Ψ_k Newsletter

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

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Contents

1 Editorial

In this *Newsletter* readers will find a number of reports on a variety of workshops which have recently taken place. They are placed in all sections dedicated to TMR networks and the ESF programme. The report on the *IX Workshop on Computational Materials Science*, which took place in Villasimius, contains also abstracts of invited talks. In the section dedicated to **General Workshop/Conference Announcements** there are announcements of two interesting events, in the field of strongly correlated systems, that will take place in the 'Newton Institute' in Cambridge. Announcements of available positions are given in the **General Job Announcements** section. Additional announcement, of interest to EU nationals only, can be found in the **TMR1** section. As always, we have a number of abstracts in the usual **Abstracts** section. The scientific highlight is by Mike Brooks (Karlsruhe) *et al.* on **'Crystal Field Excitations as Quasi-Particles'**. Please check the table of content for further details.

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

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

The above contains pointers to home pages of some of the members of our electronic structure community. If you maintain a home page on your activities we will be happy to include a pointer from the *Networks'* home page to your home page.

Please note that the home page of the Psi-k Networks has recently been updated. It contains useful information regarding funding of workshops and collaborative visits within the ESF Programme. Its major new feature is a separate highlight section which contains all highlight articles of the Newsletters published so far.

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

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

	function
psik-coord@daresbury.ac.uk	**messages to the coordinators, editor & newsletter**
psik-management@daresbury.ac.uk	**messages to the NMB of all Networks**
psik-network@daresbury.ac.uk	**messages to the whole Ψ_k community**

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2 General News

2.1 Psi-k2000 Conference

Schwäbisch Gmünd, 22-26 August, 2000

”Ab initio (from Electronic Structure) Calculations of Complex Processes in Materials

Call for Suggestions

As you know from the previous newsletters the Psi-k2000 Conference has its own web sever:

http://psi-k.dl.ac.uk/psi-k2000

The page contains the latest information on all matters of the Conference and also allows pre-registration to the Conference. There one can also find a suggestion form for the symposia and plenary and symposia speakers. Please take time and send us your choice for the symposia and speakers. This we need to receive within the next month or so, to be able to formulate a preliminary programme of the Conference for discussion with the Programme Committee and the International Advisory Committee. The time is pressing. We would very much appreciate everybody’s input on the symposia and speakers.

The web page is updated on daily basis. Please have a look and help us publicize the Conference and make it a success.

3 News from the TMR1 Network

"Ab Initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers"

3.1 Reports on Workshops

3.1.1 Report on the Riksgränsen Workshop, Sweden

Workshop on Interface Anisotropy and Spin and Orbital Magnetism

held in Riksgränsen, Sweden, May 5–9, 1999.

This workshop, which was partially financed by the TMR-programme "Interface and surface magnetism", the ESF-programme Ψ_k, the Swedish Natural Science Research Council (NFR) as well as the Royal Swedish Academy of Science (KVA), was from the beginning planned to be mainly tutorial. In this spirit eleven experienced researchers in the field were invited in order to give a two hour lecture with ample time for a long introduction leading up to the presentation of some recent results. This was done in hope to educate and interest young researchers, students or post-docs, which would like to learn about the field. In order to allow for a more relaxed atmosphere, we had forewarned the speakers that the audience was allowed and encouraged to interrupt them with questions and comments.

Of these speakers, three had an experimental background: Klaus Baberschke, Berlin, Björgvin Hjörvarsson, Stockholm, and Claus Schneider, Dresden. They brought up different aspects of the magnetism of thin films, emphasizing the problems of structural determinations, the morphology and their importance for the observed magnetic properties. Several different experimental techniques were covered as e.g. MOKE, FMR, and photo-electron spectroscopy. They all took opportunities to present challenges to the theoreticians in the audience.

Especially two of the theoreticians had been asked to give some background to the theory of magnetism. Peter Mohn, Wien, covered many aspects of itinerant magnetism, especially from a band-structure perspective, while Helmut Eschrig, Dresden, introduced the audience to the field of density functional theory, especially its relativistic extensions, which is the proper theoretical approach to magnetic anisotropy as well as orbital magnetism. They both also presented recent results on itinerant non-collinear magnetism. Prof. Mohn presented calculations on the exchange coupling in perovskite CMR material, while Prof. Eschrig discussed some ineffincies in present formulations of local approximations to the intra-atomic exchange-correlation field.

Stefan Blügel, Jülich, covered the field of surface magnetism, which ended up with presentations of the possible stabilization of magnetic surface alloys as in e.g. Mn/Cu. He also discussed for instance how the magnetism is changed from the bulk when one is studying the effects of the surface. While Dr.Blügel mainly covered spin magnetism, Mike Brooks, Karlsruhe, got into details of the orbital magnetism, its origin in spin-orbit coupling as well as its spectacular manifestations in the magnetic actinides. He discussed the often overlooked exchange effects on the orbital magnetism, as manifested in Hund's second rule. In his talk he pedagogically compared the magnetism of the itinerant $3d$ metals, the magnetism of the localized $4f$ as in the lanthanides, and the relativistic magnetism of the actinide $5f$.

A slightly different approach to the magnetism of thin films was covered by Peter Jensen, Berlin. He described how the temperature effects can be described within a field theoretical approach, and how that is a powerful tool in describing the many experimentally observed temperature driven spin reorientations.

Ruqiuan Wu, Los Angeles, presented how to calculate the magnetic anisotropies and magnetostrictions from first principles. He discussed different approaches to obtain the often minute energies: total energy calculations, force theorem approaches, state tracking methods, perturbational methods, as well as the recently developed torque method. At the end he presented results on the magnetostriction in the giant magnetostrictive rare earth based Laves phase compounds.

How to calculate magneto-optical spectra and hyperfine fields was discussed in the lecture by Hubert Ebert, München. Especially, the relativistic effects were discussed, which in the hyperfine fields manifest itself in the often neglected orbital contribution.

Finally, Börje Johansson and Lars Nordström, both Uppsala, shared the last lecture in order to present the background and theoretical approaches on the Invar effect respectively non-collinear magnetic ordering.

All these topics stimulated lively discussions both during the lectures as well as, most importantly, during the breaks. Even the parts of the lectures which were devoted to the "basic" introduction often led to surprisingly vivid discussions.

In addition to these invited tutorial lectures, there were nine contributed talks. Roland Mathieu, Uppsala, presented some experimental work on the exhange coupling and anisotropy of Fe/V films, while Arvid Broddefalk of the same group, presented measurements of the magnetic anisotropy in Fe/Co films. Bereshad Nonas, Jülich, presented calculations of spin and orbital moments of magnetic adatoms on a Fe substrate, while Philip Kurz, Jülich, showed his results on the non-collinear antiferromagnetic ordering of Cr and Mn layers. Geoffrey Short, York, presented some results regarding dicroism experiments he has performed. Peter James, Uppsala, presented his results regarding the calculations of the anisotropy of tetragonally strained films. Markus Eisenbach, Bristol, showed results from his model calculations of the magnetic coupling of mesoscopic magnets, while Jürgen Schwitalla, Bristol, discussed how one can calculate the width of Bloch walls. Andres Ayuela, Helsinki, presented calculations on the exchange coupling of Fe layers through Si.

In total the workshop was attended by 49 participants, of which twelve had a mainly experimental background. We were happy to see so many young researchers, which had been our main target for the workshop. Except for Ruqiuan Wu, Northridge University, California, all attendees came from within Europe, and in total eight countries were represented.

Since the sun was generous the discussions, although in daylight, tended to continue long into the night. Also the weather made it possible to enjoy the close to midnight sun. We hope the particants brought home a wider understanding of magnetism, especially of its relativistic effects as manifested in its anisotropy, as well as a good memory of the days they spent together with us north of the polar circle in the middle of the land of the lapps.

At least we will remember those days and we would like to thank all the participants, the sponsors, and especially the lecturers which had spent ample of time to prepare their talks,

The organizers from Uppsala:

Lars Nordström
Olle Eriksson
Jürgen Henk

Programme of the Workshop follows.

5 May

14.45-15.45	Registration
15.45-16.00	L. Nordström, General information and welcoming
16.00-18.00	B. Hjörvarson, Real and fictive samples. Magnetism, structure and morphology of thin films, multilayers and superlattices.
18.00-19.15	*Dinner*
19.15-21.15	P. Mohn, Theory of magnetism.

6 May

08.15-10.00	H. Eschrig, Relativistic density functional theory. Fundamentals and aspects of intra-atomic spin correlations.
10.15-12.00	Short contributions. (P. James, P. Kurz, B. Nonas, J. Schwitalla, G. Short, R. Mathieu)
12.00-18.00	*Lunch and Break for Discussions*
18.00-19.15	*Dinner*
19.15-21.00	P. Jensen, Theory for the temperature driven reorientation of the thin film magnetisation.

7 May

08.15-10.00	R. Wu, Spin-orbit coupling induced magnetic phenomena in magnetic thin films: density functional determinations.
10.15-12.00	H. Ebert, Influence of the spin-orbit coupling on the properties of magnetic multilayers and surfaces. / Magnetic hyperfine interactions.
12.00-18.00	*Lunch and Break for Discussions*
18.00-19.15	*Dinner*
19.15-21.00	K. Baberschke, Measured anisotropy in magnetic energy and in magnetic moments. / T_C and susceptibility of coupled trilayers.

8 May

08.15-10.00	S. Blügel, Properties of magnetic surfaces and overlayers.
10.15-12.00	M. Brooks, Orbital magnetism and itineracy.
12.00-18.00	*Lunch and Break for Discussions*
17.00-18.00	Short contributions. (A. Ayuela, A. Broddefalk, M. Eisenbach)
18.00-19.00	*Dinner*
19.15-21.00	C.M. Schneider, Interrelations between structure, morphology, and magnetism in ultrathin films. / Photoelectron spectroscopy of magnetic systems.

9 May

08.15-9.00	B. Johansson, Theory of Invar effect.
9.15-10.00	L. Nordström, Non-collinear magnetism.
10.00-	Summary, conclusion and departures.

3.2 Job Announcements

POST-DOCTORAL POSITION

Philips Research Laboratories Eindhoven, The Netherlands

Interface Magnetism: Giant Magnetoresistance

Candidates are invited to apply for a post-doctoral position* to work on the theory of Giant Magnetoresistance (GMR) with the Dutch partners of the Network *Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers* sponsored by the European Union's Training and Mobility of Researchers programme.

