheme for the efficient treatment of dispersion bonded systems. We show here that the accuracy of vdW-DF can be dramatically improved both for dispersion and hydrogen bonded complexes through the judicious selection of its underlying exchange functional. New and published exchange functionals are identified that deliver much better than chemical accuracy from vdW-DF for the S22 benchmark set of weakly interacting dimers and for water clusters. Improved performance for the adsorption of water on salt is also obtained.

(J. Phys.: Cond. Matt. **22**, 022201 (2010))

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Carbon in palladium catalysts: a metastable carbide

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Abstract

The catalytic activity of palladium towards selective hydrogenation of hydrocarbons depends on the partial pressure of hydrogen. It has been suggested that the reaction proceeds selectively towards partial hydrogenation only when a carbon-rich film is present at the metal surface. On the basis of first-principles simulations, we show that carbon can dissolve into the metal because graphite formation is delayed by the large critical nucleus necessary for graphite nucleation. A bulk carbide Pd₆C with a hexagonal 6-layer fcc-like supercell forms. The structure is characterized by core level shifts of 0.66-0.70 eV in the core states of Pd, in agreement with experimental x-ray photoemission spectra. Moreover, this phase traps bulk-dissolved hydrogen, suppressing the total hydrogenation reaction channel and fostering partial hydrogenation.

Journal of Chemical Physics 132, 024711 (2010)

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New Type of Magnetic Tunnel Junction Based on Spin Filtering through a Reduced Symmetry Oxide: FeCo|Mg₃B₂O₆|FeCo

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Abstract

Magnetic tunnel junctions with high-tunneling magnetoresistance values such as Fe|MgO|Fe capitalize on spin filtering in the oxide region based on the band symmetry of incident electrons. However, these structures rely on magnetic leads and oxide regions of the same cubic symmetry class. A new magnetic tunnel junction (FeCo|Mg₃B₂O₆|FeCo) is presented that uses a reduced symmetry oxide region (orthorhombic) to provide spin filtering between the two cubic magnetic leads. Complex band structure analysis of Mg₃B₂O₆ based on density functional calculations shows that significant spin filtering could occur in this system. This new type of magnetic tunnel junction may have been fabricated already and can explain recent experimental studies of rf-sputtered FeCoB|MgO|FeCoB junctions where there is significant B diffusion into the MgO region.

(Nano Letters 10, 263 (2010), <http://pubs.acs.org/doi/full/10.1021/nl9034362>)

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Cluster scattering effects on phonon conduction in graphene

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Abstract

The phonon-scattering cross section associated with isotopic clusters is evaluated from first principles and used to estimate the reduction in thermal conductance of wide graphene samples. A strong sensitivity of the thermal conductivity to clustering is predicted for micrometer-sized samples at low temperatures. Important differences are obtained between the atomistically computed cross section, and existing analytical approximations, emphasizing the importance of atomistic investigations of thermal transport. Finally, possible techniques are suggested for synthesizing graphene containing isotopic clusters.

(Phys. Rev. B 81, 045408 (2010), <http://prb.aps.org/abstract/PRB/v81/i4/e045408>)

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Magnetism at surfaces and defects in icosahedral Al-Pd-Mn quasicrystals

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Abstract

In our recent work [Krajčí and Hafner, Phys. Rev. B **78**, 224207 (2008)] we have demonstrated that the ground state of bulk i-Al-Pd-Mn quasicrystals is non-magnetic. Mn atoms located at specific sites can acquire a large magnetic moment if they have at least two Pd neighbors in the first coordination shell. Such configurations can be created by substitutional Al/Pd defects which can be formed at low energetic cost because at these sites the overlap between the pseudo-Mackay and Bergman clusters building the quasicrystalline structure leads to conflicting assignments of the chemical decoration. Besides the large magnetic moments formed on these special Mn-sites, we have found a broad diffuse background of smaller magnetic moments on many different Mn atoms induced by the large Mn moments. In the present work we extend these investigations to magnetism at the fivefold surface of the quasicrystal and at isolated point defects, with particular attention to the formation of induced moments. For the stable fivefold surface we find that Mn atoms located in the surface layer carry indeed large magnetic moments of up to $3 \mu_B$ and that smaller magnetic moments (aligned both parallel and antiparallel to the surface moments) are induced at distances of up to 10 \AA below the surface. We have considered three types of isolated point (vacancies and substitutional defects) around a Mn atom and investigated the formation of magnetic moments on the Mn atom and of induced moments on the surrounding sites. For both the magnetization induced below a magnetic surface and the magnetization induced around an Al/Pd substitutional defect, the induced moments show an irregular dependence on the distance for the inducing "source" moment, but a marked dependence on the location of the Mn atom in the occupation domain in six-dimensional hyperspace. Mn atoms with a large coordinate in perpendicular space show large induced moments. Based on the analysis of the local paramagnetic density of states we demonstrate that the formation of a large induced moment is caused by a large polarizability of these Mn atoms, which is related in turn to a rather loosely packed local environment. Per Mn atom, the sum of the source moment (created by a special substitutional defect in the bulk quasicrystal or by the reduced coordination of a Mn atom at the surface) and of the induced moments reaches values of 6 to $8 \mu_B$, i.e. much higher than the limit set by Hund's rule for the spin-moment of a free Mn atom.

(Published in Phys. Rev. B **80** 214419 (2009))

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Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: ab-initio transition path sampling.

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Abstract

The dehydrogenation of propane over acidic chabazite has been studied using ab-initio density-functional simulations in combination with static transition-state searches and dynamic transition-path sampling (TPS) methods at elevated temperatures. The acidic zeolite has been modeled both using a small cluster and a large periodic model consisting of two unit cells, the TPS simulations allow to account for the effect of temperature and entropy. In agreement with experimental observations we find propene as the dominant reaction product and that the barrier for the dehydrogenation of a methyl group is higher than that for a methylene group. However, whereas all studies based on small cluster models (including the present one) conclude that the reaction proceeds via the formation of an alkoxy intermediate, our TPS studies based on a large periodic model lead to the conclusion that propene formation occurs via the formation of various forms of propyl cations stabilized by entropy, while the formation of an alkoxy species is a relatively rare event. It was observed only in 15 % of the reactive trajectories for methyl dehydrogenation and even in only 8 % of the methylene dehydrogenation reactions. Our studies demonstrate the importance of entropic effects and the need to account for the structure and flexibility of the zeolitic framework by using large periodic models.

(JOURNAL OF CHEMICAL PHYSICS 131: 214598 DEC 7 2009)

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First principles theory of dilute magnetic semiconductors

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Abstract

This review summarizes recent first-principles investigations of the electronic structure and magnetism of dilute magnetic semiconductors (DMS), which attract much attention for applications in spintronics. Details of the electronic structure of transition metals doped III-V and II-VI semiconductors are described, especially how the electronic structure couples to the magnetic properties of an impurity. In addition, the underlying mechanism of the ferromagnetism in DMS is investigated from the electronic structure point of view, in order to establish a unified picture which explains the chemical trend of the magnetism in DMS. Recent efforts to fabricate high- T_C DMS requires accurate materials design and reliable T_C predictions for DMS. In this connection, we discuss a hybrid method (ab initio calculations of effective exchange interactions coupled to Monte Carlo simulations for the thermal properties) as a practical method for calculating the Curie temperature of DMS. We discuss calculated ordering temperatures for various DMS systems and its usefulness is demonstrated. Moreover, in order to include all the complexity in the fabrication process of DMS into advanced materials design, we simulate spinodal decomposition in DMS and try to assess the effect of the inhomogeneity in DMS. Finally, we review recent work on first principles theory of transport properties of DMS. Our discussion is mainly based on electronic structure calculations within the local density approximation (LDA) to density functional theory.

(Review of Modern Physics, accepted)

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Electronic Band Structure of Zirconia and Hafnia Polymorphs from the GW perspective

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Abstract

The electronic structure of crystalline ZrO_2 and HfO_2 in the cubic, tetragonal and monoclinic phase has been investigated using many-body perturbation theory in the GW approach based on density functional theory (DFT) calculations in the local-density approximation (LDA). ZrO_2 and HfO_2 are found to have very similar quasiparticle band structures. Small differences between them are already well described at the LDA level indicating that the filled f -shell in HfO_2 has no significant effect on the GW corrections. A comparison with direct and inverse photoemission data shows that the GW density of states agrees very well with experiment. A systematic investigation into the structural and morphological dependence of the electronic structure reveals that the internal displacement of the oxygen atoms in the tetragonal phase has a significant effect on the band gap.

(accepted at: Phys. Rev. B)

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An alloy catalyst in a reactive environment: the example of Ag-Cu particles for ethylene epoxidation

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M. Hävecker,³ D. Teschner,³ Valerii I. Bukhtiyarov,⁵ Frank Girgsdies,³
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Abstract

Combining first-principles calculations and in situ photoelectron spectroscopy, we show how the composition and structure of the surface of an alloy catalyst is affected by the temperature and pressure of the reagents. The Ag-Cu alloy, recently proposed as an improved catalyst for ethylene epoxidation, forms a thin Cu-O surface oxide, while a Ag-Cu surface alloy is found not to be stable. Several possible surface structures are identified, among which the catalyst surface is likely to dynamically evolve under reaction conditions.

(submitted to: Phys. Rev. Lett.)

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Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metal-Phthalocyanine Dimers

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Abstract

Noncovalent interactions, of which London dispersion is an important special case, are essential to many fields of chemistry. However, treatment of London dispersion is inherently outside the reach of (semi)local approximations to the exchange-correlation functional as well as of conventional hybrid density functionals based on semilocal correlation. Here, we offer an approach that provides a treatment of both dispersive interactions and the electronic structure within a computationally tractable scheme. The approach is based on adding the leading interatomic London dispersion term via pairwise ion-ion interactions to a suitably chosen nonempirical hybrid functional, with the dispersion coefficients and van der Waals radii determined from first-principles using the recently proposed “TS-vdW” scheme (Tkatchenko, A.; Scheffler, M. *Phys. Rev. Lett.* 2009, 102, 073005). This is demonstrated via the important special case of weakly bound metal-phthalocyanine dimers. The performance of our approach is additionally compared to that of the semiempirical M06 functional. We find that both the PBE-hybrid+vdW functional and the M06 functional predict the electronic structure and the equilibrium geometry well, but with significant differences in the binding energy and in their asymptotic behavior.

(published in: *J. Chem. Theory Comput.* **6**, 81 (2010).)

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6 Presenting Other Initiatives

6.1 PEtot: A planewave pseudopotential DFT code for large system calculations

(<https://hpcrd.lbl.gov/~linwang/PEtot/PEtot.html>)

PEtot is a planewave pseudopotential DFT code developed in Lawrence Berkeley Laboratory for large system calculations. It uses both norm conserving and ultrasoft pseudopotentials. It deploys three levels of parallelizations: on planewave G-vector, on band index, and on k-points. It has several options for wavefunction solutions, including band-by-band, all-band conjugate gradient, and all band DIIS method. It can be scaled to thousands of processors. It can calculate both periodic systems and isolated systems (for Poission equation). It can be used to relax the atomic positions. It is written in Fortran 90 with MPI for communications. The source codes are available for download. A norm conserving pseudopotential library generated from J.L. Martins's program and an ultrasoft pseudopotential library generated from D. Vanderbilt's program are also included in the downloadable package.

(Licence Details: PEtot is released under the GNU General Public License)

Lin-Wang Wang

Lawrence Berkeley National Laboratory

7 SCIENTIFIC HIGHLIGHT OF THE MONTH: "Recent Developments in KKR Theory"

Recent Developments in KKR Theory

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Abstract

In contrast to its original version that deals with the band structure of periodically ordered solids more or less like any other all-electron band structure method, the modern version of the KKR (Korringa-Kohn-Rostoker) method represents the electronic structure of a system directly and efficiently in terms of its single-particle Green's function (GF). This appealing feature and the wide applicability connected with it, is achieved by the use of multiple scattering theory (MST) for the electronic structure calculations. The basic ideas behind the resulting KKR-GF-method are outlined and the various techniques to deal with the underlying multiple scattering problem are reviewed. The second part of the contribution presents various applications of the KKR-GF-method meant to demonstrate its great flexibility and wide applicability. These should also reflect the many developments of the KKR-GF-method or methods based on it, respectively, that were made during the last years by many work groups.

7.1 Introduction

The KKR method for electronic structure calculations goes back to the work of Korringa [1], and Kohn and Rostoker [2], who introduced the original version of the scheme for periodically ordered solids. In contrast to other all-electron band structure methods based on the variational principle the KKR starts from the Schrödinger equation formulated as an integral equation; i.e. the Lippmann-Schwinger equation for Bloch states involving the free-electron Green's function $G^0(\vec{r}, \vec{r}', E)$. This was expected to lead to higher accuracy compared to other methods. The ansatz for the Bloch wave function used within the KKR-method implies a minimal basis set provided by energy and angular momentum dependent partial waves, with a corresponding low dimension resulting for the eigenvalue problem. Since its introduction the KKR method has been continuously further developed² with its domain of application enormously widened. This

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²In fact, the title of the contribution has been borrowed from a status report given on occasion of a conference on band structure techniques in 1972 [3].

is primarily based on the fact that the KKR scheme can be interpreted in terms of multiple scattering theory (MST). This implies that the KKR method is not restricted to periodic solids but can also be applied to finite systems as well, leading to Slater's $X\alpha$ -multiple scattering method for molecules [4]. Although a minimal basis set is used, the KKR-method is numerically quite demanding in practice because one has to evaluate the free-electron Green's function $G^0(\vec{r}, \vec{r}', E)$ in terms of so-called structure constants. Nevertheless, a rather efficient version of the KKR-method could be implemented by Moruzzi, Janak, and Williams [5] who summarised their results for pure elements in a well-known book [6]. However, as the KKR-method uses energy-dependent basis functions its original version based on the variational principle does not lead to a simple algebraic eigenvalue problem, but the energy eigenvalues have to be searched by scanning the energy with zeros of the secular determinant indicating the eigenvalues. This great drawback was removed by Andersen introducing the linear approximation for the basis functions [7]. As a consequence the original KKR-method is rarely used anymore nowadays as it was replaced by the LMTO (linear muffin-tin orbital) method as its linearised version.

This sounds like the fate of a prehistoric creature. This is by no means the case, as there is another branch of developments on the KKR-method.³ It seems that it was Beeby who first realized that the KKR-formalism or, equivalently, multiple scattering theory can be used to get access to the Green's function (GF) of the system under consideration [8], leading finally to the KKR-GF-method. Representing the electronic structure in terms of the Green's function gives a large number of advantages as compared to the use of eigenvalues and eigenfunctions. Beeby exploited these when considering properties of substitutional impurities in solids that break the Bloch symmetry [8]. Another example is the treatment of disorder in alloys for which Korringa [9] and Beeby [10] suggested the average t-matrix approximation (ATA). In the following the basic ideas of the KKR-GF-method are sketched. In particular, the many developments of the scheme that have been made during the last two or three decades are reviewed. The various applications presented are meant to demonstrate the great flexibility of the KKR-GF-method as it is used and further developed by many active groups throughout the world.⁴ The close connection between the original version of the KKR and the LMTO-method was already mentioned. Accordingly, the properties and features of the KKR-GF described will in general also apply to the TB-LMTO-GF [11] and the EMTO [12] methods as these also supply the electronic Green's function. In fact, several developments of the KKR-GF-method go back to corresponding work on these methods [11, 13].

7.2 Basic idea of the KKR-GF method

The KKR method is based on a decomposition of a system (molecule, atomic cluster, solid etc.) into atomic regions. Originally, this was done using the muffin-tin-construction (see Fig. 1). To calculate the electronic structure of the total system, as a first step an atomic region is treated as an isolated system embedded in a free-electron environment. Solving this single-site problem in a non-relativistic way implies to calculate the angular momentum l - and energy-dependent solutions $R_l(r, E)$ of the radial Schrödinger equation for a given potential. In a next step the

³otherwise this contribution would end here

⁴See for example the website www.kkr-gf.org that was installed very recently.

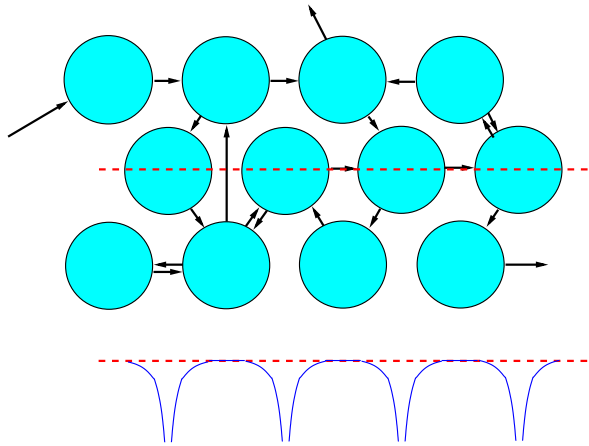


Figure 1: Central idea of multiple scattering theory: decomposition of electronic motion into scattering at atomic sites and free-electron like propagation in between. The bottom of the figure gives a sketch for the potential along the dashed line.

solutions inside the atomic regions are matched coherently with each other assuming a free-electron like behaviour in the inter-atomic or interstitial region [14]. Obviously, matching can be achieved only for certain energies corresponding to the energy eigenvalues of the system. These are found by solving a secular equation expressed in terms of the properties of the radial wave functions $R_l(r, E)$ at the boundary of the atomic regions and a structural matrix $G_{LL'}^{0nn'}(E)$ connecting atomic sites n and n' , with $L = (l, m)$ representing the orbital angular momentum and magnetic quantum numbers. Obviously, the eigenvectors to the secular equation together with the radial functions $R_l(r, E)$ determine the eigenfunction of the total system. The l -dependency of the basis functions $R_l(r, E) Y_L(\hat{r})$, with $Y_L(\hat{r})$ a spherical harmonic, allows for a chemically intuitive interpretation of the results and leads to a minimal basis set. For example, for transition metals it is in general sufficient to use basis functions up to $l_{max} = 2$ rendering the KKR-method a minimal basis set method. In addition, using numerical energy-dependent basis functions obviously ensures corresponding accuracy for the eigenvalues and eigenfunctions. The energy-dependency of the basis functions, however, leads to the great disadvantage that the resulting secular equation does not correspond to an algebraic eigenvalue problem but the eigenvalues have to be found by scanning the energy through an appropriate regime. For this reason the original KKR-method as an eigenvalue scheme is hardly used any more nowadays for self-consistent electronic structure calculations.

Instead of interpreting the scheme sketched above as a mere matching technique one can interpret it in terms of multiple scattering theory. The potential connected with an atomic region gives rise to scattering of an incoming electronic wave into an outgoing one. With the partial wave functions $R_l(r, E)$ available this can be represented by a phase shift $\delta_l(E)$ or in a more general way by a corresponding single-site scattering t-matrix $t_{LL'}^n(E)$. The free-electron like propagation between scattering centres is described by the free-electron Green's function $G^0(\vec{r}, \vec{r}', E)$. Within the adopted angular momentum representation this is expressed in terms of the structural Green's function matrix $G_{LL'}^{0nn'}(E)$ already mentioned. The matching condition referred to above, now corresponds to the requirement that the wave function coming in at an atomic site has to be identical to the superposition of the waves outgoing from all other sites. This

point of view not only gives access to the energy eigenvalues and eigenfunctions of the system (see above) but also in a rather direct way to its single electron Green's function $G(\vec{r}, \vec{r}', E)$. The main features of the resulting KKR-Green's function (KKR-GF) method, that keeps all attractive features of the original KKR-method but avoids the tedious eigenvalue search, are reviewed in the following.

7.3 The single-site problem

Having chosen the decomposition of space (muffin-tin-, ASA- or Wigner-Seitz-construction), the underlying Hamiltonian (non-, scalar- or fully relativistic) including a potential term (e.g. a DFT-LSDA potential), the first step of any KKR-GF calculation is to seek the exact numerical solution of the resulting single-site problem, i.e. the energy dependent scattering solution of the given single electron Hamiltonian. For a spherical potential the corresponding solutions have pure angular momentum character L . On the other hand, for aspherical (also termed "full") potentials centred at atomic sites n and represented by an angular momentum expansion [15–19]:

$$V^n(\vec{r}) = \sum_L^{l_{max}^{(V)}} V_L^n(r) Y_L(\hat{r}) \quad (1)$$

the potential terms $V_L^n(r)$ with $L \neq (0, 0)$ lead to a coupling of angular momentum channels and non- or scalar-relativistic solutions of the form

$$R_L^n(\vec{r}, E) = \sum_{L'}^{l_{max}} R_{L'L}^n(\vec{r}, E) Y_L(\hat{r}). \quad (2)$$

The partial wave functions $R_{LL'}^n(\vec{r}, E)$ have to be determined by solving a set of coupled radial differential equations. This may be done directly or by making use of a Born series expansion [18, 20]. The latter approach is very efficient as it starts from a solution to the spherical part of the potential and accounts for the non-spherical terms in an iterative way. For spin-polarised systems and a collinear spin configuration assumed, calculations for spin up and down are done subsequently for a spin-dependent scalar potential. For non-collinear spin configurations it is advantageous to solve the single-site problem using a local frame of reference with its z -direction along the magnetic moment of the considered atomic region [21]. If the variation of the magnetisation direction within the atomic region can be ignored, the spin-dependent part of the potential is diagonal with respect to the spin and one again has a standard spin-dependent problem to solve. In case that the variation of the magnetisation is non-negligible the Born series technique can be applied again starting from the solution to the collinear part of the potential [22]. Obviously, the resulting solutions have no unique spin character any more.

Having solved for the wave functions up to a angular momentum cut-off, l_{max} , the single-site t-matrix $t_{LL'}^n(E)$ is obtained from the wave functions $R_L^n(\vec{r}, E)$ at the boundary of the atomic region. To set up the Green's function $G(\vec{r}, \vec{r}', E)$, the wave functions $R_L^n(\vec{r}, E)$ are normalised using the t-matrix giving the normalised wave functions $Z_L^n(\vec{r}, E)$, that are regular at the origin [23]. In addition, an irregular wave function $J_L^n(\vec{r}, E)$ has to be calculated in an analogous way (see below), that fulfils certain boundary conditions at the surface of the atomic regime [23]. For fully relativistic calculations on the basis of the four-component Dirac formalism [24], the

situation is completely analogous with the spherical harmonics $Y_L(\hat{r})$ replaced by spin-angular functions $\chi_\Lambda(\hat{r})$ ($\Lambda = (\kappa, \mu)$ with κ and μ the relativistic spin-orbit and magnetic quantum numbers) and the radial wave functions $R_L^n(\vec{r}, E)$ by the large and small components $g_\kappa^n(r, E)$ and $f_\kappa^n(r, E)$, respectively [25]. Calculations for spin-polarised systems, however, become more complicated now as the spin-dependent part of the potential breaks the full rotational symmetry and leads to a coupling of partial waves as in Eq. (2) even if one restricts to spherical potential functions ($l_{max}^{(V)} = 0$ in Eq. (1)) [26, 27]. In the most general situation the potential couples not only to the spin but also to the orbital degree of freedom of the electron. This holds for calculations within CDFT (current density functional theory) [28], if the Breit interaction is included within fully relativistic calculations [29] or if correlation effects are treated by a scheme going beyond standard LDA (see below). This situation can be dealt with in analogy to the spin-dependent case leading to more terms to be considered for the set of coupled radial equations. As long as the orbital-dependent terms do not change the symmetry, however, the number of coupled wave functions (corresponding to the sum over L' in Eq. (2)) does not change.

For situations in which the LDA or LSDA, respectively, seem to be inadequate, one may set up the potential defining the single-site problem in a more sophisticated way. In the case of the non-relativistic spherical implementation of the so-called local SIC (self interaction correction) [30,31] this does not cause any technical problems as the potential becomes only l -dependent with no coupling among the partial waves induced. For the OP (orbital polarisation) [32], the LDA+U [33], as well as the DMFT (dynamical mean field theory) [34], on the other hand, the effective potential depends on the m -character of the wave function in addition. This implies that the corresponding single-site problem has to be dealt with on a full-potential level. In particular it turns out that the additional potential terms occurring within the LDA+U and DMFT schemes are strictly spoken non-local. For the DMFT, with the correlation effects represented by a self-energy matrix $\Sigma_{LL'}(E)$, these become complex and energy-dependent dependent in addition [34].

When solving the single-site problem, obviously the entire complexity of the underlying geometrical description and Hamiltonian (aspherical potential, non-collinear magnetism, spin-orbit coupling, Breit interaction, non-local potentials within LDA+U or DMFT etc.) is accounted for. Accordingly, the resulting regular and irregular wave functions $Z_L^n(\vec{r}, E)$ and $J_L^n(\vec{r}, E)$ as well as the corresponding single-site t-matrix $t_{LL'}^n(E)$ carry all information on the complete Hamiltonian. The resulting single-site solutions could of course be used as numerical basis functions within any all-electron method that determines energy eigenvalues and eigenfunctions on the basis of the variation principle; as e.g. the LAPW, LMTO or ASW. Apart from few exceptions, as for example in the spin-polarised relativistic case [35,36], this is hardly done. Instead solutions to a simplified scalar-relativistic single-site problem with a spherical potential are used in general, dealing with all additional complexity of the Hamiltonian within the variational step.

7.4 Multiple scattering

With the single-site t-matrix available the next step of a KKR-GF calculation is to solve the multiple scattering problem. This task can be solved very elegantly by using the scattering path operator $\tau^{nn'}$ introduced by Györffy and Stott [37], that transfers an electronic wave incoming at site n' into a wave outgoing from site n with all possible scattering events that may take place

in between in a self-consistent way. Adopting an angular momentum representation (see above) this requirement implies for the corresponding matrix the following implicit equation of motion

$$\underline{\tau}^{nn'}(E) = \underline{t}^n(E) \delta_{nn'} + \underline{t}^n(E) \sum_{k \neq n} \underline{G}^{0nk}(E) \underline{\tau}^{kn'}(E), \quad (3)$$

with $(\underline{\tau}^{nn'})_{LL'} = \tau_{LL'}^{nn'}$ etc. For a finite system this equation is solved straight forwardly by a matrix inversion [38]:

$$\underline{\tau}(E) = [\underline{t}(E)^{-1} - \underline{G}^0(E)]^{-1}, \quad (4)$$

where $\underline{M} = [\underline{t}^{-1} - \underline{G}^0]$ is the so-called real-space KKR-matrix, with $[\underline{\tau}]^{nn'} = \underline{\tau}^{nn'}$, $[\underline{G}^0]^{nn'} = \underline{G}^{0nn'}$ and $[\underline{t}]^{nn'} = \underline{t}^n \delta_{nn'}$.⁵ Obviously, the dimension of the various matrices is determined by the number of sites (atoms) in the system and the angular momentum cut-off l_{max} . For a non- or scalar-relativistic formulation \underline{G}^0 can be calculated easily from analytical expressions. For the fully relativistic case \underline{G}^0 is obtained from its non-relativistic counterpart by a simple Clebsch-Gordan transformation [39]. For a finite system the solution to the multiple scattering problem given by Eq. (4) is obviously exact. It is also useful if an extended system is approximated by a finite subsystem as it is justified for example when dealing with EXAFS spectra [39, 40]. A cluster representation of the atomic environment is also used within the locally self-consistent multiple scattering (LSMS) method [41]. As each inequivalent atom is represented by its own cluster or local interaction zone (LIZ), respectively, the method scales strictly with the system size N leading to an Order- N method.

Dealing with a three-dimensional periodic system Eq. (3) can also be solved exactly by Fourier transformation leading to [23]:

$$\underline{\tau}^{nn'}(E) = \frac{1}{\Omega_{\text{BZ}}} \int_{\Omega_{\text{BZ}}} d^3k [\underline{t}(E)^{-1} - \underline{G}^0(\vec{k}, E)]^{-1} e^{i\vec{k}(\vec{R}_n - \vec{R}_{n'})}, \quad (5)$$

with the (reciprocal space) structure constants matrix $\underline{G}^0(\vec{k}, E)$ being the Fourier transformed of the real-space structure constants matrix $\underline{G}^0(E)$. Accordingly, working on a fully relativistic level $\underline{G}^0(\vec{k}, E)$ is again obtained from its non-relativistic counterpart by a simple Clebsch-Gordan transformation [42].