The aim of the theoretical work is to bridge the gap between realistic ab-initio descriptions of the electronic structure in layered magnetic materials (P.J. Kelly: University of Twente and Philips Research Laboratories Eindhoven) and phenomenological transport models of GMR (G.E.W. Bauer: Delft University of Technology) . Candidates should have considerable experience of first-principles electronic structure calculations. Knowledge of tranport theory would be very welcome but is not a prerequisite.. The post-doc. will have the opportunity to participate in a number of collaborations with experimentalists in Eindhoven, Delft and Twente as well as with other non-Dutch nodes of the Interface Magnetism network. The research position is expected to be based in Enschede (Twente) and the post-doc will maintain intensive contact with Delft and Eindhoven.

Applications should be sent to
Prof. P.J. Kelly,
Faculty of Applied Physics,
University of Twente,
P.O. Box 217,
7500 AE Enschede,
The Netherlands

Additional information may be obtained from:

p.j.kelly@tn.utwente.nl, Tel.: +31-53-4893166, Fax: +31-53-4892910 or
bauer@duttnto.tn.tudelft.nl, Tel.: +31-15-2784719, Fax: +31-40-2781203

* Only nationals of Member States or Associated States of the EU (but not the Netherlands) are eligible for the position allocated to the Dutch node.

4 News from the TMR2 Network

'Electronic Structure calculations of materials properties and processes for industry and basic science'

4.1 Report on the Workshop on "Catalysis from First Principles"

M. Mavrikakis and J.K. Nørskov

The workshop on "Catalysis from First Principles" gathered a pool of about 50 physicists, chemists, and chemical engineers both from industry and academia in the Magleås Conference Center, Høsterkøb, Denmark for 3 days last May. A brief report drawn from the 28 presentations and the subsequent discussions follows. The overall impression from the workshop is that DFT calculations are now an equal with experiments in understanding chemical phenomena at surfaces and the calculations are entering a new role as a source for input into research and development in heterogeneous catalysis.

To set the stage, B. Clausen (Haldor Topsøe) started by giving the details of the development of a new Ni-Au alloy catalyst promising significant improvements for the steam reforming process. A combination of DFT calculations with several experimental characterization (EXAFS, TEM, STM) and synthesis techniques was instrumental in developing this new catalyst. M. Neurock (University of Virginia) closed the Alloy Catalysis session by presenting his group's work on analyzing the elementary reaction steps for the hydrogenation of Maleic Anhydride on Pd-Re catalysts based on DFT and MC simulations.

D. King (Cambridge University) presented the latest results of his group's work on understanding methane partial oxidation to syngas over Pt surfaces using supersonic beam studies. Main emphasis was placed on the dissociation mechanism and reaction products for methane on Pt single crystals, which could serve as a nice benchmark for ab-initio calculations. The main products of the dissociation process depend on several factors, but in most cases CH and C are formed on the Pt surface. A. Alavi (The Queen's University of Belfast) and A. Eichler (Technical University of Vienna) presented results from calculations for the CO oxidation reaction on Pt(111). Moreover, the latter discussed the dissociation path of O2 on Pt(111), whereas the former addressed the reactivity of subsurface hydrogen on Ni (111). Along the same lines, A. Bottcher (Humboldt University, Berlin) presented experimental results for the role of subsurface oxygen on the reactivity of Ru surfaces for CO oxidation.

F. Besenbacher (University of Aarhus) presented the latest results of his STM group on several studies directly linking to major catalytic processes: (1) hydrogen adsorbed on top of Pt adatoms was shown to substantially increase the adatom diffussivity on Pt surfaces, a problem of fundamental importance for explaining sintering in catalysis, and (2) the first atomically resolved STM images of MoS2 nano-crystals on Au surfaces were presented, which can provide a benchmark for electronic structure calculations on HDS catalysts. A. Chaka (Lubrizol) demonstrated how state-of-the-art quantum chemistry and electronic structure methods are used in the understanding and design of new lubricants with improved antiwear resistance.

The second day of the workshop started with a session focussing on recent experimental and theoretical advances in hydrotreating catalysts, with particular emphasis on hydrodesulfurization (HDS) catalysis, as presented by H. Topsøe (Haldor Topsøe) and followed by a DFT study of thiophene HDS on the MoS2 edge (P. Raybaud, IFP). Later on in the morning, C. Campbell (University of Washington) gave an update on micro-calorimetry data for an array of metals deposited on several single crystal metal oxide surfaces and discussed consequences for supported catalysts. T. Kluener (FHI-Berlin) presented wave packet calculations for the interpretation of experimental data on the photo-induced desorption of NO from NiO(100). D. Bird (University of Bath) closed the morning session with a discussion of H2 dissociation on Cu(111) and an understanding of the results using simplified total energy functionals.

The first afternoon session of the second day was focussed on oxide catalysts and included 3 talks: (1) E. Derouane University of Liverpool) presented open problems and challenges in liquid phase zeolite-catalyzed chemicals synthesis, (2) R. van Santen (Eindhoven University of Technology) discussed several examples where theory and experiment play a complimentary role in understanding zeolite-catalysis, and (3) K. Hermann (FHI-Berlin) presented his group's latest results for the formation of OH and H2O on V2O5 surfaces, based on DFT cluster studies.

The second day of the workshop was closed with a session opened with H-J. Freund (FHI-Berlin) presenting results on the effect of particle size on transition metal reactivity. M. Mavrikakis (Technical University of Denmark), who spoke immediately afterwards, described results of DFT calculations substantiating the importance of strain and steps in understanding the catalytic activity of transition metals. B. Hammer (Aalborg University) and I. Chorkendorff (Technical University of Denmark) subsequently discussed the effect of steps on the reactivity of Ru single crystal surfaces, the former with DFT studies for the NO dissociation, and the latter with molecular beam and thermal experiments probing the sticking probability of N2. A. Gross (technical University of Munich) closed the day with results of ab-initio based tight-binding calculations of the dynamics of H2 dissociation on Pd(100).

A thought provoking mixture of theory and experiment was presented on the last day of the workshop; J. Dumesic (University of Wisconsin) discussed the effect of Sn on the reactivity of Pt catalysts as illustrated by a combination of micro-calorimetric experiments and electronic structure calculations. M. Barteau (University of Delaware) described his group's investigations of oxametallacycle chemistry of Ag surfaces, emphasizing the importance of theory for the correct identification of elusive reaction intermediates. B. Lundqvist (Chalmers University of Technology) gave a delightful overview of the development of theoretical methods necessary for treating adsorption and reactions on metal surfaces. C. Stampfl (FHI-Berlin) reported on her latest work towards a First-Principles theory for surface thermodynamics. G. Kresse (Technical University of Vienna) and O. H. Nielsen (Technical University of Denmark) closed the workshop by giving accounts on the current state-of-the-art of the computational methods used and their projections for upcoming developments.

Overall, the workshop was successful in identifying meeting points between theory and experiment and suggesting directions that theory can take in order to meet the expectations and needs of the experimental community. The importance of theory for addressing open questions related to the catalytic activity of metals was clearly illustrated, and at the same time the dawn of a new era for catalysis, based on the ab-initio design of new catalysts, was shown as the new reality.

4.2 Report on Hands-on Workshop on FHI98md Computer Code

Workshop on

Calculation of Material Properties using Total Energy and Force Methods and *ab initio* Molecular Dynamics

(Trieste, 9 - 18 August 1999)

This 10-days course was directed by Peter Kratzer from the Fritz-Haber-Institut (FHI) in Berlin. Co-directors were Jorge Kohanoff (ICTP, Trieste), Jörg Neugebauer (FHI), and Matthias Scheffler (FHI). The workshop was concerned with detailed presentations on basic aspects of density-functional theory (DFT), pseudopotentisl concepts, *ab initio* molecular dynamics (md), time-dependent DFT, and many-body schemes. In addition to the talks, there were practical, hands-on sessions, in which the use of the FHI98md computer code (DFT-md calculations with pseudopotentials and a plane wave basis set) and the construction of pseudopotentials was taught.

Because of the limited number of available terminals, the number of participants had to be limited to 80 people. However, 235 people had applied. We tried our best to create an as-fair-as-possible selection, but obviously could not do justice to all applicants. Thus, here come a big **"SORRY"** to those we had to reject.

Participants and tutors have written reports with their viewpoints concerning the activity (see below). The "participants' viewpoint" was written by Sigrid Kuempel (a German Ph.D. student in Hawaii/USA), Claudia Ramirez (a Mexican Ph.D. student in Kiel/Germany), and Maria Alfredsson (a postdoc from Sweden working in London/GB).

And the "tutors' viewpoint" was written by Sixten Boeck (diploma student in Berlin) and Tosja Zywietz (Ph.D. student in Berlin).

The program, and with a click also abstracts and transparencies of some talks, can be found at

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

The participants' viewpoint

For us this workshop was a big success. There is the basic fact that we learned a lot about Density Functional Theory (DFT) in general and the FHI98md program in particular. Then we had the opportunity to meet people from other groups working on similar or different ideas. Suddenly we could exchange viewpoints and learn about methods, while our own group would not be creating so many different perspectives. Also, having the chance to talk to the authors of the code and to share in their experience with the program package was very important and helpful.

The days started with talks ranging from general introductions to the DFT to more specific subjects at the end of the workshop, which gave a flavour of how to extend the basic ideas of DFT or “new” properties to calculate. Unfortunately, the theories, in the more specialized seminars, were sometimes too sparsely explained to be understood, unless you were already familiar with the subject. However, in this way everybody attending the course should be satisfied, from new Ph.D. students to more experienced speakers.

The afternoon practical sessions (as the whole workshop) were very well organized, starting with a short/general theoretical introduction to ’the problem of the day’. With so big a group of people, some very familiar with the FHImd code and others who had never used it before, it is obviously difficult to find a common denominator. There was the question, if there should have been a more basic introduction into the specifics of the program on the first day, to make the input files less mystic. But the tutors were very helpful, whenever we ran into problems, and the scripts to run the programs were well prepared. Most probably there will be questions coming up, once we now get home and try to use the program on our own, changing all the parameters to adopt them to our system. But since we have met so many people here, it will be easy to get in touch with them via email and resolve the problem.