The KKR-matrix $\underline{M}(\vec{k}, E) = [\underline{t}(E)^{-1} - \underline{G}^0(\vec{k}, E)]$ in Eq. (5) is identical to the secular matrix occurring within the original KKR method. Accordingly, varying the energy E for the wave vector \vec{k} fixed $\underline{M}(\vec{k}, E)$ will indicate an eigenvalue $E_{\vec{k}}$ by a jump of its phase. This interrelation is the basis for Lloyd's formula [43–46] that gives the integrated density of states $N(E)$ in terms of the imaginary part of the logarithm of the determinant of $\underline{M}(\vec{k}, E)$. This approach can be applied not only to ordered and disordered (see below) solids [47, 48] but also to finite systems [49]. It allows in particular to handle the single particle energy term within total energy calculations in a very elegant way [48]. Closely connected with this, Lloyd's formula gives a very sound basis when dealing with magnetic properties, like the exchange coupling constants J_{ij} (see below), on the basis of the so-called magnetic force theorem [50, 51].

The calculation of the structure constants matrix $\underline{G}^0(\vec{k}, E)$ was for a long time the bottleneck when applying the original KKR-method. However, several schemes have been developed for an

⁵The energy argument has been dropped here and in the following where appropriate.

efficient evaluation of $\underline{G}^0(\vec{k}, E)$ [5,52] allowing to calculate it on-the-fly with much less effort than needed to invert the KKR-matrix $\underline{M}(\vec{k}, E)$. For systems having only two-dimensional periodicity appropriate schemes have been developed as well to solve the corresponding multiple scattering problem leading to the so-called layer KKR (LKKR) method [53, 54]. These are extensively used when dealing with LEED [55] or angle-resolved photo emission (ARPES) [56] but also for SCF-calculations for layered systems [54]. The numerical effort to deal with the Brillouin zone integral in Eq. (5) or its two-dimensional counterpart can substantially be reduced if the symmetry of the system is exploited. For this purpose a scheme was worked out to find the non-zero matrix elements and to reduce the integration regime to the irreducible part of the Brillouin zone [57]. The scheme is applicable in particular for the spin-polarised relativistic case for which unitary as well as anti-unitary magnetic point group operations have to be considered. In addition, it allows also to handle more complex Brillouin zone integrals involving products of scattering path operators occurring in the context of linear response formalism (see below).

7.5 The single electron Green's function and Dyson's equation

Having solved the multiple scattering problem the retarded single-electron Green's function $G(\vec{r}, \vec{r}', E)$ can be written as [23, 58]:

$$\begin{aligned}
G(\vec{r}, \vec{r}', E) = & \sum_{LL'} Z_L^n(\vec{r}, E) \tau_{LL'}^{nn'}(E) Z_{L'}^{n'\times}(\vec{r}', E) \\
& - \sum_L [Z_L^n(\vec{r}, E) J_L^{n\times}(\vec{r}', E) \Theta(r' - r) \\
& + J_L^n(\vec{r}, E) Z_L^{n\times}(\vec{r}', E) \Theta(r - r')] \delta_{nn'} , \tag{6}
\end{aligned}$$

where \vec{r} (\vec{r}') lies in the atomic cell n (n') representing cell-centred coordinates and \times indicates a so-called left-hand side solution [59]. If the spin of the electron is accounted for explicitly, e.g. when dealing with non-collinear spin-configurations the Green's function $G(\vec{r}, \vec{r}', E)$ is a 2×2 -matrix function [22]. In case of fully relativistic calculations using four-component wave functions $Z_\Lambda^n(\vec{r}, E)$ and $J_\Lambda^n(\vec{r}, E)$, respectively, $G(\vec{r}, \vec{r}', E)$ is a 4×4 -matrix function [29].

The expression for $G(\vec{r}, \vec{r}', E)$ given in Eq. (6) follows in a natural way if multiple scattering is represented by the scattering operator $\underline{\tau}$ with a corresponding normalisation of the wave functions (Bristol-Oak-Ridge convention). An alternative to this is to use the so-called structural Green's function matrix \underline{G} instead that is related to $\underline{\tau}$ by $\underline{G} = \underline{\tau}^{-1} \underline{\tau} \underline{\tau}^{-1} - \underline{\tau}^{-1}$ together with regular and irregular wave functions $R_L^n(\vec{r}, E)$ and $H_L^n(\vec{r}, E)$, respectively, normalised accordingly (Jülich convention) [60].

With the Green's function $G(\vec{r}, \vec{r}', E)$ available all properties of interest can be calculated straight forwardly. For example the particle density $n(\vec{r})$ and density of states $n(E)$ are given by:

$$n(E) = -\frac{1}{\pi} \Im \text{Trace} \int_{\Omega_n} d^3r G(\vec{r}, \vec{r}, E) \tag{7}$$

$$\rho(\vec{r}) = -\frac{1}{\pi} \Im \text{Trace} \int^{E_F} dE G(\vec{r}, \vec{r}, E) , \tag{8}$$

where the trace applies if $G(\vec{r}, \vec{r}', E)$ is given in matrix form. It's worth to note that for $n(E)$ and $\rho(\vec{r})$, needed for example within SCF calculations, only site-diagonal scattering path operators

$\underline{\tau}^{nm}$ are required. For a more detailed representation of the electronic structure than supplied by the DOS $n(E)$, the Bloch spectral function $A_B(\vec{k}, E)$ may be used that is defined as the Fourier transformed of $G(\vec{r}, \vec{r}', E)$ [58]:

$$A_B(\vec{k}, E) = -\frac{1}{\pi N} \Im \text{Trace} \sum_{n, n'}^N e^{i\vec{k}(\vec{R}_n - \vec{R}_{n'})} \int_{\Omega} d^3r G(\vec{r} + \vec{R}_n, \vec{r} + \vec{R}_{n'}, E). \quad (9)$$

Thus, $A_B(\vec{k}, E)$ can be seen as a \vec{k} -resolved density of states function. For a perfectly ordered system, in particular, $A_B(\vec{k}, E)$ is just a sum of δ -functions $\delta(E - E_{\vec{k}})$ that represents the usual dispersion relation $E_{\vec{k}}$.

Obviously, the KKR-GF method supplies all information on the electronic structure that may also be supplied by any other band structure method that represents the electronic structure in terms of energy eigenvalues and eigenfunctions. However, using the Green's function from the very beginning to represent the electronic structure provides a large number of advantages.

The definition of the Green's function and all expressions given above is not restricted to real energies E but also holds for arbitrary complex energies z .⁶ The fact that $G(\vec{r}, \vec{r}', E)$ is analytical [61] allows, in particular, to perform the energy integration in Eq. (8) on a contour in the complex energy plane [62, 63] with typically around 30 energy mesh points needed. This results in an efficiency comparable to linear band structure methods without making use of the linear approximation (with respect to the energy) for the basis functions [64].

One of the major benefits of working with the Green's function $G(\vec{r}, \vec{r}', E)$ is the use of the Dyson equation:

$$G(\vec{r}, \vec{r}', E) = G^{\text{ref}}(\vec{r}, \vec{r}', E) + \int_{\Omega_{\text{pert}}} d^3r'' G^{\text{ref}}(\vec{r}, \vec{r}'', E) \mathcal{H}_{\text{pert}}(\vec{r}'') G(\vec{r}'', \vec{r}', E). \quad (10)$$

This equation allows to get the Green's function $G(\vec{r}, \vec{r}', E)$ of a system described by a Hamiltonian $\mathcal{H} = \mathcal{H}_{\text{ref}} + \mathcal{H}_{\text{pert}}$ in terms of the Greens function $G^{\text{ref}}(\vec{r}, \vec{r}', E)$ for a simpler reference system described by \mathcal{H}_{ref} and a perturbation $\mathcal{H}_{\text{pert}}$. In fact, this equation supplies the formal background for the scheme sketched above where the free-electron system supplies the reference system, i.e. $G^{\text{ref}}(\vec{r}, \vec{r}', E) = G^0(\vec{r}, \vec{r}', E)$, and the perturbation $\mathcal{H}_{\text{pert}}$ is given by the potential $V(\vec{r})$ of the system to be considered.

The Dyson equation allows for many interesting situations to deal with the multiple scattering problem in a very efficient way. Replacing the single-site scattering t-matrix of the real system by t-matrices $\underline{t}^{\text{TB}}$ that are derived from a repulsive potential one gets by solving the corresponding multiple scattering problem the Green's function $G^{\text{TB}}(\vec{r}, \vec{r}', E)$ for this artificial new reference system. In contrast to the free-electron Green's function $G^0(\vec{r}, \vec{r}', E)$, this new auxiliary Green's function $G^{\text{TB}}(\vec{r}, \vec{r}', E)$ decays very rapid in space, i.e. with increasing distance $|\vec{r} - \vec{r}'|$. As a consequence the corresponding scattering path operator $\underline{\tau}^{\text{TB}nm'}$ is essentially zero if the distance of sites n and n' is greater than the next-nearest neighbour distance. Solving now the multiple scattering problem for the real system using the Green's function of the new reference system

⁶The symbol E will still be used in the following for the energy, without implying a restriction to the real axis.

one gets for its scattering path operator $\underline{\underline{\tau}}$ the following set of equations [60]:

$$\underline{\underline{G}}^{\text{TB}} = \underline{\underline{G}}^0 [\underline{\underline{1}} - \underline{\underline{t}}^{\text{TB}} \underline{\underline{G}}^0]^{-1} \quad (11)$$

$$\underline{\underline{\tau}}_{\Delta} = [\Delta \underline{\underline{t}}^{-1} - \underline{\underline{G}}^{\text{TB}}]^{-1} \quad (12)$$

$$\Delta \underline{\underline{t}} = \underline{\underline{t}} - \underline{\underline{t}}^{\text{TB}} \quad (13)$$

$$\underline{\underline{G}} = (\Delta \underline{\underline{t}}^{-1}) \underline{\underline{\tau}}_{\Delta} (\Delta \underline{\underline{t}}^{-1}) - (\Delta \underline{\underline{t}}^{-1}). \quad (14)$$

Because of the sparseness of the matrix $\underline{\underline{G}}^{\text{TB}}$ one has now a sparse matrix problem to deal with as for the tight binding (TB) formalism. The main idea behind the resulting TB-KKR-GF [60, 65] goes back to a similar scheme used within the TB-LMTO [66]. Analogous to this case the TB-KKR-GF method becomes an order(N)-method with its numerical effort scaling linearly with the system size if the structure of the system can be exploited [60]. Using an efficient scheme to deal with the auxiliary TB-reference system, this allows to deal with systems containing thousands of atoms [67].

So far the TB-KKR-GF has been primarily applied to two-dimensional periodic layered systems for which a hybrid representation of the scattering path operator $\underline{\underline{\tau}}^{II'}(\vec{k}_{\parallel}, E)$ is used, with I and I' layer indices and \vec{k}_{\parallel} a vector of the corresponding two-dimensional reciprocal space. For a given \vec{k}_{\parallel} the multiple scattering problem with respect to the layer index has then a TB-structure, that can be solved with established techniques [11, 65].

As an example Fig. 2 shows results of TB-KKR-GF calculations for a Co mono layer on top of a Pt(111) substrate. For the first calculation the substrate was approximated by a slab of

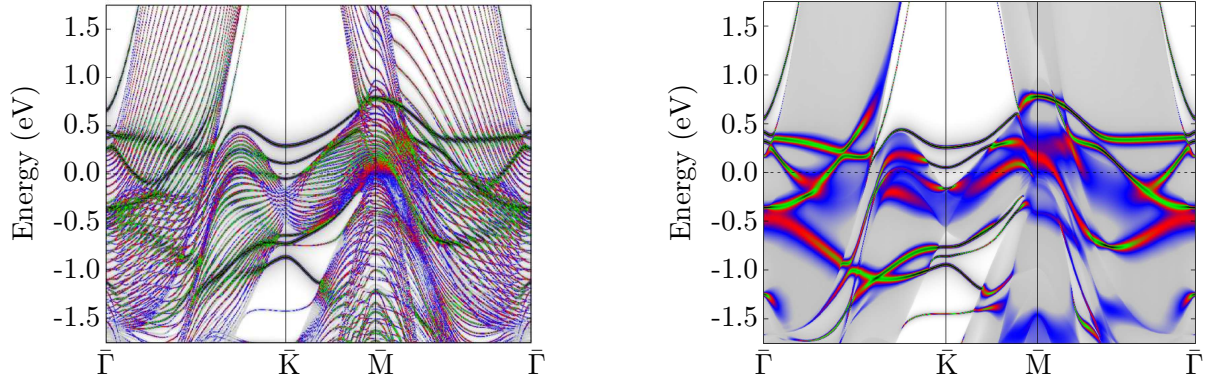


Figure 2: Co-projected Bloch spectral function $A_{\text{B}}(\vec{k}_{\parallel}, E)$ for a Co mono-layer on top of a Pt (111) substrate. Left: a slab geometry with 38 atomic layers was used. Right: the Pt(111) substrate was represented by a semi-infinite solid.

38 (111)-oriented Pt-layers. The Bloch spectral function $A_{\text{B}}(\vec{k}, E)$ projected onto the Co-layer shown in Fig. 2 (left) can now be seen as a \vec{k}_{\parallel} -resolved partial DOS of Co. Obviously, it shows many discrete bands that are caused by the spatial confinement imposed by the slab geometry. Dealing with a Co-mono layer on top of a semi-infinite Pt(111) substrate instead, the artificial confinement is removed and the spurious features of the local electronic structure are gone.

7.6 Embedding of atoms clusters in a perfect host system

For the examples considered above the reference system for the Dyson equation is just a suitable auxiliary system. Another important application of the Dyson equation is the embedding of a perturbing subsystem into a host reference system. The most simple case is the substitutional embedding of an impurity atom into an otherwise perfect three-dimensional periodic host, with a perturbation of its neighbouring atoms. Because the impurity breaks the Bloch symmetry of the system standard band structure schemes can handle the problem only by using the super cell approach. To keep the interaction of neighbouring impurity cells negligible, large enough super cells have to be used.

This problem can be completely avoided by making use of the Dyson equation. Dealing with a metallic host the perturbation caused by a substitutional impurity is typically restricted to few neighbouring atomic shells due to screening. The integration regime Ω_{pert} in Eq. (10) can be restricted accordingly. Representing the Green's functions by means of multiple scattering theory Eq. (6) the Dyson equation is transformed to an equivalent algebraic equation for the scattering operator that can be solved easily:

$$\underline{\underline{\tau}}^{\text{imp}} = [(\underline{\underline{t}}^{\text{imp}})^{-1} - (\underline{\underline{t}}^{\text{host}})^{-1} - (\underline{\underline{\tau}}^{\text{host}})^{-1}]^{-1}, \quad (15)$$

where the site index of the matrices is restricted to the atomic sites within the regime Ω_{pert} . In Eq. (15) $\underline{\underline{\tau}}^{\text{host}}$ is the scattering path operator matrix for the corresponding cluster of unperturbed host atoms with single site t-matrices $\underline{\underline{t}}^{\text{host}}$. $\underline{\underline{\tau}}^{\text{imp}}$ is the scattering path operator matrix representing the embedded atom cluster with the substitutional impurity atom at the centre and the single site matrices collected in $\underline{\underline{t}}^{\text{imp}}$. As mentioned, the size of the cluster can be restricted typically to few neighbouring atomic shells around the impurity atom. For specific problems much larger clusters may be necessary. An example for this is the investigation of satellites in Cu-NMR that can be ascribed to Cu-atoms in the vicinity of a magnetic 3d-impurity atom. In experiment signals from Cu-atoms up to the 6th neighbouring shell could be identified and confirmed by KKR-GF-based calculations [68]. Another example is an investigation of the so-called giant magnetic moments caused by the spin-polarisation of Pd in the vicinity of an embedded magnetic 3d-impurity atom. In this case even for clusters with 8 atomic shells around the impurity, containing 683 atoms all together, an appreciable polarisation of the Pd atoms on the outermost cluster shell was found [69].

In Fig. 3 the first results of a more exotic application of the embedding scheme are presented. The left part of the figure shows the electronic charge distribution around a vacancy in Al. From this the corresponding potential seen by a positron was constructed [70] and a KKR-GF calculation for the positron was performed subsequently. The right panel of Fig. 3 shows the corresponding DOS for the positron on the vacancy and the neighbouring Al sites. As one can see a bound state for the positron emerges that is localised on the vacancy site. From the DOS for the neighbouring Al sites it is clear that the positron state is not completely restricted to the vacancy regime but spills out over the neighbouring sites. In fact, only about 63 % of the positron charge is localised at the vacancy site. The corresponding charge distribution for a single positron trapped on the vacancy site shown in the middle panel of Fig. 3 demonstrates this as well. It should be noted that the lifetime of the positron that can be measured in experiment

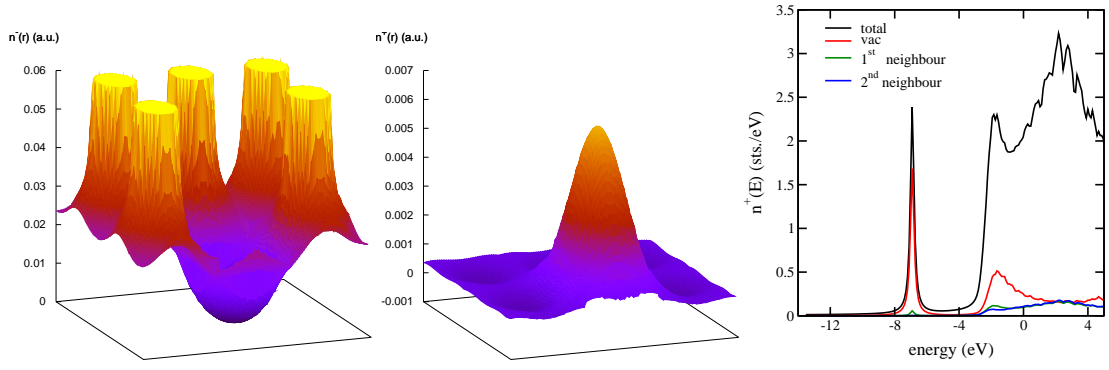


Figure 3: Left: electronic charge distribution $n^-(\vec{r})$ around a vacancy in fcc-Al showing the charge depletion at the vacancy site. Middle: charge distribution $n^+(\vec{r})$ for a single positron trapped in the vacancy regime. Right: DOS $n^+(E)$ for the positron on the vacancy and Al sites of the neighbouring two atom shells, respectively. The δ -like peak for the bound positron state is smeared out to a Lorentzian line due to the use of complex energies with a corresponding imaginary part.

is determined by the overlap of the positronic and electronic charge distributions [70]. As it is obvious from the results shown in Fig. 3 the lifetime of the positron will be modified if an additional impurity atom becomes nearest neighbour to the vacancy. In fact, positron life time measurements are a well established experimental tool to investigate impurity-vacancy dimers that play a very important role for metallurgical properties [70].

The embedding scheme described above is of course not restricted to three-dimensional bulk systems as a host but can be applied straight forwardly to clusters deposited on a substrate. This was demonstrated by many investigations on the magnetic properties of transition metal clusters deposited on various substrates [71–74]. As a corresponding example Fig. 4 shows a pyramid-shaped cluster of Fe- and Pt-atoms with a fcc-like structure deposited on a Cu (001)-substrate. The table next to the figure gives the spin and orbital magnetic moments resulting

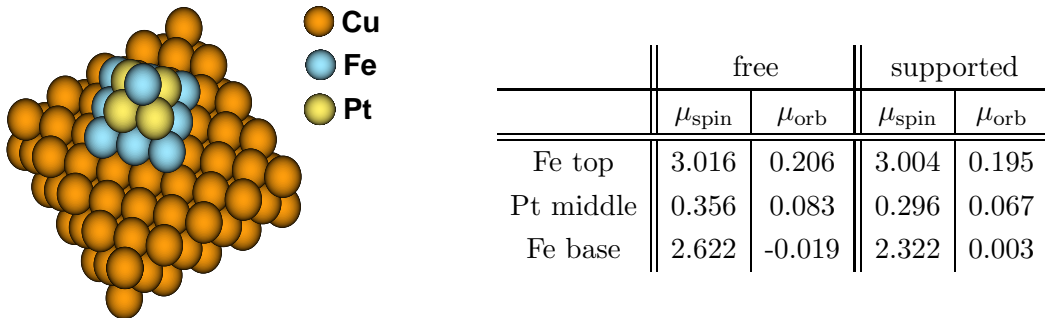


Figure 4: Pyramid-shaped FePt-cluster with a fcc-like structure deposited on a Cu (001)-substrate. The table gives the spin and orbital magnetic moments for the deposited cluster as well as for a free cluster with the same structure.

from a fully relativistic KKR-GF calculation. The table gives in addition results of corresponding calculations for a free FePt-cluster that has the same structure as the deposited one and that has been treated by the real space version of the KKR-GF method for finite systems. As one notes the resulting spin moments for the Fe atoms are quite high and similar to that for bulk

FePt with CuAu structure. For the Fe-atom at the top of the pyramid the moments in both cluster systems are more or less the same implying that the substrate has very weak influence in the case of the deposited FePt cluster. For the Fe-atom in the middle of the basal plane of the clusters there is an appreciable difference however. As one would expect on the basis of the Stoner-criterion for spontaneous spin magnetism, the spin moment is smaller for the deposited cluster due to bond formation with the substrate and a corresponding increase of the d-band width for the Fe-atoms in the basal plane.

There are many more applications of the KKR-GF embedding technique to surface nano structures containing up to several hundreds of atoms. In particular the influence of adatoms and embedded impurity atoms on the surface electronic structure was studied in detail this way [75]. Another interesting example is the investigation of quantum corrals [76] and the occurrence of so-called mirages induced by enclosed magnetic impurity atoms [77]. Several investigations were devoted to the exchange coupling within a magnetic nano structure (see below) or the coupling of magnetic adatom moments via the substrate [78]. For finite anti-ferromagnetic nano wires deposited on a ferromagnet, the so-called even-odd effect was studied by means of non-collinear calculations showing the central importance of the number of atoms in the wire for its magnetic ground state [79]. The KKR-GF embedding scheme is applicable without modification to any other two-dimensional system. An example for this are half-infinite electrodes separated by vacuum and connected by a single wire [80,81]. In the case of magnetic wires non-collinear spin structures as well as their transport properties have been investigated even in a fully relativistic way [82].

For most KKR-GF-based embedded cluster calculations it was assumed so far that the cluster atoms occupy substitutionally perfect lattice sites of the host systems; this implies that possible lattice relaxations have been ignored. However, this is not a necessary restriction as various schemes have been worked out to account for lattice relaxations within KKR-GF calculations for embedded systems. For relatively small relaxations in the order of few percent the Green's function of the host reference system can be re-expanded around the shifted atomic positions by a so-called U-transformation [83,84]. This has been applied with great success for bulk systems [84] as well as surface systems [85]. In case of more pronounced shifts of the atomic positions or when dealing with interstitial impurities an auxiliary sub lattice can be introduced [86–88]. In addition, a scheme has been developed that allows to embed clusters with a structure completely unrelated to that of the host system as it occurs for example when dealing with segregation in a bulk material [89,90].

7.7 Treatment of chemical disorder

Dealing with disordered substitutional alloys the chemical disorder destroys obviously the Bloch symmetry even if a perfect underlying lattice is assumed. Using a standard band structure method this situation can again be handled only by making use of the super cell technique. This implies that one is restricted to concentrations that can be represented by stoichiometric compounds and that one has to use large super cells if the concentration of one of the components in the alloy is low. In addition, one has to average over several atomic configurations in the super cell to get the configurational average corresponding to the disordered state.

Attempts to construct a configurationally averaged wave function for a disordered solid does not seem to be very sensible [14]. Seeking for the configurational average of the electronic Green's function, on the other hand, makes sense and various schemes have been suggested for this purpose in particular on the basis of multiple scattering theory [14]. Obviously construction of a configurational average is most simple if any correlation concerning the occupation of neighbouring sites is ignored i.e. short-range order is excluded and a random distribution of the components is assumed with the alloy composition being the only restriction. On the basis of this single-site approximation Korringa [9] and Beeby [10] suggested to represent a disordered alloy by a single-site t-matrix $\underline{t}^{\text{ATA}}$ that is obtained by the concentration-weighted average over the components; e.g. $\underline{t}^{\text{ATA}} = x_A \underline{t}^A + x_B \underline{t}^B$ for a binary disordered alloy $A_{x_A} B_{x_B}$. This average t-matrix approximation (ATA), however, leads to a Green's function that does not guarantee a positive definite DOS for real energies. This problem could be removed in a mathematically sound way by the Coherent Potential Approximation (CPA) of Soven [91] that introduces an auxiliary CPA medium by demanding that embedding one of the components into the CPA medium should reproduce in the concentration average the properties of the CPA medium. This central idea of the CPA is represented by Fig. 5. Expressing it in terms of the KKR-GF

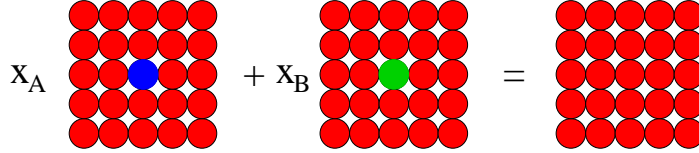


Figure 5: Basic idea of the Coherent Potential Approximation (CPA): the embedding of one of the components of an alloy $A_{x_A} B_{x_B}$ into the CPA-medium should not change its properties if the concentration-weighted average is taken.

formalism this means that the average should cause no additional scattering compared to the CPA-medium [92]:

$$x_A \underline{\tau}^{A nn} + x_B \underline{\tau}^{B nn} = \underline{\tau}^{\text{CPA } nn} . \quad (16)$$

In line with the single site approximation the component projected scattering path operator matrices $\underline{\tau}^\alpha$ ($\alpha = A, B$) are given by Eq. (15) with the CPA-medium as a host and the cluster size reduced to the single central atom. Eq. (16) imposes implicitly a condition to be met by the single-site t-matrix $\underline{t}^{\text{CPA}}$ of the CPA-medium. In addition, $\underline{t}^{\text{CPA}}$ has to lead to the CPA scattering path operator $\underline{\tau}^{\text{CPA } nn}$, e.g. via Eq. (5). Due to this implicit definition of $\underline{t}^{\text{CPA}}$ it has to be calculated by solving these so-called CPA equations iteratively starting from a reasonable guess as e.g. $\underline{t}_{\text{start}}^{\text{CPA}} = \underline{t}^{\text{ATA}}$ [93]. The resulting description of the configurational average via $\underline{t}^{\text{CPA}}$ and $\underline{\tau}^{\text{CPA } nn}$ is the best solution that can be achieved on the basis of the single-site approximation. It can be shown, in particular, that the CPA is exact up to fourth order in the scattering t-matrices with respect to the CPA medium [91].

Within the combined KKR-GF-CPA scheme the Green's function for the alloy is given by the concentration weighted average according to Eq. (16) with [14]:

$$G(\vec{r}, \vec{r}', E) = \sum_{\alpha} x_{\alpha} G^{\alpha}(\vec{r}, \vec{r}', E) , \quad (17)$$

with the component projected Green's function G^{α} given by Eq. (16) using the component-projected $\underline{\tau}^{\alpha nn'}$ and specific wave functions Z^{α} and J^{α} . The expression makes clear that the CPA

provides an averaged but component specific information on the electronic structure as it may be probed by element-specific experimental techniques like NMR, Mößbauer spectroscopy [94] or XAS (x-ray absorption spectroscopy) [95].