So, what were the important facts we learned?
We think, first of all, we learned a lot about the physical principles on which the program is based, so that we will not just use the program as a black box that somehow produces data (which could after all be dangerous, as we might produce nonsense output without knowing it). The speakers (and the practical sessions) succeeded in conveying how important it is to choose and test for the right parameters. We should not be happy, if our program claims to be converged, but we actually have to test, if it converges to a meaningful value. In addition it was helpful to see, that optimizing the parameters, even if it first takes a little while, will save us lots of CPU time in the long run, so we should not be too lazy and skip it. We obviously also profited from the well prepared practical sessions, where we could see how useful shell-scripts (or small programs) can be in analyzing the huge amount of data these kind of programs produce. In addition, we got a lot of new ideas for our own work: We learned how to calculate quantities that we maybe had ignored up to now, but that are very interesting and important to describe the systems we are working with.

So, were there things that could have been improved? Well, naturally, the next time we want to see the total eclipse of the sun, not just 95% (even though the organizers were very well prepared and helped us to create filters to save our eyes; *THANK YOU*).

The tutors’ viewpoint

While the morning sessions were dedicated to the theoretical aspects of density functional theory, plane wave pseudopotential calculations and also some applications, the afternoon sessions were designed to provide practical knowledge about the FHI98md program. The practical sessions were divided into an introductory talk about the specific application of the program followed by computer exercises. The applications ranged from simple physical aspects as e.g. calculations of bulk properties to more advanced topics like surface structures, band structures and molecular dynamics simulations.

The computer exercises were designed such that even beginners were able to deal with the tasks. However, at the beginning of the workshop the knowledge of the participants was very inhomogeneous with some “real” experts and some people who had never used UNIX before. Nevertheless, we had the impression that all participants were getting along with the exercises quite well and after a few days the group became more and more homogeneous. The participants were mainly working in two-member groups and could solve the problems mostly independent without the help of a tutor.

While at the beginning the questions we had to answer were mainly related to technical details of the program, more and more physical questions showing a deeper understanding were asked towards the end of the first week. Getting all this questions was very helpful for us, too. The questions pointed towards technical aspects which were somehow unclear in the manuals and helped to recognize problems of handling the program.

Of course, the preparation for the workshop was quite a bit of work, but we learned a lot by ourselves and enjoyed talking to people from all over the world. Besides the official part of the workshop there was time enough to meet with the participants, and to learn about their personal background. Some interesting contacts may have emerged out of the official as well as the recreational part of the workshop.

5 News from the ESF Programme

”Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces”

5.1 Reports on Workshops

5.1.1 Report on E-MRS Spring Meeting

Symposium 3 – 1999 E-MRS Spring Meeting:

June 1-4, 1999

”Progress in Computational Materials Science”.

With 102 presentations, consisting of 50 talks and 52 posters, this symposium ran for the full 3 1/2 days allowed for the technical sessions. The talks were well attended and often led to lively debate. The material was distributed over 9 sessions: electronic structure (first principles), electronic structure (empirical methods and beyond), defects, mechanical properties, semiconductors, magnetism (electronic structure), micromagnetism, growth, and novel techniques. While the various subfields of computational materials science have often developed their own peculiar techniques, at this symposium one could clearly witness a closer integration of the diverse methodologies and some real progress towards hybrid methods. Many speakers also outlined areas of current and future progress, enhancing the pedagogical value of the meeting.

To study simultaneously electronic structure and dynamics, the Car-Parrinello technique has become a real “workhorse” and it is the method of choice for systems of up to a few hundred atoms observed over time periods on the order of 10 ps. For larger systems or longer times, tight-binding molecular dynamics has established itself as the preferred approach. Several authors reported applications of these methods to novel fields such as biomolecules and pharmacological systems, besides the more traditional materials (metals, semiconductors, etc.). Classical electronic band structure methods continue to be very useful tools yielding a great deal of information, from binding energies and activation barriers to excited states.

Classical particle-based simulations, using the Monte Carlo (MC) or molecular dynamics (MD) approaches, increasingly rely on energetic information obtained from first-principles calculations, rather than resorting to a phenomenological description. With continuing advances in computer power, MC and MD now permit the study of mesoscopic systems and in some cases approach the scale of macroscopic objects. The largest system reported at the symposium had over 5,000,000 atoms, with time-scales in MD simulations approaching milliseconds (on the order of tens of millions of time-steps). Spectacular though these numbers may be, only continuum methods permit studies of truly macroscopically large systems, over long time scales (in some cases ranging on the order of centuries). Impressive work along those lines was reported on electromigration, metallic foams, and micromagnetism, to name just a few. Here too, major progress has been made in the last few years.

Clearly the main challenge in the years ahead will be the integration of the various methods to span time and length scales. Some work in this direction was presented at the meeting and showed very encouraging signs that major breakthroughs can be expected in this direction in the next few years. There was also strong evidence of the continuing efforts to use the tools of computational materials science to study "real" materials: systems with imperfections or highly complex unit cells, in high-energy collisions, or interacting with solvents.

Many of the talks were attended by participants whose main interests were in other, more applied, symposia, indicating that computational materials science is being perceived as having something relevant to contribute to industrial processes and design. This trend can only grow stronger in the future as methodologies continue to become more refined and computer capacities (both in terms of speed and storage) continue to increase. It seems a plausible conclusion that on the eve of the twenty-first century, computational materials science is thriving and is here to stay.

List of invited speakers

W. Andreoni (Ruschlikon), M. Ben-Amar (Paris), X. Blase (Lyon), R. W. Chantrell (Bangor), L. Colombo (Milan), B. Delley (Villigen), M. W. Finnis (Belfast), T. Frauenheim (Paderborn), K. W. Jacobsen (Lyngby), E. A. Kotomin (Riga), C. Massobrio (Strasbourg), M. J. Puska (Helsinki), F. Rammerstorfer (Vienna) and P. Weinberger (Vienna)

Publication

A special issue of Computational Material Science, edited by Elsevier, will be published with a selection of the accepted papers. The volume should have around 350 pages.

Programme

The programme can be found, for a certain time, on the WEB:

http://www-emrs.c-strasbourg.fr/PSympC.htm

Acknowledgements

Financial assistance for the symposium was provided by the European Science Fundation through the program Ψ_k, the TMR networks, TMR1 "Interface Magnetism" and TMR2, Starlab, CCP3, Université Louis Pasteur from Strasbourg and Institut de Physique et Chimie de Strasbourg. The support from these organizations et particularly from the Ψ_k was essential and is gratefully acknowledged.

Hugues Dreyssé and Luc T. Wille

The organizers of the symposium

5.1.2 Report on Workshop in Villasimius

IX Workshop on Computational Materials Science

held 10 to 13 September 1999 in Villasimius (Cagliari), Sardinia, Italy

The ninth edition of the Workshop on Computational Materials Science [formerly known as Computational Condensed Matter (1990-1994) Italian-Swiss (1990-1997) Workshop] was held on the south-eastern coast of Sardinia, Italy from 10 to 13 September. The main sponsors were Regione Autonoma Sardegna (the regional government of Sardinia) and the Ψ_k European Science Foundation Program; UNESCO bestowed its prestigious patronage. Nearly 70 participants gathered at the Workshop, in the pleasant framework of the Tanka Village sea resort, in an informal atmosphere also favored by excellent weather. As customary in this workshop, social and scientific programs blended together nicely (a two-evening poster session was the highlight) favoring intense discussion and contacts.

The traditional focus of this workshop is ab initio electronic structure, mostly within density-functional theory. Tight binding and ab initio molecular dynamics, as well as less-common topics such as polarization theory have been well represented in past editions. While keeping with the tradition of past meetings, this workshop has devoted some attention to semiempirical and model approaches, to statistical mechanics, and experiment. This implies (given the sum rule on the workshop length) that the cross section of each single topic is somewhat smaller than usual, but this program formula had the definite merit of opening up new perspectives and contacts in the form of new or unfamiliar viewpoints, besides the obviously necessary confrontation with inputs from experiment. A somewhat arbitrary classification of the 18 one-hour invited talks shows that there were 10 ab initio ones, 4 on statistical mechanics-related topics, 3 on semiempirical, classical, and analytical methods, and 1 experimental.

A part of the ab initio studies focused on DFT basics, such as DFT beyond the adiabatic approximation and current density-functional theory (Gross), and polarization-localization theory (Resta). Beyond-DFT methods and applications were discussed for spectral properties by Godby, and for quantum dynamics by Baroni and Kohanoff; the latter also discussed applications to hydrogen phase transitions. Molteni presented DFT calculations on biological molecules. Semiempirical methods were called into play by Smit in his talks on large scale simulations of phase equilibria and diffusion of hydrocarbons in zeolites; Molinari discussed instead methodologies and numerous results on semiconductor quantum nanostructures, serving also as introduction to the exciting experimental talk by Cingolani on quantum wires and dots, and conduction in DNA-made contacts. The statistical mechanics part was shared between disordered systems (Marinari), path searches in protein folding (Seno), epitaxial growth (Wolf), and a refreshing overview on granular matter (Wolf).

The over 25 posters presented in two lively evening sessions focused mostly on ab initio (with some semiempirical tight binding blend) simulations. Among the topics touched upon, let us mention Wannier functions studies of localization in amorphous systems, ab initio MD on laser-induced fullerene transformations, metal and semiconductor surface dynamics and roughening, lattice dynamics of semiconductors, polarization effects in nitride quantum structures, electronic structure of nanowires, etc.

The abstract of the lectures, and the list of posters follows below.

INVITED TALKS

Reptation Quantum Monte Carlo: a new method for simulating interacting bosons and fermions

Stefano Baroni

INFM and SISSA, Trieste, Italy

Abstract not available

Physics and technology of nanostructures: recent trends and perspectives

Roberto Cingolani

INFM – Dipartimento di Fisica, Università di Lecce, Italy

I will review the present status of the physics and technology of nanostructures: the most recent trends in the study and application of semiconductor quantum dots and the novel ideas for hybrid mesoscopic systems. In particular I will discuss the few electron transitions in single quantum dots and the issues connected to electron-electron and electron-hole correlation. Quantum dots lasers and devices will also briefly commented. In the second part of the lecture I will present a few new ideas about the possibility of integrating organic matter and nanotechnology systems, namely DNA-based electronic devices, basic molecular computation and hybrid organic/inorganic structures.

Electronic exchange and correlation in excited states, and the space-time GW method

Rex W. Godby

Department of Physics, University of York, York YO10 5DD, U.K

I shall review the contrasting and complementary roles of density-functional theory (DFT) and *ab initio* many-body perturbation theory (MBPT) in condensed-matter physics.

Our *ab initio* MBPT work is based on Hedin's GW approximation, and uses our recent "space-time" method, in which the Green's function G and the screened Coulomb interaction W are represented in the real-space and imaginary-time domain, increasing the efficiency of the calculation of W and the self-energy Σ, and its scaling with system size. The availability of the full self-energy $\Sigma\left(\mathbf{r},\mathbf{r}',\omega\right)$ gives access to such quantities as the electron density and total energy, in addition to quasiparticle energies and the spectral function.

I shall also present the results of studies using Hubbard model systems [2] (for which exact results may be calculated), which address the accuracy of the GW approximation, and candidate extensions beyond GW for more strongly correlated electrons, for the spectral function, total energy, etc.

GW calculations for surface excitations, charge densities, and wide-gap semiconductors

Rex W. Godby

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I shall present applications of the space-time method for *ab initio* GW calculations that was described in my earlier talk.

First, we have studied an Al(111) surface. The GW self-energy automatically includes the image potential not present in any local-density approximation for exchange and correlation. We solve the energy-dependent quasiparticle equations to obtain surface state wavefunctions, and calculate the effective local potential experienced by electrons in the near-surface region.

The electronic charge density of Si and Ge has been calculated using GW. The implications of the results for GW total energy calculations will be explored.

Results will also be presented for GaN, a wide-gap semiconductor.

Density Functional Theory Beyond the Born-Oppenheimer Approximation

E. K. U. Gross, **Nikitas Gidopoulos**, and **Martin Lüders**

Intitut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We develop a density-functional formalism to treat the complete system of electrons and nuclei in a molecule or solid. To this end, the adiabatic or Born-Oppenheimer decomposition of the total wavefunction is reexamined. We prove, that if one does not a priori choose the electronic wavefunction to be an eigenfunction of the electronic Born-Oppenheimer Hamiltonian, but instead determines it by free variation under the constraint of being normalized to one for each nuclear configuration, then the resulting scheme becomes *exact*. In other words, any exact eigenstate of the electron-nuclear Hamiltonian can be written as such an "adiabatic" product. The variational principle leads to an equation for the nuclear wavefunction which coincides with the corresponding equation in the Born-Oppenheimer approximation. The electronic equation, however, contains new terms which couple the electronic and the nuclear wavefunctions and account for the electron-nuclear correlation beyond the Born-Oppenheimer level. On the basis of these equations we then develop a density functional formalism. As a first application, we show how to deal with strong electron-phonon coupling in the density functional theory for superconductors [1,2]. Numerical calculations of the critical temperature of some materials will be presented.

1. L.N. Oliveira, E.K.U. Gross, and W. Kohn, Phys. Rev. Lett. **60**, 2430 (1988).
2. S. Kurth, M. Marques, M. Lüders, and E.K.U. Gross, Phys. Rev. Lett. **83** (1999), in press

Current-density functional theory: New functionals and the calculation of orbital magnetic moments in bulk ferromagnets

E. K. U. Gross

Intitut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Abstract not available

High pressure phases of hydrogen: the role of electrostatic interactions and quantum nuclear effects

Jorge Kohanoff

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In spite of being the simplest element in the periodic table, hydrogen exhibits a rich phase diagram with an interesting collection of phase transitions of varied nature. In this presentation I will describe this phase diagram as has emerged during the years, from optical spectroscopy studies in diamond anvil cells and shock wave thermodynamic measurements, to state-of-the-art electronic structure calculations, ab initio molecular dynamics simulations, and quantum Monte Carlo results.

Beginning at room pressure, I will give an overview of the phenomenology of the solid phases at low temperatures. Three molecular phases of quite different nature have been observed experimentally: a low-pressure phase where the H_2 molecules rotate freely due to the quantization of these rotations, a second phase at higher pressures where the rotations are hindered and turned into large amplitude librations, and a puzzling third phase characterized by a strong infrared vibronic activity. Since diffraction studies are not yet possible at these pressures, ab initio calculations constitute a crucial tool for understanding the structural properties of these phases. In this perspective, I will present the results of ab initio calculations for these phases, and also phonon spectra and IR activities obtained from density functional perturbation theory calculations. Then, I will discuss the role played by electrostatic interactions and quantum nuclear delocalization effects in stabilizing the different phases, and how these aspects are connected with experimental data like vibrational frequencies and infrared absorption. Still within the context of low-temperature phases, I will continue by addressing the issue of the the long-sought metal-insulator transition and the dissociation transition under pressure, to end by describing the sequence of structural transitions in atomic phase, including a brief discussion about the relevance of the quantum character of the protons.

In the final part of the presentation I will concentrate on the high temperature region of the phase diagram, by describing the plasma (atomic, fluid and metallic) in some detail, and decreasing pressure until the region of molecular formation is reached. I will discuss the issue of molecular dissociation and metallization at high temperatures and, in this context, address the issue of the controversial plasma phase transition.

Introducing the quantum character of light nuclei in electronic structure calculations

Jorge Kohanoff

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In traditional electronic structure calculations, the atomic nuclei (or ions) are treated as classical particles. While this is certainly a good approximation for most of the elements in the periodic table, its validity becomes questionable for the lighter elements like hydrogen, helium, and first row elements. Depending on the context, the proper treatment of these nuclei as quantum particles can be a crucial ingredient to describe correctly the physics. In the past, quantum nuclear dynamics was studied using simplified models. More recently, A. Gross et al. proposed a strategy that consists of fitting a high-dimensional potential energy surface (PES) to first-principles calculations, and then performing the quantum dynamical simulations in that PES [1]. While this is certainly an appealing methodology, the number of dimensions is limited to a small number (six at most). To overcome it, the PES has to be computed *on-the-flight*. In this presentation I will discuss two different approaches which have been recently developed, and basically merge the well-established first-principles electronic structure technology with a quantum description of the atomic nuclei.

The first method is based on a path integral description of the nuclear variables, while the electronic degrees of freedom are treated within the adiabatic approximation. Monte Carlo [2] and Molecular Dynamics [3] sampling techniques for the path integral will be discussed, and applications to molecular systems and condensed phases will be presented. Difficulties in sampling rapidly oscillating, real-time propagators (the phase problem) are so severe that the only feasible possibility is to deal with a purely imaginary-time propagator (which is positive definite). As a consequence, the *ab initio* path integral formalism is well-suited for computing finite-temperature, *static* quantum-statistical properties, e.g. particle distributions, free energies, etc. A direct measure of quantum dynamical properties is not possible, although an indirect insight can be obtained by studying imaginary-time correlations.

The second method is currently under development [4], and is based on an energy functional that depends on nuclear and electronic densities. For ground state properties, these two densities are optimized simultaneously, in a self-consistent way. The two-density functional includes three types of correlations: (a) electronic, which are treated within the standard density functional approach (LDA or GGA), (b) nuclear, where the main ingredient is the self-interaction correction, and (c) electron-nuclear, which is the most delicate one and has to be appropriately approximated. In order to do this, we have developed a number of approximate electron-nuclear correlation functionals that are computationally amenable. Firstly, we propose a mean-field approach consisting of neglecting e-n correlations altogether. The computational cost is of the same order of a traditional electronic structure calculation, the main difference being that the e-n interaction is calculated for a spread nuclear distribution instead of point charges. Results for ground state properties are remarkably good within this approximation. Then, we introduce an approximate electron-nuclear correlation which is implemented onto the mean-field approach, and systematically improves the results. Finally, we introduce a first order approximation in which the potential acting on the nuclei is calculated by solving the electronic problem on a grid of real-space points. This is computationally more demanding than the mean-field, although its cost should be comparable to the path integral approach. Up to now we have concentrated on static properties but, in contrast to the path integral formalism, this two-density functional methodology admits a generalization to dynamical processes.

[1] A. Gross, S. Wilke, and M. Scheffler, Phys. Rev. Lett. **75**, 2718 (1995).

[2] R. O. Weht, J. Kohanoff, D. A. Estrin, and C. Chakravarty, J. Chem. Phys. 108, 8848 (1998).

[3] D. Marx and M. Parrinello, Z. Phys. B **95**, 143 (1994); J. Chem. Phys. **104**, 4077 (1996).

[4] N. Gidopoulos and J. Kohanoff (in preparation).

Disordered and complex systems: from the mean field paradigm to the realistic models

Vincenzo Marinari

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Do finite dimensional spin glasses share the unusual and interesting behavior of the Parisi Solution of the Mean Field Theory? We will report about a large amount of mainly numerical work trying to clarify this issue. Optimized Monte Carlo methods will be the basis of our work, and we will discuss among other about equilibrium and out-of-equilibrium issues, and about the existence of a transition in finite magnetic field. Our tentative answer to the question will be yes.

Optical and addition spectra of quantum wires and dots: the effects of Coulomb interactions

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Abstract not available

Modelling photoreactions in proteins by density functional theory

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Photoactive proteins are an important class of biomolecules that offer potential technological applications. In the first hundreds of femtoseconds of their photocycle, the absorption of a photon produces conformational changes that trigger a cascade of chemical reactions culminating in a specific biological signal. Given the short time of the initial photoreaction, which usually implies a double bond isomerisation, it is experimentally difficult to see how this isomerisation proceeds and how it is converted in a protein-wide structural change; therefore simulations could be extremely helpful for accurately characterizing the structural and electronic changes initially induced by light.

I will present some attempts to investigate photochemical reactions by density functional theory based methods. Excited states are treated within a recently developed density functional theory scheme which allows us to perform geometry optimisation and molecular dynamics in the first excited singlet state. The effects of the protein environment can be included by combining the quantum mechanical treatment of the chromophore with the classical treatment of the environment. Results on the photoisomerisation of rhodopsin will be shown.

This work has been done in collaboration with I. Frank (Institut für Physikalische Chemie, University of Munich) and M. Parrinello (Max-Planck-Institut für Festkörperforschung, Stuttgart).

The many-body phase operator: macroscopic polarization and electron localization in extended systems.

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The dipole moment of any finite and neutral system, having a square-integrable wavefunction, is a well defined quantity. The same quantity is ill–defined for an extended system, whose wavefunction invariably obeys periodic (Born-von Kármán) boundary conditions. Despite this fact, macroscopic polarization is a theoretically accessible quantity, for either uncorrelated or correlated many–electron systems: in both cases, polarization is a rather “exotic” observable. For an uncorrelated—either Hartree–Fock or Kohn–Sham—crystalline solid, polarization has been expressed and computed as a Berry phase of the Bloch orbitals (since 1993) [1-3]. The case of a correlated and/or disordered system received a definitive solution only very recently [4]: this latest development allows us to present here the theory from a novel and very general viewpoint, where a key role is played by the “many–body phase operator”, whose main properties will be discussed. This same operator provides the relevant information about the *localization* of the electronic wavefunction [5].