Since its first successful numerical implementation [96] the KKR-GF-CPA scheme was applied with great success to many different alloy systems. In particular using the Bloch spectral function $A_B(\vec{k}, E)$ for the discussion of the electronic structure of disordered systems [58] turned out to be very useful. As an example the top row of Fig. 6 shows results for the Bloch spectral function $A_B(\vec{k}, E)$ of ferromagnetic fcc-Fe_{0.2}Ni_{0.8} as a function of the energy and wave vector $\vec{k} \parallel [100]$ [97]. The uppermost plot gives the total Bloch spectral function while the plots below give its minority

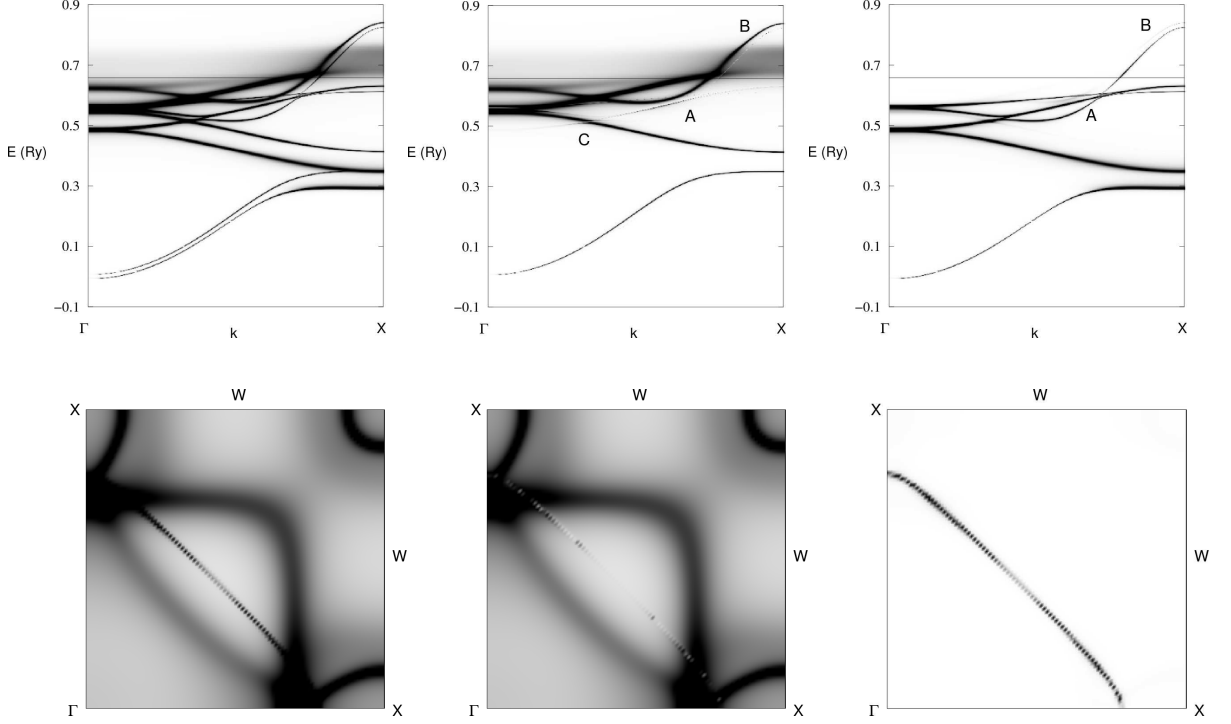


Figure 6: Top row: Gray-scale representation of the Bloch spectral function $A_B(\vec{k}, E)$ (in atomic units) for fcc-Fe_{0.2}Ni_{0.8} with $\vec{k} \parallel [100]$ and the magnetisation $\vec{M} \parallel [001]$. The white background corresponds to $A_B(\vec{k}, E) = 0$, while the black regions represent $A_B(\vec{k}, E) \geq 50$ a.u.; i.e. the cusps of $A_B(\vec{k}, E)$ have been cut for a more resolved representation. The column in the middle and at the end of a row give $A_B(\vec{k}, E)$ decomposed into their minority and majority spin part, respectively. Bottom row: $A_B(\vec{k}, E)$, but for the energy fixed to the Fermi energy E_F and \vec{k} lying in the (010)-plane; i.e. the horizontal axis gives the component of \vec{k} perpendicular to \vec{M} , while the vertical axis gives that parallel to \vec{M} [97].

and majority spin contribution. As one notes for the selected concentration the spectral function resembles very much the dispersion relation $E_{\vec{k}}$ of pure Ni. However, due to the disorder in the alloy the curves are smeared out implying that the wave vector \vec{k} is not a good quantum number any more. In addition, one notes that the impact of disorder is much more important for the minority than for the majority spin channel. This is because the resonance of the d-states of Fe and Ni is very close to each other for the majority band while – due to the different local exchange splitting – they are shifted against each other for the minority spin channel. The same

behaviour can be seen for the plots in the bottom row of Fig. 6 that represent the Fermi surface of the alloy. The width and variation of the Bloch spectral function at the Fermi level can be used to deduce a \vec{k} -dependent life time $\tau_{\vec{k}}$ of the electrons and a corresponding group velocity $v_{\vec{k}}$. This has been exploited by Butler and Stocks to calculate the residual resistivity of $\text{Ag}_x\text{Pd}_{1-x}$ on the basis of the Boltzmann formalism (see below) [98].

In the middle column of Fig. 6 one notices very weak features that correspond to the majority spin spectral function. This mixing of the spin channels is caused by spin-orbit-coupling that has been accounted for by performing spin-polarised fully relativistic calculations. For the transport properties of ferromagnetic alloys this spin-mixing has important consequences as it gives among other rise to the galvano-magnetic properties; i.e. the anomalous magneto-resistance (AMR) and the spontaneous Hall-effect (SHE) [99, 100].

As mentioned before, the CPA is a single-site theory and for that reason does not give direct access to features in the electronic properties caused by short-range order (SRO). Nevertheless, as was demonstrated by Györffy and Stocks [101], SRO phenomena may be investigated in terms of concentration waves. Another route is to investigate the electronic structure of clusters with specific configurations embedded into the CPA-medium [102]. This embedded cluster method (ECM) has been used for example to study the variation of the nuclear spin lattice relaxation time of Cu and Pt in $\text{Cu}_x\text{Pt}_{1-x}$ [103] and of the hyperfine fields of Fe and Ni in $\text{fcc-Fe}_x\text{Ni}_{1-x}$ alloys [104] with their local environment. In all cases it turned out that the average over all investigated configurations agrees very well with the CPA-result.

It should be stressed that the CPA is not restricted to deal with chemical disorder in three-dimensional alloy systems but can be used for inhomogeneous systems as well. Important examples for the latter are the inter diffusion at interfaces [105–107] and surface segregation [108] for which one has to deal with a layer dependent concentration profile. Also in case of finite systems as free and deposited alloy clusters [109] the CPA has been applied successfully. Furthermore, exploiting the alloy analogy the CPA scheme was transferred to deal with the thermal fluctuations of magnetic moments in ferromagnets leading to the disordered local moment (DLM) scheme [110, 111]. Within a non-relativistic approach the single-site averaging leads for the paramagnetic state of a pure ferromagnet effectively to a binary alloy that has components with their moments oriented up and down, respectively, having each a concentration $x = 1/2$. An extension of the DLM to layered systems allowed to determine the magnetic ordering temperature for 3 and 7 layers of Fe on Cu(100) as a function of the Cu coverage in very satisfying agreement with experiment [112]. Recently, corresponding work was done for rare earth systems revealing the magnetic ordering tendencies as a function of the volume and the c/a -ratio [113]. In this case correlation effects were accounted for by making use of the local SIC [30]. Combining local SIC and CPA causes obviously no conceptual or technical problems within the KKR-GF formalism because both schemes make use of the single-site approximation. The same holds for the combination of the CPA used to deal with disordered alloys and the LDA+U [33] or DMFT [34, 114] to account for correlation effects beyond LSDA – as long as the latter schemes are used on a site-diagonal, i.e. single-site level.

In spite of the great success of the CPA many more sophisticated schemes have been worked out in the past to avoid the single-site approximation and to include SRO effects directly within

the primary electronic structure calculation [14]. Recently, a cluster extension of the single-site CPA – called non-local CPA (NL-CPA) – was suggested that is based on ideas borrowed from averaging techniques developed in many body theory [115,116]. As Fig. 7 shows the basic idea of the NL-CPA is very similar to that of the CPA: embedding a cluster with given atomic configuration into the NL-CPA medium should not change its properties if the average over all possible configurations of the cluster is taken. Within multiple scattering formalism this can be

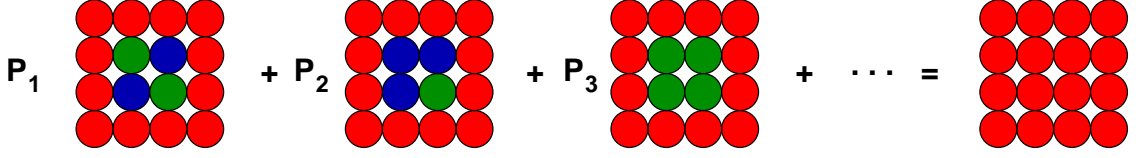


Figure 7: Basic idea of the non-local CPA (NL-CPA): embedding a cluster with given atomic configuration into the NL-CPA medium should not change its properties if the average over all possible configurations of the cluster is taken.

expressed again by the corresponding scattering path operators:

$$\sum_{\text{config } \gamma} P_{\gamma} \underline{\underline{\tau}}_{\gamma} = \underline{\underline{\tau}}^{\text{NL-CPA}}, \quad (18)$$

where the site index of the matrices runs over all sites within the cluster. The summation in Eq. (18) is performed over all possible atomic configurations γ of the cluster with the probability P_{γ} . For a completely disordered system the probabilities P_{γ} are all the same, but they differ if ordering or clustering occurs.

Fig. 8 shows results for the spin and orbital magnetic moment of Pt in disordered fcc-Fe_{0.5}Pt_{0.5} as obtained by the NL-CPA [117]. For these calculations clusters with $N_c = 4$ atoms on the

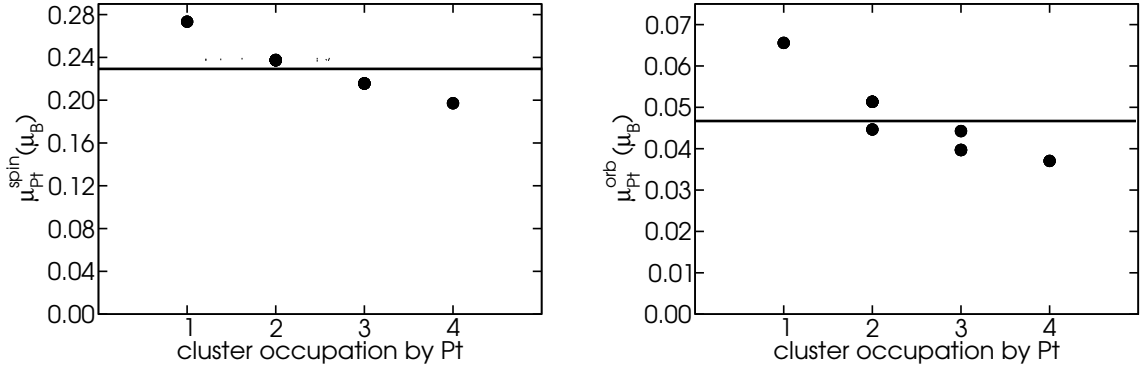


Figure 8: Spin (left) and orbital (right) magnetic moment of Pt in fcc-Fe_{0.5}Pt_{0.5} as obtained by the NLCPA. The various data points show the moments for individual sites of all occurring cluster configurations for $N_c = 4$ as a function of the occupation of the cluster by Fe and Pt atoms, respectively. The horizontal lines represent the average NLCPA result, that nearly coincides with the CPA result [117].

fcc-lattice have been used; i.e. 2^4 configurations have been considered. The various data points give the moments as a function of the number of Pt atoms within the cluster (1-4). One notes that the induced Pt spin moment increases if the number of Fe atoms in the cluster increases (from the right to the left). For the spin moment obviously only the number of Fe atoms in

the cluster matters, i.e. the specific geometrical arrangement of the atoms within the cluster is more or less unimportant. For the orbital magnetic moment, on the other hand, that is very sensitive to the electronic structure at the Fermi level, the specific geometry matters as well as it is reflected by finding different moments for a given number of Fe atoms in the cluster.

There are already several further developments based on the NL-CPA and interesting corresponding applications to be found in the literature that demonstrate the great potential of this new scheme [116, 118, 119] (see also below).

7.7.1 Magnetic Anisotropy and Exchange interaction

Magnetic anisotropy denotes the dependency of the total energy of a system on the orientation of its magnetisation. For transition metal systems the magnetic anisotropy energy is usually split into a contribution, connected with the spin-orbit coupling and one associated with the dipole-dipole interaction of the individual magnetic moments [120, 121]. The latter one $\Delta E_{\text{dip}}(\hat{n}, \hat{n}')$ is treated classically by evaluating a corresponding Madelung sum [121, 122]. The magnetic anisotropy energy $\Delta E_{\text{SOC}}(\hat{n}, \hat{n}')$ connected with spin-orbit coupling, on the other hand, is determined by total energy calculations with the magnetisation oriented along directions \hat{n} and \hat{n}' , respectively, and taking the difference. Obviously, for both orientations a full SCF calculation has to be performed. This can be avoided by making use of the so-called magnetic force theorem that allows to approximate $\Delta E_{\text{SOC}}(\hat{n}, \hat{n}')$ by the difference of the single particle or band energies for the two orientations obtained using a frozen spin dependent potential [120]. This simple scheme has been used among other things for surface layered systems. In particular for $\text{Fe}_n/\text{Au}(001)$ it was found that the spin-orbit coupling term $\Delta E_{\text{SOC}}(\hat{n}, \hat{n}')$ and the dipole-dipole term $\Delta E_{\text{dip}}(\hat{n}, \hat{n}')$ are of the same order of magnitude leading to a change from out-of-plane to in-plane anisotropy if the number n of Fe layers is increased above three [121]. By decomposing the band-energy via the DOS in a layer-resolved way the anisotropy energy $\Delta E_{\text{SOC}}(\hat{n}, \hat{n}')$ could be decomposed accordingly [123]. A corresponding analysis of $\Delta E_{\text{SOC}}(\hat{n}, \hat{n}')$ shows in general that the dominating contributions originate from interface or surface layers, respectively.