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2. R. Resta, Il Nuovo Saggiatore **9**(5/6), 79 (1993); Europhysics News **28**, 18 (1997).
3. R. Resta, *Berry Phase in Electronic Wavefunctions*, Lecture Notes for the “Troisième Cycle de la Physique en Suisse Romande” (Lausanne, 1996). Available online (194K) at the URL: http:///www-dft.ts.infn.it/˜resta/publ/notes_trois.ps.g

4 R. Resta, Phys. Rev. Lett. **80**, 1800 (1998).

5 R. Resta and S. Sorella, Phys. Rev. Lett. **82**, 370 (1999).

Localized orbitals in molecules and in extended systems: Theory and computations.

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The insulating state of matter is characterized by the excitation spectrum, but also by qualitative features of the electronic ground state. The insulating ground wavefunction in fact: (i) displays vanishing DC conductivity; (ii) sustains macroscopic polarization; and (iii) is *localized.* The idea that the insulating state of matter is associated to electron localization was first proposed by W. Kohn in a landmark paper [1]. We have given [2] a sharp definition of the concept of electron localization, rather different from Kohn's, and deeply rooted in the modern theory of polarization. In fact we link the two features (ii) and (iii) above, by means of essentially the same formalism, based on the many–body phase operator introduceded in the previous lecture.

In the special case of an uncorrelated (either Hartree–Fock or Kohn–Sham) crystalline solid, the localization of the many–body wavefunction is measured—according to our definition—by the spread of the Wannier orbitals, previously discussed by Marzari and Vanderbilt [3]. I will also show that for uncorrelated molecules the present theory of localization recovers the basic features of Boys' localization in quantum chemistry [4]. Finally, I will present some preliminary results about localized orbitals in semiconductors [5].

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3 N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997).

4 S.F. Boys, Rev. Mod. Phys. **32**, 296 (1960); J.M. Foster and S.F. Boys, *ibid.* 300.

5 C. Sgiarovello, M. Peressi, and R. Resta, in preparation.

An optimal procedure to extract interaction potentials for Protein Folding

C. Micheletti,(1) **F. Seno**,(2) **J.R. Banavar**,(3) and **A. Maritan**,(1)

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(3) *Department of Physics and Center for Material Physics, the Pennsylvania State University, University Park, USA*

A formidable challenge in molecular biology is the prediction of the three-dimensional structures of the native state of proteins from the sequences of their amino acids [1]. An essential ingredient to solve this problem is the task of deducing the coarse-grained interaction potentials between the amino acids [2]. Here we outline a strategy to accomplish such goal based on the search of those potentials which are able to recognize the native state of a protein as a stable local minimum. The method is implemented by exploiting several numerical and analytical tools which have been recently developed by our group [3,4,5]. The results are extremely promising: despite the fact that we have used simple forms for Hamiltonians, the exctracted potentials are able to stabilize simultaneously 10 different proteins to an average distance (per residue) less than 3 Å from the native state.

1. T.E. Creighton, *Proteins: Structures and Molecular Properties*, W.H. Freeman, New York (1992).
2. S. Miyazawa and R.L. Jernigan, Macromolecules **18**, 534 (1985).
3. F. Seno, A. Maritan, and J.R. Banavar, Proteins: Struct., Funct., Genet. **22**, 81 (1995).
4. J. van Mourik, C. Clementi, A. Maritan, F. Seno, and J.R. Banavar ,J. Chem. Physics **110**, 10123 (1998).
5. G. Settanni, C. Micheletti, J. Banava,r and A. Maritan, *Depermination of optimal effective interactions between amino acids in globular proteins*, SISSA preprint (1999).

Monte Carlo simulations of chain molecules

B. Smit
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Abstract not available

Simulating phase equilibria

B. Smit
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Abstract not available

Charged granular matter

Dietrich E. Wolf and **Tim Scheffler**
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Granular materials like dry sand are classical many particle systems which differ significantly from solids and liquids in their dynamical behaviour. They seem to have some properties in common with solids, like the ability of granular packings to sustain shear, and other ones with fluids, like the ability to flow through a hopper. Upon looking more closely, however, it turns out that such similarities are only superficial: Force localization or arching in granular packings and the plastic yield behaviour are distictly different from solids, cluster instabilities and nonlinear internal friction make granular flow very different from that of ordinary, Newtonian fluids. After a short introduction into the physics of granular materials this talk will focus on granular flow, the properties of which can be explained, if two essential physical ingredients are understood: The interaction of the granular flow with the container walls and the phenomenon of collisional cooling. The latter term means the reduction of relative motion due to collisions which irreversibly convert kinetic energy into heat. Finally some recent results will be presented, which show how collisional cooling is modified, if all particles carry the same charge.

Epitaxial growth: Theory and simulation

Dietrich E. Wolf, **Lothar Brendel**, and **Alexander C. Schindler**
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Molecular beam epitaxy is an experimentally sophisticated, though conceptually simple technique to manipulate the composition of a growing crystal film on the atomic scale. Multilayers with carefully composed materials show novel electronic and magnetic properties which make them technologically interesting. Starting with a high symmetry substrate and choosing appropriate growth conditions, one often observes layer-by-layer growth, which means that freshly deposited atoms form two dimensional islands that coalesce before a significant amount of material condenses in the next atomic layer. Layer-by-layer growth is only transient due to kinetic roughening or growth instabilities. After a general introduction this talk will address the question, how strain due to lattice mismatch between substrate and growing film affects layer-by-layer growth. As an example it will be discussed, whether compressive or tensile strain will improve layer-by-layer growth of Pt on strained Pt(100).

POSTERS

Ab Initio Calculation of the Structural and Dynamical Properties of Layered Semiconductors, Christoph Adler and Pasquale Pavone
Theoretische Physik, Universität Regensburg, Germany

Structural and electronic properties of {311} defects in silicon: a tight-binding molecular dynamics investigation, , Paola Alippi and Luciano Colombo, INFM and Department of Materials Science, University of Milan, (Italy)

Macroscopic polarization and built-in electrostatic fields in III-V nitride multi-quantum-wells, F. Bernardini,[1] V. Fiorentini,[1] A. Di Carlo,[2] F. Della Sala,[2] and P. Lugli,[2] (1) INFM e Dipartimento di Fisica, Università di Cagliari, Italy, (2) Dip. di Ingegneria Elettronica, Università degli Studi di Roma "Tor Vergata", Italy.

Investigating detergent behaviour in a solvated membrane-bound protein by MD simulation, Matteo Ceccarelli and Massimo Marchi, INFM and CECAM-ENS Lyon, France

Oxygen Adsorption on Rh(110) Surface, Gabriele Cipriani, Stefano Baroni, and Stefano de Gironcoli SISSA/ISAS and INFM, Trieste, Italy.

Atomic and electronic structure of high-energy twist grain boundaries in silicon and carbon, Fabrizio Cleri, INFM and ENEA, Divisione Materiali Avanzati, Centro Ricerche Casaccia

Efficient real-space approach to TDDFT for the dielectric response of periodic systems, F. Kootstra, P.L. de Boeij, and J.G. Snijders, Theoretical Chemistry, Materials Science Centre, University of Groningen

Valence Stability in Lanthanide Systems Anna Delin, Lars Fast, Börje Johansson, Olle Eriksson, and John Wills, Uppsala University, Uppsala, Sweden

Ab–initio molecular dynamics simulation of laser–induced transformation of fullerite, Alfredo Gambirasio,[1] Marco Bernasconi,[1] Giorgio Benedek,[1] Pier Luigi Silvestrelli,[2] and Michele Parrinello[3] (1) INFM and Dipartimento di Scienza dei Materiali, Universitá di Milano–Bicocca, (2) Dipartimento di Fisica "G. Galilei", Universitá di Padova, (3) Max–Planck–Institut für Festkörperforschung, Stuttgart, Germany

Structural models of amorphous carbon and amorphous carbon surfaces Rainer Härle and Alfonso Baldereschi, Institute of Applied Physics, EPF-Lausanne, and IRRMA, 1015 Lausanne, Switzerland

Lattice dynamics from mixed-basis density-functional perturbation theory: Application to sapphire R. Heid,[1] D. Strauch,[1] and K.-P. Bohnen,[2] (1) Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany, (2) Forschungszentrum Karlsruhe, Institut für Nukleare Festkörperphysik, Karlsruhe, Germany

Silicon diffusion in $TiSi_2$ competing phases by tight binding molecular dynamics Marcella Iannuzzi, Paolo Raiteri, and Leo Miglio, INFM and Dept. of Material Science, University of Milano-Bicocca

Ab initio study of dynamical properties and thermal expansion in some Be surfaces, Michele Lazzeri and Stefano de Gironcoli, INFM and SISSA, Trieste, Italy.

Vacancies in Ge and SiGe, J. Lento, M. Pesola, J.-L. Mozos, and R. M. Nieminen, Laboratory of Physics, Helsinki University of Technology

Ab-initio molecular dynamics with a classical pressure reservoir: simulation of pressure-induced amorphization in a Si_35H_36 cluster, R. Martoňák, C. Molteni,* and M. Parrinello, Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany, * Cavendish Laboratory - Theory of Condensed Matter, Madingley Rd, Cambridge CB3 OHE UK

Coordination defects in a-Si and a-Si:H: topological characterization and electronic properties from first principles calculations, M. Peressi,[1] M. Fornari,[1,2] S. de Gironcoli,[3] A. Baldereschi,[1,4] N. Marzari,[2] and L. De Santis[3], (1) INFM and Università di Trieste (Italy), (2) Naval Research Laboratory, Washington DC (USA), (3) INFM and SISSA (Italy), (4) IPA - Ecole Polytechnique Fédérale, Lausanne (Switzerland)

Many-body effects on one-electron energies and wave functions: a study of the GaAs(110) surface, Olivia Pulci,[1] Friedhelm Bechstedt[1], Giovanni Onida,[2] Rodolfo Del Sole,[2] and Lucia Reining,[3] (1) Institut für Festkörpertheorie und Theoretische Optik, Friedrich-Schiller-Universität, D-07743 Jena, Germany, (2) Istituto Nazionale per la Fisica della Materia, Università di Roma Tor Vergata, Via della Ricerca Scientifica, I-00133 Roma, Italy, (3) Laboratoire des Solides Irradiés, CNRS UMR 7642/CEA, École Polytechnique, Palaiseau, France

Raman scattering for disordered and anharmonic systems, Anna Putrino, Daniel Sebastiani, Juerg Hutter, and Michele Parrinello, Max-Planck Institut für Festköperforschung - Stuttgart

Thermodynamic behavior of a carbon schwarzite, Vittorio Rosato,[1] Massimo Celino,[1] Giorgio Benedek,[2] and Sabrina Gaito,[2] (1) ENEA, Casaccia Research Centre, HPCN Project, P.O.Box 2400, 00100 Roma, (2) INFM and Dipartimento di Scienza dei Materiali, Università degli Studi di Milano-Bicocca

Schottky barriers at metal/nitride junctions, P. Ruggerone, F. Bernardini, D. Mura, and V. Fiorentini, INFM – Dipertimento di Fisica, Università di Cagliari

Co-adsorption at transition-metal surfaces: Cs+CO/Ru(0001), Ari P. Seitsonen and H. Over, Fritz-Haber-Institut, Berlin, Germany

Stability of the maximum-density droplet state in quantum dots: a quantum Monte Carlo study, Sami Siljamäki, Viktor Sverdlov, Ari Harju, Petteri Hyvönen, and Risto Nieminen, Laboratory of Physics, Helsinki University of Technology

Theoretical investigation of the lattice dynamics of relaxed GaAlSb-systems, Bernhard Steininger and Pasquale Pavone, Theoretische Physik, Universität Regensburg, Germany

Construction of Many-body Potentials for Ge, Walter Stigler and Ulrich Schröder, Institut fr̈ Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Phonon softening in Tellurium by ultrashort laser pulses, an ab-initio study, Paul Tangney,[1,2] and Stephen Fahy[2], (1) Scuola Internazionale Superiore di Studi Avanzati (SISSA/ISAS), Trieste, Italy, (2) University College, Cork, Ireland

Electronic structure calculations of quantum nanowires, Tuomas Torsti, Martti Puska, and Risto Nieminen, Laboratory of Physics, Helsinki University of Technology,

Free energies of Al vicinal surfaces from thermodynamic integration, Federica Trudu, Paolo Ruggerone, and Vincenzo Fiorentini, INFM – Dipartimento di Fisica, Università di Cagliari

5.2 Reports on Collaborative Visits

Report on a Collaborative Visit of C.Molteni, (Theory of Condensed Matter group, University of Cambridge) to the Max-Planck-Institut für Festkörperforschung, Stuttgart

11–17 July 1999

From 11 to 17 July 1999, I visited Prof. M. Parrinello and his group at the Max-Planck-Institut für Festkörperforschung in Stuttgart.

The aim of my visit was to discuss future developments of a collaboration, started when I was working at the Max-Planck-Institut, on phase transformations in nanocrystals and photoreactions.

The visit supported by the network has given me the opportunity to discuss, with various people of Prof. Parrinello group, recent results and technical aspects of the joint projects we are carrying on.

In particular, we have recently developed a new constant pressure molecular dynamics method suitable for studying, within a density functional theory (DFT) scheme, non-periodic systems under pressure, which cannot be simulated with the usual techniques for periodic systems. The idea is to immerse a DFT treated non-periodic object in a model classical liquid, described by a soft-sphere potential, which acts as a pressure reservoir; the pressure is varied by tuning the parameter of the liquid potential (R. Martonak, C. Molteni and M.Parrinello, submitted for publication 1999). We are presently applying this method to the study of structural phase transformations in semiconductor nanocrystals. While this project was originally inspired by experimental data on nanocrystals, the resulting method is fairly general, with potential applications to systems of chemical and biological interest.

We are also trying to investigate the feasibility of simulating photoprocesses in biomolecules by means of a recently developed DFT based method which allows us to perform structural relaxations and molecular dynamics simulations in the first excited singlet state (I. Frank et al., *J. Chem. Phys.* **1998**, 108, 4060-4069).

The visit has been very useful to discuss new ideas for future calculations, and I am very grateful to the network for its support.

Carla Molteni

Report on Collaborative Visit of Balazs Ujfalussy (Budapest) to The H.H. Wills Physics Laboratory, Bristol, UK

I had several points of contact with the group of Professor Balazs Gyorffy at the H.H. Wills Physics Laboratory, Bristol. Many of these originate in methodology and some in physical theories. It was very fruitful to discuss many of the concepts with Professor Gyorffy and his coworkers. During this visit from July 28,1999 to August 4, 1999 there were three fields we were concentrating on.

1. Marcus Eisenbach is working on the band theoretical study of quantum wires. As a first approximation he is using the relatively new Locally Selfconsistent Multiple Scattering (LSMS) method developed at the Oak Ridge National Laboratory [1]. I have been involved in the later developments of the LSMS code, therefore it was quite natural to help to start the project. Here the initial problem was the introduction of empty spheres. Finally we managed to successfully perform a test calculation involving empty spheres and spin-polarized Iron atoms. Doing so, I explained parts of the code and we discussed the roles of various input parameters.
2. Dr. Nektarios Lathiotakis is working on the theory of Oscillatory Exchange Coupling in alloy spacers. He is working with a computer code which I was previously also involved with. Here the problem was the modification of the existing computer code to allow the treatment of alloy spacers according to the theory developed by Dr. Lathiotakis. Specifically, in this theory selfconsistent calculations have to be performed in the Coherent Potential Approximation (CPA) before the calculation of the coupling can begin to obtain the CPA t-matrices of the spacer alloy. This is needed in a fashion, which is in every (numerical) detail compatible with the computer code developed to calculate the coupling. Therefore I implemented the SKKR CPA code and performed calculations on CuNi at various concentrations. We also discussed the necessary modifications of the code for the next step. After that calculations can be performed routinely on alloy systems to further understand the phenomena.
3. Dr. Jürgen Schwitala has been working on the ab-initio description of domain walls using the Fully Relativistic SKKR method. During the next few years our group will also study domain walls also in the framework of the next network project. Therefore it was very interesting to me to get familiar with Dr. Schwitala's work. I learned how he implemented symmetry in the code to reduce computational efforts by a factor of two in the case of uniform Bloch walls. Wee agreed that we are going to merge the current codes in the near future.

I believe it was a rather efficient visit from which both sides profited. The collaboration of course will continue, as the projects are in the most interest of both groups.

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[1] Yang Wang, G. M. Stocks, W. A. Shelton, D. M. C. Nicholson, Z. Szotek and W. M. Temmerman, *Phys. Rev. Letters.* **75**, 2867

I spent 174GBP on the ticket from Budapest to London Heathrow and return, plus 200GBP for lodging (374GBP altogether).

(Balazs Ujfalussy)

Report on the visit of Maosheng Miao (Antwerp) to Jose Luis Martins (Lisbon)

June 6–13, 1999

The groups in Antwerp and Lisbon have collaborated in the past in the study of semiconductors. Recently there has been a shift of interest to the study of molecular and organic crystals. As is well known, the LDA predicts for those types of crystals lattice constants that are much shorter than the experimental values, while the GGA corrects part of the error. The pseudopotential plane-wave codes used in the past were recently modified in Lisbon to include the option of a GGA calculation, to have new structural optimization techniques, plus a few improvements of the numerical efficiency of the codes.

Maosheng Miao visited Lisbon to get acquainted with the code modifications, and we are now collaborating in the study of poly-ethylene and of halogen crystals.

J.L. Martins

6 General Workshop/Conference Announcements

6.1 Newton Institute-ESF Conference

NON-FERMI LIQUID EFFECTS IN METALLIC SYSTEMS WITH STRONG ELECTRONIC CORRELATION

Organisers: DM Edwards; PB Littlewood; H von Loehneysen

5 - 8 January 2000

This conference will initiate the Newton Institute research programme "Strongly Correlated Electron Systems" and is organized in conjunction with the European Science Foundation programme "Fermi-liquid instabilities in correlated metals" (FERLIN) (details at: http://www.esf.org/ferlin)

Scope Of The Conference: Metals are usually described within Fermi-liquid theory. However, this description is sometimes found to break down when the interaction between electrons dominates their motion so that they become strongly correlated. New theories are being developed to describe such non-Fermi-liquid effects. The main aim of this conference is to confront theory with new experimental data covering a wide range of situations and materials where such effects occur. Specific cases to be discussed include:

- high temperature superconductors
- heavy fermion materials near quantum critical points
- fractional quantum Hall effect
- low dimensional systems

Speakers (already confirmed): J-C Campuzano, P Chaikin, A Chubukov, Coleman, J Flouquet, A Freimuth, A.Georges, S Girvin, A.Gogolin, Lonzarich, A Millis, J Nicholls, B Rainford, N Read, J Smet, F Steglich, Stockert, P Woelfle

Location and Costs: The conference will take place at the Newton Institute and accommodation for participants will be provided at Wolfson Court, adjacent to the Institute. The conference package costs 260 pounds, which includes registration fee, accommodation for four nights, a welcome buffet on Tuesday evening, 4 January, and all meals up to lunch on Saturday 8 January, when the conference ends. Limited financial support may be available to young researchers from EC countries. The conference will be restricted to about 80 participants.

Applications: Application forms and further details are available from the WWW at:
http://www.newton.cam.ac.uk/programs/scew01.html.
Completed application forms should be sent to Maureen Clark at the Newton Institute or via

email to: m.clark@newton.cam.ac.uk Closing date for the receipt of applications is 30 October 1999.

Offers of posters (numbers will be limited) with title and short (less than 10 lines) abstract should be sent to DM Edwards by 30 October via e-mail to: d.edwards@ic.ac.uk.

6.2 NATO Advanced Study Institute Workshop

"New Theoretical Approaches to Strongly Correlated Systems"

10 - 20 April 2000

A NATO Advanced Study Institute will hold a workshop on "New Theoretical Approaches to Strongly Correlated Systems". The workshop will take place at the Newton Institute in Cambridge. The dates are 10-20 April 2000.

The purpose of the workshop is to bring together researches of different profile working in the field of strongly correlated systems. The confirmed speakers include:

I. Affleck, J. Cardy, V. Emery, P. Fendley, A. Georges, T. Giamarchi, FDM Haldane, I. Kogan, G. Kotliar, S. Lukyanov. C. Nayak, A. Nersesyan, S. Sachdev, H. Saleur and F. Smirnov.