An alternative to the calculation of $\Delta E_{\text{SOC}}(\hat{n}, \hat{n}')$ via the total energy or the force theorem is to consider the torque exerted on a magnetic moment when the magnetisation is tilted away from its equilibrium orientation (easy axis). Using multiple scattering theory the torque component with respect to a rotation of the magnetisation about an axis \hat{u} can be expressed as [124]:

$$T_{\alpha\hat{u}}^{\hat{n}} = -\frac{1}{\pi} \Im \int^{E_F} dE \frac{\partial}{\partial \alpha^{\hat{u}}} [\ln \det (\underline{t}(\hat{n})^{-1} - \underline{G}^0)] . \quad (19)$$

The great flexibility of this approach has been demonstrated by investigations on the temperature dependence of the magnetic anisotropy energy of L1_1 -ordered FePt alloys [125]. Another example for its application are investigations on small deposited Fe clusters on a Pt(111) substrate [126]. Calculating the magnetic moments and anisotropy energies for various cluster sizes, the input necessary to simulate the magnetisation curves $M(B)$ for ensembles of Fe clusters could be supplied. Fig. 9 shows the results for two different temperatures compared with experimental data [126]. Obviously, the calculations based on Eq. (19) lead to a parameter set that is in very satisfying accordance with experiment.

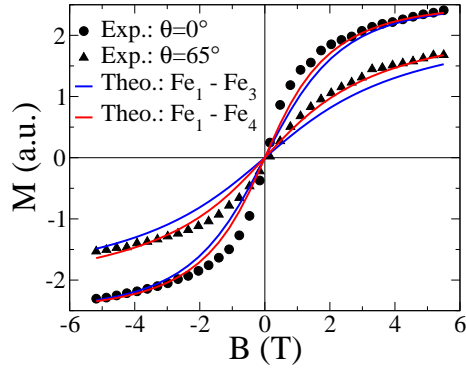


Figure 9: Experimental magnetisation curves $M(B)$ (dots) of an ensemble of Fe_n ($n=1,2,3$) clusters on Pt(111) measured at $T = 6$ K for an orientation of the magnetic field $M(B)$ along the easy axis $\hat{z}(\theta = 0^\circ)$ and rotated by $\theta = 65^\circ$ with respect to that. The full lines give corresponding theoretical results obtained on the basis of the calculated properties of Fe_n clusters and the Langevin formula. The dashed line is obtained by including in addition Fe_4 clusters in the simulation [126].

The expression for the magnetic torque given above is derived by considering the change of the single-particle energies if all magnetic moments change their orientations the same way. If only two moments change their relative orientation the corresponding change in the energy ΔE_{ij} can be expressed in an analogous way. As was shown by Lichtenstein et al. ΔE_{ij} can be expressed very elegantly within multiple scattering theory by making use of Lloyd's formula [51]. If ΔE_{ij} is expressed to lowest order with respect to the orientation angle of the moments \hat{m}_i and \hat{m}_j , one gets a one-to-one mapping of the exchange coupling energy ΔE_{ij} to the Heisenberg Hamiltonian $\mathcal{H} = -\sum_{ij} J_{ij} \hat{m}_i \cdot \hat{m}_j$, with the coupling constants J_{ij} given by [51]:

$$J_{ij} = -\frac{1}{4\pi} \text{Im} \int^{E_F} dE \text{Trace} \left(t_{i\uparrow}^{-1} - t_{i\downarrow}^{-1} \right) \tau_{\uparrow}^{ij} \left(t_{j\uparrow}^{-1} - t_{j\downarrow}^{-1} \right) \tau_{\downarrow}^{ji}. \quad (20)$$

This expression for the isotropic exchange coupling has been used extensively to supply the input for subsequent Monte-Carlo simulations on the basis of the Heisenberg Hamiltonian. This hybrid approach offers a realistic route to investigate magnetic properties at finite temperatures and has been applied with great success for bulk [127–129], layered [130–132], one-dimensional [133] as well as finite cluster systems [134, 135].

If spin-orbit coupling is accounted for the exchange coupling parameter in the Heisenberg Hamiltonian has to be replaced by a corresponding tensor:

$$\mathcal{H} = -\sum_{i \neq j} \hat{m}_i \underline{\underline{J}}_{ij} \hat{m}_j + \sum_i K(\hat{m}_i) \quad (21)$$

$$= -\sum_{i \neq j} J_{ij} \hat{m}_i \cdot \hat{m}_j - \sum_{i \neq j} \hat{m}_i \underline{\underline{J}}_{ij}^S \hat{m}_j - \sum_{i \neq j} \vec{D}_{ij} \cdot (\hat{m}_i \times \hat{m}_j) + \sum_i K_i(\hat{m}_i). \quad (22)$$

with the single-site magnetic anisotropy represented by the term $K(\hat{m}_i)$. In Eq. (22) the coupling tensor $\underline{\underline{J}}_{ij}$ has been decomposed in the standard way into its isotropic part J_{ij} , its traceless symmetric part $\underline{\underline{J}}_{ij}^S$ and its anti-symmetric part that in turn is represented in terms of the so-called Dzyaloshinsky-Moriya (DM) vector \vec{D}_{ij} . A corresponding generalisation of the non-relativistic expression for J_{ij} given in Eq. (20) to its relativistic tensor form was worked out by

Udvardi et al. [136]. An alternative expression, that offers several advantages, is given by [137]:

$$J_{ij}^{\alpha_i \alpha_j} = -\frac{1}{\pi} \Im \int dE \text{Trace} \Delta V_{\Lambda}^{\alpha_i} \underline{\tau}^{ij} \Delta V_{\Lambda'}^{\alpha_j} \underline{\tau}^{ji}, \quad (23)$$

with

$$\Delta V_{\Lambda \Lambda'}^{\alpha_i} = \int d^3r Z_{\Lambda}^{\times}(\vec{r}) \beta \sigma_{\alpha} B(r) Z_{\Lambda'}(\vec{r}). \quad (24)$$

The expressions given above have been applied recently to a number of cluster systems [138,139] with the interest focussing on the impact of the DM-interaction. For Fe, Co, and Ni dimers on Pt(111) it was found for example that the DM-interaction leads to a tilting of the individual magnetic moments in the dimer in spite of the pronounced out-of-plane anisotropy and a strong ferromagnetic isotropic exchange coupling. Another system studied was an FePt cluster on Pt(111) that has rows of Fe atoms separated by Pt atoms (see Fig. 10). The left panel of Fig. 10

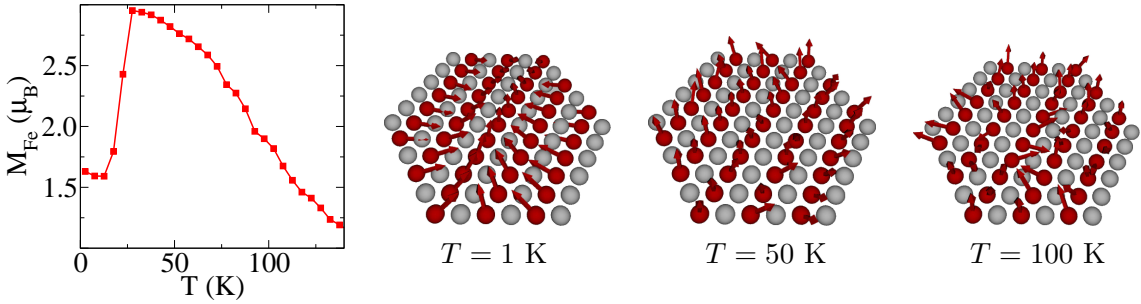


Figure 10: Left: Temperature dependence of the thermally averaged Fe moment $m_{\text{Fe}}(T)$. Around $T = 25$ K the transition from non-collinear low-temperature structure caused by the Dzyaloshinsky-Moriya interaction to the ordered ferromagnetic structure occurs. Right: Magnetic structure of $\text{Fe}_{43}\text{Pt}_{48}$ cluster for three different temperature range: non-collinear ($T = 1$ K), ferromagnetic ($T = 50$ K) and disordered paramagnetic ($T = 100$ K) [139].

shows the thermally averaged Fe moment $m_{\text{Fe}}(T)$ as a function of the temperature T that was obtained from Monte-Carlo simulations on the basis of the generalised Heisenberg Hamiltonian in Eq. (21). For high temperatures, one starts in the paramagnetic regime with the individual moments randomly oriented as it is shown by the snapshot for $T = 100$ K. With decreasing temperature the strong isotropic exchange coupling leads to a ferromagnetic alignment of the moments within each Fe row (see snapshot for $T = 50$ K). Below around $T = 25$ K the Fe-rows get coupled with their average moment tilted against each other due to the DM-interaction.

It should be emphasised that Eq. (21) is an approximate mapping of the complicated energy landscape $E(\{\hat{m}_i\})$ of a system calculated in an ab-initio way onto a simplified analytical expression. This implies corresponding limitations [138] in particular due to the use of the rigid spin approximation (RSA) [140]. A coupling tensor of the same shape as in Eq. (21) occurs for the indirect coupling of nuclear spins mediated by conduction electrons. In this case the above mentioned restrictions do not apply. As a consequence the linear response formalism on the basis of the Dyson equation can be used without restrictions to determine the corresponding nuclear spin – nuclear spin coupling tensor [141].

7.7.2 Magnetic response functions

The Green's function formalism supplies a natural basis for investigations on the response of a system to an external perturbation via the Dyson equation (10). Inserting the Dyson equation repeatedly into itself one obtains for the Green's function G^{pert} of the perturbed system a power series with respect to the perturbation $\mathcal{H}_{\text{pert}}$ expressed in terms of the Green's function G^{ref} of the unperturbed reference system. Keeping only the first order term one ends up with the linear response of the system to the perturbation:

$$G^{\text{pert}}(\vec{r}, \vec{r}', E) = G^{\text{ref}}(\vec{r}, \vec{r}', E) + \int_{\Omega_{\text{pert}}} d^3r'' G^{\text{ref}}(\vec{r}, \vec{r}'', E) \mathcal{H}_{\text{pert}}(\vec{r}'') G^{\text{ref}}(\vec{r}'', \vec{r}', E). \quad (25)$$

Considering for example the perturbation caused by a static magnetic field B_{ext} along the z-axis the corresponding perturbation $\mathcal{H}_{\text{pert}}(\vec{r})$ may be written as:

$$\mathcal{H}_{\text{pert}}(\vec{r}) = \underbrace{\beta \sigma_z \mu_B B_{\text{ext}} + \beta \hat{l}_z \mu_B B_{\text{ext}}}_{\text{Zeeman}} + \underbrace{\Delta V^{\text{xc}}(\vec{r}) + \Delta V^{\text{H}}(\vec{r})}_{\text{induced}}. \quad (26)$$

Here a relativistic formulation has been adopted with β standing for one of the standard Dirac matrices. The first two terms represent the Zeeman-type coupling of the external magnetic field to the spin and orbital angular momentum of the electrons, while the remaining terms represent the changes of the exchange-correlation (xc) and Hartree (H) potential induced by the perturbation. For non-magnetic solids the last term can usually be ignored. Focusing in this case on the spin magnetisation $m_{\text{spin}}(\vec{r})$ induced by B_{ext} the second term can also be omitted if the influence of the spin-orbit coupling is neglected. Expressing now $m_{\text{spin}}(\vec{r})$ as well as $\Delta V^{\text{xc}}(\vec{r})$ in terms of $G^{\text{pert}}(\vec{r}, \vec{r}', E)$ using Eq. (26) one ends up with an implicit equation for $m_{\text{spin}}(\vec{r})$ that in turn is linear with respect to B_{ext} . Accordingly, one gets a corresponding equation for the spin susceptibility χ_{spin} with the term connected with $\Delta V^{\text{xc}}(\vec{r})$ giving rise to the Stoner-enhancement. This scheme was used to arrive at a formulation for the Stoner-enhanced spin susceptibility that accounts for the influence of spin-orbit coupling and that is applicable also for disordered alloys [142]. Later it was extended to include also orbital contributions giving rise to the Van-Vleck-susceptibility χ_{VV} as well as spin-orbit cross-terms [143]. In an analogous way the NMR Knight-shift in metals was formulated accounting for all spin and orbital contributions [144].

Dealing with spontaneously magnetised solids the last term in Eq. (26) has also to be included. In addition the Fermi energy may be shifted due to the perturbation. Including these modifications gives access to the high-field susceptibility χ_{HF} of ferromagnetic solids [145]. In Fig. 11 results of corresponding calculations for the alloy system $\text{bcc-Co}_x\text{Fe}_{1-x}$ are shown. For the Fe-rich regime of the system the experimental data are obviously reproduced quite well by the theoretical results. For the region around $x = 1/2$ agreement is less satisfying. However, accounting for partial ordering in the system in this regime, that may be expected because the equilibrium structure for $x = 1/2$ is the CsCl-structure, agreement between theory and experiment is again very good. The right panel of Fig. 11 shows the contribution of the spin susceptibility to the total high-field susceptibility of $\text{bcc-Co}_x\text{Fe}_{1-x}$. As one notes, the partial susceptibilities of Fe and Co are quite different and give rise to the concentration dependence of the total susceptibility (left panel). In addition one can see that the spin susceptibility is only a minor contribution to the total susceptibility that is dominated by its orbital Van-Vleck-contribution. The latter one

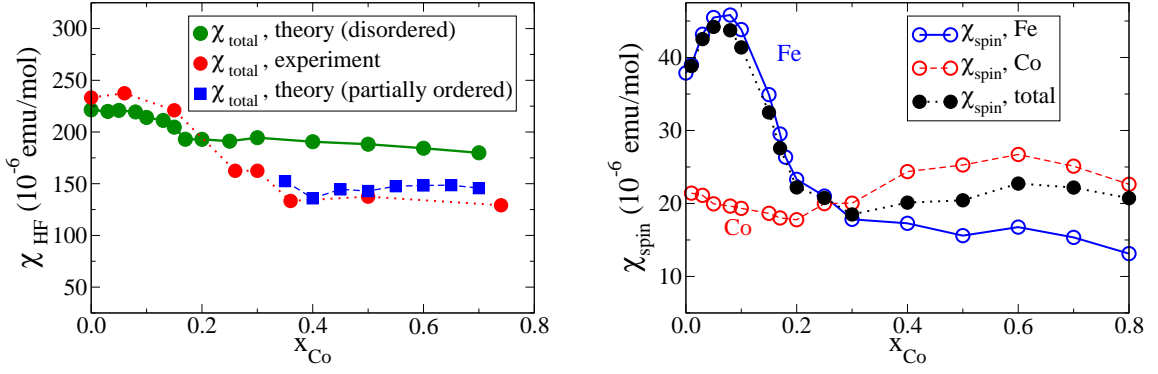


Figure 11: High-field magnetic susceptibility χ_{HF} of bcc $\text{Fe}_{1-x}\text{Co}_x$ alloys: Total susceptibility (left); green circles correspond to randomly disordered alloys, while blue squares correspond to 'partially ordered' alloys. Experimental data are given by filled circles; (right) Element-resolved contributions to the spin magnetic susceptibility χ_{spin} of Fe and Co in disordered $\text{Fe}_{1-x}\text{Co}_x$ [145].

is more or less concentration independent and is accompanied by an appreciable Landau-type contribution χ_{Lan} . Here, it should be noted that $\mathcal{H}_{\text{pert}}$ given in Eq. (26) does not give access to χ_{Lan} . However, as was shown by Benkowitzsch and Winter [146] for the non-relativistic case, χ_{Lan} can be determined by starting from a spatially oscillating magnetic field $\vec{B}_{\vec{q}}(\vec{r})$ and considering the coupling of the orbital current density to the corresponding magnetic vector potential $\vec{A}_{\vec{q}}(\vec{r})$. A corresponding relativistic formulation suitable for magnetic solids was used to calculate χ_{Lan} included in the total high-field susceptibility χ_{HF} given in Fig. 11.