Further details and the application form can be found on

http://www.newton.cam.ac.uk/programs/scew02.html

Alexei Tsvelik

7 General Job Announcements

At the Chair of Physical Chemistry I at the

University of Konstanz (Germany)

there are openings for

Post-doc and Graduate Positions

The candidates are expected to work on one or more of the following topics:

- Experimental and theoretical studies of the electronic structure of matter (molecules, solids and particularly materials with confining geometries),
- Compton scattering of synchrotron radiation, x-rays and gamma rays for the determination of electron momentum distributions (chemical bonding, intermolecular interactions, phase transitions, interfaces etc.),
- Focusing X-ray optics and X-ray spectrometers,
- Position-sensitive X-ray fluorescence spectroscopy,
- Properties and experimental determination of density matrices and quantum-mechanical phase space densities, or
- Theory of the scattering cross-section of bound electrons

and should participate in the teaching activities of the Chair to an adequate extent. There is the possibility to join the research activities in the project "Electronic properties of extended systems in confined geometries" of the SFB 513 (Nano-structures at interfaces and surfaces).

Applications with curriculum vitae and a complete list of publications should be sent to

Prof.Dr.Dr.hc. Wolf Weyrich
Lehrstuhl für Physikalische Chemie I
Fakultaet für Chemie
Universität Konstanz
Fach M721
78457 Konstanz, Germany

E-mail: Weyrich@chclu.chemie.uni-konstanz.de
Fax: +49-7531-88-3139

Postdoctoral Position(s) in Computational Materials Science

One or more post-doctoral positions will become available shortly in the Institute of Solid State Research (IFF) of the Forschungszentrum Jülich. These positions will be within the framework of a "Transfer Project" funded by the Federal German Ministry for Education and Research (BMBF) and industrial partners. Other groups involved in the project are those of: K. Binder (Universität Mainz), D. Heermann (Universität Heidelberg), K. Kremer (Max-Planck-Institut für Polymerforschung, Mainz), and M. Parrinello (Max-Planck-Institut für Festkörperforschung, Stuttgart).

The goal of the project is to develop, extend, and apply modern methods of computer simulation to problems of current interest, including those of our industrial partners. A long-term aim is to extend the applicability of density functional (DF) methods to larger systems, and to provide more reliable force fields for use in classical simulations of very large systems. In addition to basic problems in DF theory, our group will focus on simulations involving structure and reactions of organic molecules and polymers, and the structure and properties of silicates and other minerals.

The successful applicant(s) will have extensive experience in the area of density functional theory and its applications; experience with Car-Parrinello techniques would be an advantage. Molecular dynamics and Monte Carlo calculations using classical force fields are also planned.

Requests for further information and applications should be addressed to:

R. O. Jones
Forschungszentrum Jülich
I F F
D-52425 Jülich, Germany

e-mail : `r.jones@fz-juelich.de`
Tel. : (+49) 2461-614202
Fax : (+49) 2461-612850

Information about recent work of the group can be found under the URL:
http://www.fz-juelich.de/iff/personen/R.Jones

POST-DOCTORAL FELLOWSHIP OPPORTUNITY FOR SWEDISH SCIENTISTS

at MIT in the groups of Mario Molina, Institute Professor, and Bernhardt Trout

This is a special fellowship for Swedish students or scientists, with expertise in first-principles calculations, who would be interested in spending 1-2 years doing environmental research at MIT as a Wallenberg Fellow. These fellowships were established specifically for Swedish Post-Docs to perform environmental research at MIT. The stipends are extremely competitive (40,000 USD/yr, after taxes plus research funding), and MIT will provide a rich, multi-disciplinary research environment.

The details of the research would be worked out between the fellowship applicant and the PI's, but the general research area will be applying first-principles molecular dynamics to elucidate heterogeneous chemical processes in the stratosphere. It will be a collaborative project geared towards addressing computationally important questions that are also being addressed experimentally at MIT. The computational/theoretical work will be performed by the fellow in collaboration with experimentalists at MIT.

The URL is included below for more information:

http://curricula.mit.edu/cei/Wallenberg/index.html

Please respond to Bernhardt Trout, trout@mit.edu.

Bernhardt Trout
Assistant Professor
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email: trout@mit.edu

Mailing address:
77 Massachusetts Avenue, 66-556
Cambridge, MA 02139

POSTDOCTORAL POSITIONS

CENTER OF COMPUTATIONAL MATERIAL THEORY

Two post-doctoral Research Associate positions are available immediately at the Center of Computational Materials Theory (CCMT) at California State University Northridge. Our research interests include thin film magnetism, optics, mechanical properties, surface catalysis and strongly correlated electron systems using modern electronic structure and molecular dynamics approaches. Candidates with experience in electronic structure calculations or molecular dynamics would be given preference. The CCMT has currently four faculty members, five postdocs and several students and has excellent computer facilities. Please send or e-mail your CV and letters of recommendation to:

Nicholas Kioussis
Department of Physics
California State University Northridge
18111 Nordhoff Str.
Northridge, CA 91330-8268
e-mail: nkioussi@newton.csun.edu

POST-DOCTORAL POSITION(S) AT HUT

The COMP group at Laboratory of Physics, Helsinki University of Technology, has one or more openings for a post-doctoral research associate.

The research interests of the group cover various aspects of computational condensed-matter and materials physics, including electronic properties of materials, statistical physics and complex systems, and disordered materials. A central research theme is multi-scale modelling and simulation of materials properties and processing. Further information can be obtained from the web address

www.fyslab.hut.fi

The senior personnel includes Profs. Risto Nieminen, Tapio Ala-Nissil and Martti Puska, and Drs. Mikko Alava and Juhani von Boehm. They also answer enquiries concerning actual research opportunities.

The successful candidate should have a Ph.D. or equivalent in physics, chemistry or materials science. Experience in computational methods is desirable. The terms of the contract are flexible, and the salary competetive.

Interested persons are requested to send applications to:

Prof. Risto Nieminen
COMP/Laboratory of Physics
P.O. Box 1100
FIN-02015 HUT
Finland

e-mail: rni@fyslab.hut.fi

Ph. D. Position in Condensed Matter Theory

A Ph. D. position is available in the theory department (director P. Bruno) of the Max-Planck-Institut fuer Mikrostrukturphysik in Halle (Saale), Germany, for up to three years. The subject of the work is the first-principle calculations of surfaces and interfaces of complex oxides. The candidate for this position will develop a computational code based on the Green's function method. A diploma degree (or equivalent) as well as a strong background in solid state theory are required for this position. Experience is appreciated in the multiple scattering theory and computer programming (Fortran).

Application from women, minorities and disabled persons are encouraged.

Candidates should send their application including a curriculum vitae, copies of examination certificates and names of two referees to:

Arthur Ernst
Max-Planck-Institut fuer Mikrostrukturphysik
Weinberg 2
D-06120 Halle (Saale)
Germany
tel: +49-345-5582-666
fax: +49-345-5511-223
e-mail aernst@mpi-halle.de

8 Abstracts

Magnetism and magneto-structural effects in transition-metal sulphides

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[‡] *Institut für Material Physik, Universität Wien,*
Sensengasse 8, A-1090 Wien, Austria
and
Centre for Computational Material Science, Sensengasse 8, A-1090 Wien, Austria

Abstract

Recent density-functional studies of the structural and electronic properties of a wide range of transition-metal sulphides (Raybaud *et al.*, J. Phys.: Condens. Matter 9 (1997) p. 11085, *ibid.* p. 11107) are extended to consider the effect of magnetic ordering in sulphides formed by 3d - transition metals. We find that CrS is well described as an itinerant antiferromagnet and that the magnetic ordering leads to a substantial increase of the equilibrium volume and a reduction in the axial ratio of the NiAs-type lattice. MnS(NaCl-structure) is correctly described as a high-spin type-II antiferromagnet (AFM) with a very large magneto-volume effect, but the semiconducting gap is underestimated - probably due to the neglect of correlation effects. Correlation effects are also important for stabilizing the high spin AFM type-III state of MnS_2 over the low spin-state. The phase transitions between nonmagnetic (NM) NiAs-type FeS and antiferromagnetic troilite are well described by spin density functional theory, but the formation of a semiconducting gap and the magnitude of the magnetic moments and exchange-splitting can be explained only by postulating correlation effects of intermediate strength. FeS_2 (pyrite or marcasite) and CoS are predicted to be nonmagnetic, while cubic CoS_2 is well characterised as an itinerant weak ferromagnet. NiS and NiS_2 are predicted to be nonmagnetic by local spin-density theory, in contrast to experiment.

(Accepted, J. Phys. Condensed Matter)
Manuscripts available from: david.hobbs@univie.ac.at

Atomic structure and vibrational properties of icosahedral B_4C boron carbide

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46 Allée d'Italie, 69007 Lyon, France
[5] *Institut Romand de Recherche Numérique en Physique des Matériaux, EPFL,*
Ecublens, 1015 Lausanne, Switzerland

Abstract

The atomic structure of icosahedral B_4C boron carbide is determined by comparing existing infra-red absorption and Raman diffusion measurements with the predictions of accurate *ab initio* lattice-dynamical calculations performed for different structural models. This allows us to unambiguously determine the location of the carbon atom within the boron icosahedron, a task presently beyond X-ray and neutron diffraction ability. By examining the inter- and intra-icosahedral contributions to the stiffness we show that, contrary to recent conjectures, intra-icosahedral bonds are harder.

(accepted to: Physical Review Letters)
Postscript-file available from: vast@bruyeres.cea.fr

Energetics of Divalent and Trivalent Cu in YBCO

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[3] *Institute of Physics and Astronomy, University of Aarhus,*
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Abstract

An *ab initio* local spin density study of $YBa_2Cu_3O_6$ and $YBa_2Cu_3O_7$ is presented. The method includes self-interaction corrections for the Cu *d* states, which enables a description of various valency configurations of both plane and chain Cu atoms. For $YBa_2Cu_3O_6$ the antiferromagnetic state is described with planar Cu occurring in a divalent state and with a near degeneracy of divalent and trivalent Cu chain. For $YBa_2Cu_3O_7$ the most favorable configuration consists of the CuO_2 plane in the trivalent configuration. However, in comparison with $YBa_2Cu_3O_6$, for planar Cu a substantially reduced energy separation between the trivalent and the divalent configurations is observed. The band structure of $YBa_2Cu_3O_7$, with all Cu sites in the trivalent configuration, in the immediate vicinity of the Fermi level, is very similar to the standard LSD picture.

(Submitted to Phys. Rev. Lett.)
Manuscripts available from: W.M.Temmerman@dl.ac.uk

Magnetic properties of disordered CoCu alloys:a first principles approach

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and
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JD Block,SectorIII,Salt Lake City, Calcutta-700091,India

Abstract

Crystalline $\mathrm{Co}_x\mathrm{Cu}_{1-x}$ alloys show interesting magnetic behavior over the entire concentration regime. We here present a fully self-consistent first principles electronic structure studies of the electronic structure and magnetic properties of the system.We present results for the variation of density of states, magnetic moment, spin susceptibility and Curie temperature.