The formalism sketched here is not restricted to a static perturbation. Corresponding work on the frequency and wave-vector dependent dynamic spin susceptibility has been done for example on pure Pd on a non-relativistic level [147].

7.7.3 Transport properties

Another important field for the application of linear response formalism is electronic transport. As mentioned above, Butler and Stocks demonstrated the use of the KKR-GF-CPA to calculate the residual resistivity of disordered alloys on the basis of the Boltzmann formalism [98]. Later on an expression for the electronic conductivity of alloys was developed by Butler on the basis of the Kubo-Greenwood formalism and the KKR-GF-CPA that allows to express the elements of the symmetric conductivity tensor $\underline{\underline{\sigma}}$ in terms of the auxiliary conductivities $\tilde{\sigma}_{\mu\nu}$ [148]:

$$\tilde{\sigma}_{\mu\nu} = -\frac{4m^2}{\pi\hbar^3\Omega} \left(\sum_{\alpha,\beta} \sum_{\substack{L_1,L_2 \\ L_3,L_4}} x_\alpha x_\beta \tilde{J}_{L_4,L_1}^{\alpha\mu}(z_2, z_1) \left[\{1 - \chi\omega\}^{-1} \chi \right]_{\substack{L_1,L_2 \\ L_3,L_4}} \tilde{J}_{L_2,L_3}^{\beta\nu}(z_1, z_2) \right. \\ \left. + \sum_{\alpha} \sum_{\substack{L_1,L_2 \\ L_3,L_4}} x_\alpha \tilde{J}_{L_4,L_1}^{\alpha\mu}(z_2, z_1) \tau_{L_1,L_2}^{\text{CPA}00}(z_1) J_{L_2,L_3}^{\alpha\nu}(z_1, z_2) \tau_{L_3,L_4}^{\text{CPA}00}(z_2) \right), \quad (27)$$

with $z_{1(2)} = E_F \pm i\epsilon$. Here the quantities $J_{LL'}^{\alpha\mu}$ are matrix elements of the μ -component of the current density operator \vec{j} for the alloy component α , with $\tilde{J}^{\alpha\mu}$ involving in addition the component projected scattering path operators $\underline{\tau}^\alpha$. The term χ stands for a sum over all

scattering path operators $\tau_{L,L'}^{\text{CPA } 0n}(z_1)\tau_{L'',L'''}^{\text{CPA } n0}(z_2)$ with $n \neq 0$ and the expression in curly bracket accounts for the so-called vertex corrections.

Results of a corresponding application to disordered $\text{Ag}_x\text{Pd}_{1-x}$ are shown in Fig. 12 [149]. The

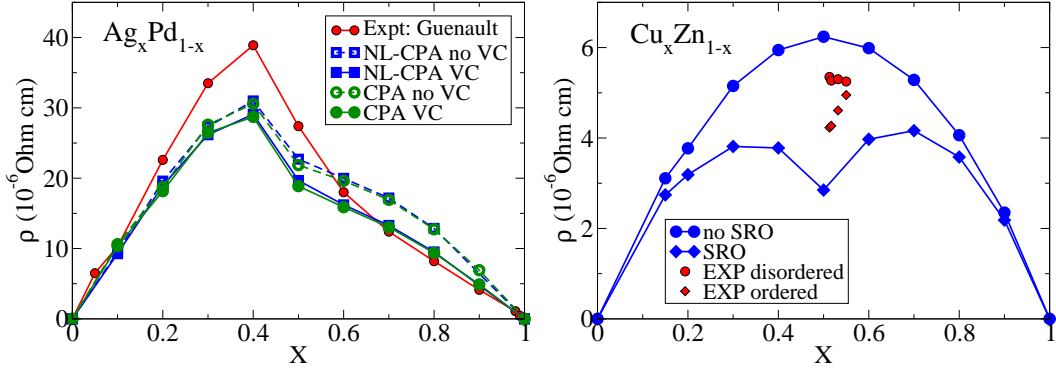


Figure 12: Left: Residual resistivity in disordered $\text{Ag}_x\text{Pd}_{1-x}$ alloys as a function of the concentration x . Results are shown obtained on the basis of the CPA and NL-CPA including (VC) and excluding (no VC) the vertex corrections. Experimental results are shown in addition. Right: Residual resistivity in disordered bcc- $\text{Cu}_x\text{Zn}_{1-x}$ alloys as a function of the concentration obtained using the NL-CPA. Results are shown including (SRO) and excluding (no SRO) atomic short-range order together with corresponding experimental data [149].

calculations have been performed with and without inclusion of the so-called vertex corrections. As one notes these have an impact on the residual resistivity only on the Ag-rich side of the alloy system. In addition, one finds that the experimental data are reproduced quite well by the calculations implying in particular that the single-site CPA is completely sufficient to deal with the residual resistivity of randomly disordered alloys. This is also confirmed by calculations based on the NL-CPA formalism [149]. As Fig. 12 shows corresponding results are indeed in very good agreement with the resistivity obtained by using the CPA.

In addition, Fig. 12 shows the residual resistivity in disordered bcc- $\text{Cu}_x\text{Zn}_{1-x}$ alloys as a function of the concentration obtained using the NL-CPA including the vertex corrections [149]. Assuming a random distribution of the alloy components a simple parabolic variation of the resistivity with concentration is found. On the other hand, assuming SRO according to the CsCl-structure within the NL-CPA cluster a pronounced reduction in the resistivity is found as it is expected from the corresponding experimental data that are also shown in Fig. 12.

The scheme to implement the Kubo-Greenwood (KG) equation for disordered alloys sketched above (see Eq. (27)), can also be used to introduce a layer-resolved conductivity $\sigma^{II'}$ appropriate for two-dimensional periodic systems [150–152], with I and I' being layer indices. This approach was later extended to finite frequencies [153, 154] supplying a suitable basis for investigations on the spin-orbit induced magneto-optical Kerr-effect of magnetic surface layer systems [153, 155, 156], that can show a pronounced enhancement of the Kerr rotation as a function of the layer thickness. As an alternative to the Kubo-Greenwood formalism, transport in two-dimensional systems may also be described in terms of a layer-resolved conductance $g^{II'}$ introduced within the framework of the Landauer-Büttiker (LB) formalism [157, 158]:

$$g^{II'} \propto \int d\vec{k}_{\parallel} \sum_{\substack{n \in I \\ n' \in I'}} \text{Trace} \left[\underline{J}^n \underline{G}^{nn'}(\vec{k}_{\parallel}, E_F) \underline{J}^{n'} \underline{G}^{nn'\dagger}(\vec{k}_{\parallel}, E_F) \right], \quad (28)$$

with the matrix elements of the perpendicular component of the current density operator \vec{j} :

$$J_{\Lambda\Lambda'}^n = \frac{1}{V_n} \int_{S_n} d^2r R_{\Lambda}^{n\times} j_{\perp} a_{\perp} R_{\Lambda'}^n. \quad (29)$$

The Kubo-Greenwood and Landauer-Büttiker approaches have been used extensively to investigate the giant magneto resistance (GMR) [159–161] and the tunnelling magneto resistance (TMR) [162–165] of FM/SP/FM trilayer systems consisting of ferromagnetic (FM) leads separated by a non-magnetic metallic or insulating, respectively, spacer (SP). Corresponding studies were dealing among other with the influence of the relative orientation of the magnetisation in the magnetic leads [160,166] or spin-flip processes due to spin-orbit coupling [165]. Corresponding results of relativistic calculations for the conductance g of the trilayer system Fe/ n (GaAs)/Fe with Ga-termination are shown in Fig. 13 [165] for the magnetisation in ([110]) and out-off ([001]) plane. Although for both geometries the magnetisation of the magnetic leads are parallel, there

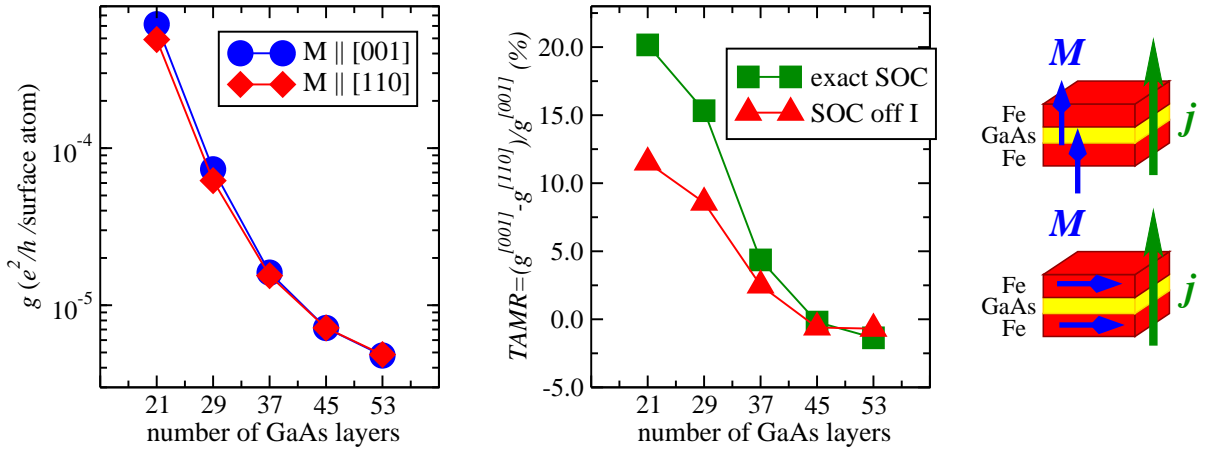


Figure 13: Left: conductance g of the trilayer system Fe/ n (GaAs)/Fe with Ga-termination for the magnetisation in ([110]) and out-off ([001]) plane. Right: sketch for the in (bottom) and out-off (top) plane geometry. Middle: first type of tunnelling anisotropic magneto resistance (TAMR) for the full spin-orbit coupling (exact SOC) and for the spin-orbit coupling suppressed for the interface layers (SOC off I).

is a pronounced dependence of the conductance on the orientation of the magnetisation due to spin-orbit coupling. The middle panel of Fig. 13 shows that the corresponding tunnelling anisotropic magneto resistance (TAMR) can be as large as 200 % for a thin GaAs-spacer. The fact that the TAMR is caused by spin-orbit coupling can be demonstrated very easily. In addition to the TAMR for the full spin-orbit coupling (exact SOC) results for the spin-orbit coupling suppressed for the interface layers (SOC off I) are shown in addition in the middle panel of Fig. 13. The drop of the TAMR by nearly a factor 2 reflects the central role of the hybridisation at the Fe/GaAs-interface for the TAMR. This gets even more important for a second type of TAMR that can be observed even with only one magnetic layer present [167]. Fig. 14 shows the corresponding set up for a Fe/(GaAs)/Au trilayer system with the magnetisation of the Fe lead in plane. Rotating the magnetisation in the plane changes the hybridisation at the interface due to spin-orbit coupling and gives rise to a corresponding variation of the conductance with the rotation angle. As Fig. 14 shows, the experimental results [167] for this second type of TAMR are reasonably well reproduced by the calculations [168]. Again the central role of spin-orbit

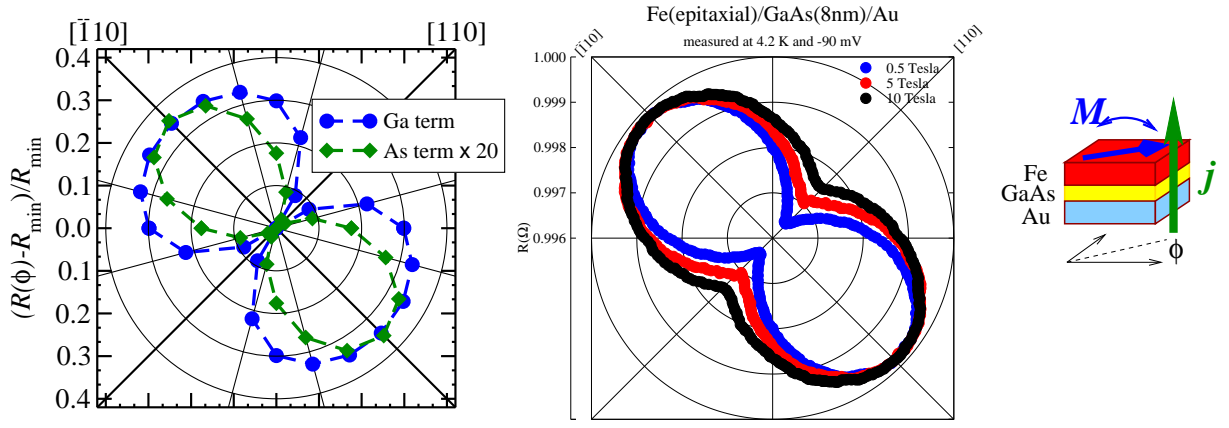


Figure 14: Left: theoretical results for the second type of TAMR in Ga and As terminated Fe/29(GaAs)/Au. Middle: corresponding experimental results for Fe/GaAs(8nm)/Au. Right: sketch of the geometry.

coupling can easily be demonstrated by model calculations with the strength of the spin-orbit coupling manipulated.

The transport theory for layered systems presented above can be applied more or less directly to lead/wire/lead systems. Corresponding investigations accounted in particular for the influence of spin-orbit coupling and a non-collinear spin configuration within the wire [82]. The effect of a finite bias voltage on the TAMR was already investigated using the sketched linear response schemes [164]. A more general description can be achieved by use of the steady state Keldysh or non-equilibrium Green's function approach. A first implementation of this numerically quite demanding scheme within the KKR-GF formalism could already be presented [169,170].

7.7.4 Electron Spectroscopy

When dealing with electron spectroscopies multiple scattering theory offers especially great advantages compared to any other scheme for electronic structure calculations. A most prominent example is EXAFS (extended X-ray absorption fine structure) [171]. An adequate theoretical description has to deal with matrix elements with respect to the electron-photon interaction operator with a tightly bound core state and an extended final state involved. As the final state lies in the energy range of about 50 – 1500 eV above the Fermi level, the energy-dependence of the final state wave function cannot be ignored. For the same reason non-dipole contributions to the matrix element may become important. The finite life time of the final state caused by various relaxation processes is usually accounted for by a corresponding complex and energy dependent self-energy $\Sigma(E)$ [172]. Finally, the influence of the environment of the absorber atom on its electronic structure has to be included in a transparent way – again up to very high energies. All these requirements are met by applying multiple scattering theory to a finite cluster centred at the absorber atom. In particular a connection of the oscillations observed in an EXAFS spectrum and the atomic configuration around the absorber atom can be established in a transparent way. A similar situation occurs for many other core level spectroscopies [39, 40, 173, 174].

In the case of a crystalline solid most detailed information on its electronic structure can be

obtained by use of angle-resolved photo emission spectroscopy (ARPES) applied to the valence band. An appropriate theoretical description of ARPES is supplied by the so-called one-step model of photo emission that expresses the photo electron current $j_{\vec{k}m_s}^{\vec{q}\lambda}(E_f)$ by making use of Fermi's golden rule [56, 175–177]:

$$j_{\vec{k}m_s}^{\vec{q}\lambda}(E_f) \propto \Im \int d^3r \int d^3r' \left[\mathcal{T} \phi_{\vec{k}m_s}^{\text{LEED}}(\vec{r}, E_f) \right]^\dagger X_{\vec{q}\lambda}(\vec{r}) G(\vec{r}, \vec{r}', E_i) X_{\vec{q}\lambda}^\dagger(\vec{r}') \mathcal{T} \phi_{\vec{k}m_s}^{\text{LEED}}(\vec{r}', E_f) \quad (30)$$

with

$$\phi_{\vec{k}m_s}^{\text{LEED}}(\vec{r}, E_f) = \Xi_{m_s} e^{i\vec{k}\vec{r}} + \int d^3r' G(\vec{r}, \vec{r}', E_f) V(\vec{r}') \Xi_{m_s} e^{i\vec{k}\vec{r}'} . \quad (31)$$

Here the initial valence band states at energy E_i are represented by the Green's function $G(E_i)$. The final state at energy $E_f = E_i + \hbar\omega$ – a so-called time-reversed LEED-state – is constructed on the basis of the Lippmann-Schwinger-equation involving the Green's function at energy E_f , Ξ_{m_s} represents the spin part of the free-electron wave function characterized by the quantum number m_s and \mathcal{T} is the time reversal operator. Finally, $X_{\vec{q}\lambda}(\vec{r})$ is the electron-photon interaction operator for radiation with wave vector \vec{q} and polarisation λ .

Again evaluating the expression for the photo electron current by means of multiple scattering theory allows to account in an appropriate way for matrix-elements, finite life time effects represented by a corresponding self-energy $\Sigma(E)$ and – most important in the UV-regime – for the surface of the system. This allows in particular for a proper inclusion of contributions to the photo electron current due to surface states. In fact, many experimental and theoretical investigations are focused recently on the influence of spin-orbit coupling giving rise to the so-called Rashba-splitting for the surface states [178, 179]. As for all other electronic properties disorder in the system may be accounted for by means of the CPA within an ARPES calculation based on multiple scattering theory [176, 180].

During the last one or two decades the resolution of ARPES experiments could be substantially improved allowing for a very detailed mapping of the electronic properties of solids. Results of a corresponding investigation on Ni(110) at a photon energy of $\hbar\omega = 21$ eV are shown in Fig. 15 and compared to the bulk spectral function calculated on the basis of the LSDA [181]. Obviously, the various features of the experimental spectra cannot be described in a satisfying way on that basis indicating the non-negligible influence of correlation effects not accounted for by LSDA. In fact, calculations of the spectral function on the basis of the LSDA+3BS (three body scattering) many-body formalism describe the spectra in a much better way [181], but still neglect the influence of matrix-elements and of the surface. Application of the KKR-GF-formalism, on the other hand, allowed to account for these on the basis of the one-step model of photo emission [182]. In addition, correlation effects were accounted for by making use of the LSDA+DMFT scheme [34]. As Fig. 15 shows this coherent approach leads to a very satisfying agreement of the calculated photo current and the experimental one.

During the last years ARPES experiments were continuously pushed to higher photon energies up to the keV-regime to reduce the surface sensitivity of this spectroscopy and to probe primarily the electronic structure of the bulk this way. Apart from many technical problems this raises

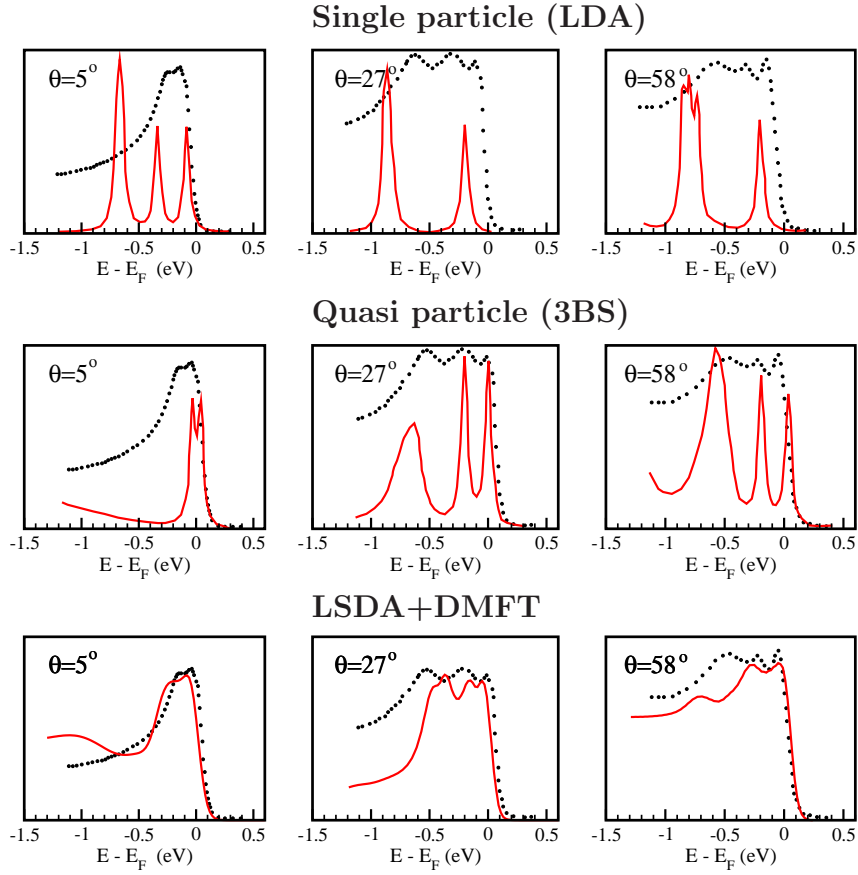


Figure 15: Spin-integrated ARPES spectra from Ni(011) along $\bar{\Gamma}-\bar{Y}$ for three different angles of emission. Upper row: comparison between LSDA-based calculations and experiment [181]; middle row: comparison between experiment and non-self-consistent quasi particle calculations neglecting matrix element and surface effects [181]; lower row: spin-integrated LSDA+DMFT spectra including photo emission matrix elements (this work). Theory: solid red line, experiment: black dots [182].

several questions concerning the interpretation of the ARPES spectra on the experimental side. Also for the calculation of ARPES spectra in the soft or hard X-ray regime extensions have to be introduced as the momentum of the photon cannot be neglected any more and non-dipole contributions may get important. Fig. 16 shows results of corresponding investigations on the ARPES of W(110) for a photon energy of $\hbar\omega = 260$ eV [183]. Obviously, the calculations based on the one-step model reproduce the experimental spectral data rather well. In addition, one notes that the spectra essentially follow the dispersion relation $E_{\vec{k}}$ calculated for bulk W rather well indicating that for the selected photon energy indeed primarily the bulk band structure is probed. The experimental data shown in Fig. 16 were recorded at $T = 300$ K. For higher temperatures but also for higher photon energies the influence of lattice vibrations gets more and more pronounced leading finally to spectra that essentially reflect the DOS of the system [183]. Theoretical schemes to deal with this complex situation have already been suggested [184] that should allow for corresponding calculations of the spectra in the near future.

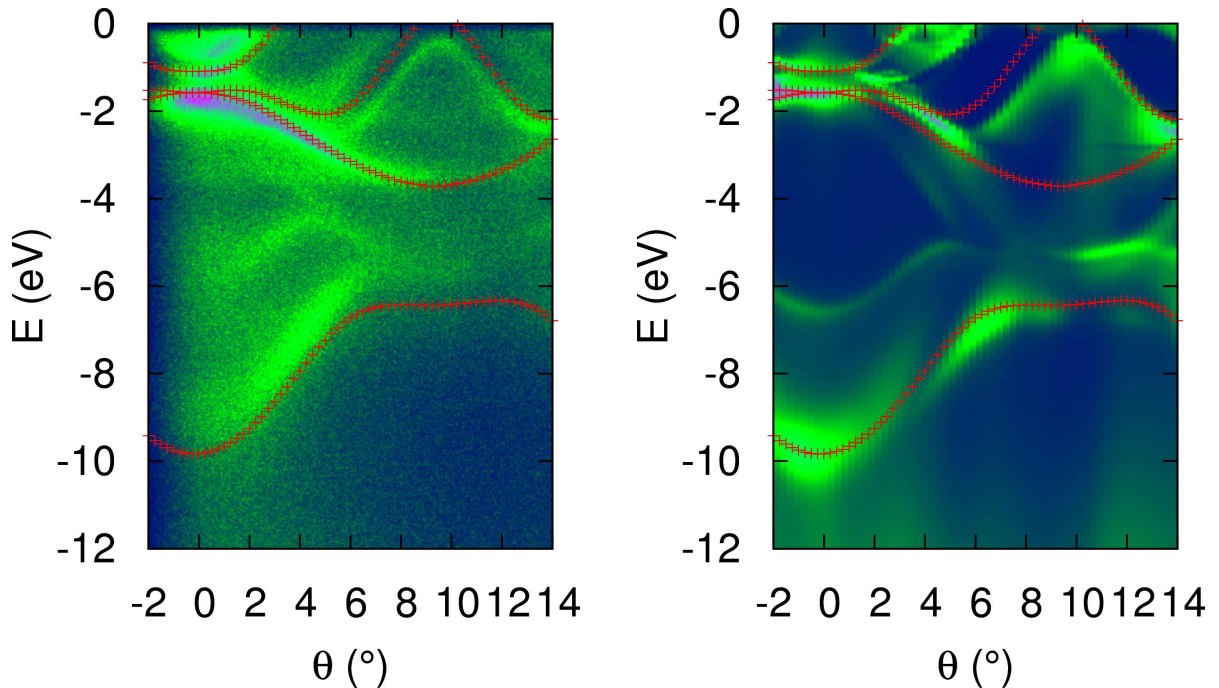


Figure 16: Plots of the experimental (left) and theoretical (right) photo current intensity for the excitation from the valence bands of W(110) at $T = 300$ K with a photon energy of $\hbar\omega = 260$ eV as a function of the initial state energy and the angle of emission with respect to the surface normal. The emission angle corresponds essentially to a probing of initial states with \vec{k} along the Γ -to-N line in the Brillouin zone with a corresponding dispersion relation $E_{\vec{k}}$ included [183].

7.8 Concluding remarks

The various examples presented in some detail⁷ were meant to demonstrate that the KKR-GF-method provides a very flexible framework to deal with a wide range of systems and properties using one and the same formalism without using unnecessary simplifications or artificial boundary conditions.⁸ One of the reasons for the flexibility of the KKR-GF is the fact that it is an all-electron method using a minimal, numerical and energy-dependent basis set. This allows to deal, for example, with hyperfine interaction, EXAFS or valence band photo-emission accounting for all their specific features and to interpret the results in a chemically intuitive way. The most important feature, however, is that the KKR-GF supplies the electronic Green's function directly. This is of great advantage when dealing with spectroscopic properties or making contact with many-body schemes that go beyond LDA as in these cases representing the electronic structure in terms of the Green's function is the standard starting point. Connected with the availability of the Green's function is the use of the Dyson equation that can be exploited in many different ways. One branch is the description of complex systems on the basis of a simpler reference system. The other branch is the straight forward investigation of all type of response quantities. Finally, one should mention the treatment of disorder by means of the CPA or NL-CPA with their application not at all restricted to chemical disorder in alloys.

⁷In fact these reflect only some of the activities of the authors; i.e. much more examples can be found via the various references given, that are by no means complete ...

⁸This statement does not imply the claim that other methods are not able or useful to deal with the systems or properties considered here.

Of course, the various features of the KKR-GF method give also rise to some disadvantages. Solving the single-site problem for the full complexity of the underlying Hamiltonian, for example, implies accuracy but also corresponding numerical effort. This can be reduced, however, to a large extent by the Born series technique. Another more serious drawback is the use of fixed atomic positions for the reference system making atomic relaxation somewhat cumbersome. However, various techniques are available now that should allow to account for atomic relaxations more or less routinely. Obviously, these minor technical problems are more than outweighed by the many advantages offered by the KKR-GF method.

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