(submitted to Journal of magnetism and magnetic materials)
Latex-file available from : subhra@boson.bose.res.in

Electric field-induced changes in STM images of metal surfaces

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[3] *Department of Physics, Brookhaven National Laboratory,*
Upton, New York 11973

Abstract

Electric field-dependent changes of scanning tunneling microscopy (STM) images of metal surfaces, metallic surface alloys, and ultra-thin magnetic films are predicted. We present a two-state model that demonstrates the general conditions leading to an inversion of the corrugation pattern as a function of field strength, and relate the effects to field-induced changes of the potential barrier. This image reversal for a pure metal surface corresponds to a change from a normal to an anticorrugated STM image. For ordered surface alloys, a switch of the imaged chemical species is possible, and may even cause a change from a p(1×1) to a c(2×2) image at different fields. We explicitly demonstrate the effects by first-principles calculations of the Fe(001) surface.

(accepted in Chem. Phys. Lett.)
copy available from: s.bluegel@fz-juelich.de

Non-Collinear Magnetism of Cr and Mn Monolayers on Cu(111)

Ph. Kurz, G. Bihlmayer, and S. Blügel
Institut für Festkörperforschung, Forschungszentrum Jülich,
D-52425 Jülich, Germany

Abstract

Cr and Mn monolayers on a triangular lattice are prototypical examples of frustrated spin-systems in two dimensions. Collinear and non-collinear magnetic structures of these systems on Cu(111) substrate are investigated on the basis of first-principles total-energy calculations using the full-potential linearized augmented plane-wave method extended by the vector spin-density description for the interstitial and vacuum region. The search for the magnetic minimum-energy configurations included unit cells with one, two, and tree atoms and continuous paths of non-collinear magnetic states connecting high symmetry states. For Cr the energy minimum was found for a 120° spin configuration in a $(\sqrt{3}\times\sqrt{3})$R30° unit cell, which is in agreement to what is expected from a classical nearest-neighbor Heisenberg model with antiferromagnetic interactions. For Mn the same result is expected but a surprise was found: the minimum energy was found for a collinear row-wise antiferromagnetic structure.

Acknowledgement includes: Program Training and Mobility of Researchers 'Interface Magnetism' (Contract: EMRX-CT96-0089) and 'Electronic Structure' (Contract: FMRX-CT98-0178) of the European Union.

(submitted to J. Appl. Phys., proceedings of the 44th Annual Conference on Magnetism and Magnetic Materials)
copy available from: s.bluegel@fz-juelich.de

First-principles investigation of the stability of 3d monolayer/Fe(001) against bilayer formation

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Abstract

We determined the ground-state spin configurations and the total energies of 3d transition-metal monolayer and bilayer films on Fe(001) within the c(2×2) unit cell. We found by energy analysis that V, Cr, and Mn layers prefer the layered antiferromagnetic coupling, and Fe, Co, and Ni layers favor the ferromagnetic coupling to Fe(001). One exception is the Mn monolayer, which favors the c(2×2) ferrimagnetic superstructure. We discuss the stability of the 3d transition-metal monolayer films on Fe(001) against the bilayer formation and found, that with the exception of Cr, all monolayers on Fe(001) are stable against bilayer formation. We have confirmed that the interlayer relaxations do not change the overall features of the present results. The results are based on the full-potential linearized augmented plane-wave method combined with the generalized gradient approximation.

Acknowledgement includes: Program Training and Mobility of Researchers 'Interface Magnetism' (Contract: EMRX-CT96-0089) and 'Electronic Structure' (Contract: FMRX-CT98-0178) of the European Union.

(submitted to J. Appl. Phys., proceedings of the 44th Annual Conference on Magnetism and Magnetic Materials)
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Developing the MTO Formalism

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Abstract

The TB-LMTO-ASA method is reviewed and generalized to an accurate and robust TB-NMTO minimal-basis method, which solves Schrödinger's equation to Nth order in the energy expansion for an overlapping MT-potential, and which may include any degree of downfolding. For $N=1$, the simple TB-LMTO-ASA formalism is preserved. For a discrete energy mesh, the NMTO basis set may be given as: $\chi^{(N)}(\mathbf{r}) = \sum_n \phi(\varepsilon_n, \mathbf{r}) L_n^{(N)}$ in terms of *kinked* partial waves, $\phi(\varepsilon, \mathbf{r})$, evaluated on the mesh, $\varepsilon_0, ..., \varepsilon_N$. This basis solves Schrödinger's equation for the MT-potential to within an error $\propto (\varepsilon - \varepsilon_0) ... (\varepsilon - \varepsilon_N)$. The Lagrange matrix-coefficients, $L_n^{(N)}$, as well as the Hamiltonian and overlap matrices for the NMTO set, have simple expressions in terms of energy derivatives on the mesh of the Green matrix, defined as the inverse of the screened KKR matrix. The variationally determined single-electron energies have errors $\propto (\varepsilon - \varepsilon_0)^2 ... (\varepsilon - \varepsilon_N)^2$. A method for obtaining orthonormal NMTO sets is given and several applications are presented.

(To be published in Lectures in Physics, Springer Verlag)
Manuscripts available from: http://xxx.lanl.gov/abs/cond-mat/9907064

Electronic structure and exchange interactions of the ladder vanadates CaV_2O_5 and MgV_2O_5

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$^{(1)}$*Institute of Metal Physics, Ekaterinburg GSP-170, Russia*
$^{(2)}$*Max-Plank-Institut für Festkörperforschung, D-70569 Stuttgart, FRG*

Abstract

We have performed *ab-initio* calculations of the electronic structure and exchange couplings in the layered vanadates CaV_2O_5 and MgV_2O_5. Based on our results we provide a possible explanation of the unusual magnetic properties of these materials, in particular the large difference in the spin gap between CaV_2O_5 and MgV_2O_5.

(Submitted to Phys. Rev. B)
Manuscripts available from: dasgupta@phy.iitb.ernet.in

Band structure and atomic sum rules for x-ray dichroism

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Abstract

Corrections to the atomic orbital sum rule for circular magnetic x-ray dichroism in solids are derived using orthonormal LMTOs as a single-particle basis for electron band states.

(Submitted to Phys. Rev. Lett.)
Manuscripts available from: oka@and.mpi-stuttgart.mpg.de

Cuprate core level line shapes for different Cu-O networks

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Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Abstract

We have studied the Cu core level photoemission spectra in the Anderson impurity model for cuprates with different Cu-O networks, dimensionalities (zero, one, two and three) and Cu valencies (two and three). We focus on the shape of the leading peak and obtain very good agreement with the experimental data. We show how the shape of the spectrum is related to the valence electronic structure and the Cu-O network but also that other atoms can play a role.

A reprint of this paper can be obtained from cond-mat in
"http://xxx.uni-augsburg.de/abs/cond-mat/9903138" Germany
or in the
"http://xxx.lanl.gov/abs/cond-mat/9903138" USA

(Accepted to Phys. Rev. Lett.)

Probing the magnetic $5f$ density of states above the Fermi level in metallic uranium compounds by x-ray magnetic circular dichroism

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[5] *European Synchrotron Radiation Facility, BP 220,*
F-38043 Grenoble, France

Abstract

We present x-ray magnetic circular dichroism (XMCD) measurements performed at the uranium $M_{4,5}$ edges of the heavy-fermion superconductors UBe$_{13}$ and UPt$_3$. Contrary to what is expected for uranium compounds, the dichroic signal at the M_5 edge exhibits a double lobe structure, comprised of a positive and negative peak. Therefore, out of the eight metallic uranium compounds, so far investigated by XMCD, five present a single-lobe and three a double-lobe structure at the M_5 edge. We show that the observed line shape can be used to study the magnetic character of the $j = 7/2$ level of the empty $5f$ density of states.

(Submitted to Phys. Rev. B)
Manuscripts available from: G.vanderLaan@dl.ac.uk

Relativistic effects in the magnetism of UFe_4Al_8

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Institut für Festkörperphysik, Technische Universität,
D-64289 Darmstadt, Germany

Abstract

The magnetic structure of UFe_4Al_8 possesses a number of unique features. There are two magnetic sublattices whose magnetic moments are almost orthogonal. Additionally, there is a canting of the magnetic moments within the Fe sublattice. We show that these features can be treated as inevitable consequences of the properties of a simpler magnetic state of the system. It is shown that the magnetism of the U sublattice is induced by the compensated antiferromagnetism of the Fe sublattice. The orthogonality of the induced and inducing moments is explained. Unusual nature of the magnetic anisotropy is demonstrated. A crucial role of the spin-orbit coupling and the inter-atomic hybridization is exposed. The symmetry criterion of the magnetic instability of a nonmagnetic sublattice in an antiferromagnetic crystal is formulated.

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Pdf-file can be obtained from sandratskii@fkp.tu-darmstadt.de

Magnetic properties of self-assembled Co clusters on Au(111) below the ferromagnetic phase transition

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Abstract

We report on the magnetic properties of Co clusters grown on Au(111) in the cluster-size range from 300 to 12000 atoms. These clusters are superparamagnetic at room temperature, while at low temperatures blocking of the thermal fluctuations leads to a macroscopic remanence. The hysteresis curves measured *in situ* by x-ray magnetic circular dichroism show that the blocking temperature scales with cluster size, following a finite-size scaling power-law behavior. We find that the blocking temperature of these clusters is substantially reduced by a thin silver overlayer, indicating a reduction in the perpendicular magnetic anisotropy at low coverages. With this change in anisotropy a clear change in the shift exponent λ can be observed.

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Stable and Metastable Structures of Cobalt on Cu(001) – an *ab initio* Study

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Abstract

We report results of density-functional theory calculations on the structural, magnetic, and electronic properties of (1×1)-structures of Co on Cu(001) for coverages up to two monolayers. In particular we discuss the tendency towards phase separation in Co islands and the possibility of segregation of Cu on top of the Co-film. A sandwich structure consisting of a bilayer Co-film covered by 1ML of Cu is found to be the lowest-energy configuration. We also discuss the a bilayer c(2×2)-alloy which due to kinetic reasons, or at strained surface regions, may play some role. Furthermore, we study the influence of magnetism an the various structures and, e.g., find that Co adlayers induce a weak spin-density wave in the copper substrate.

(submitted to: Phys. Rev. B)
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An *ab initio* study of the rutile $TiO_2(110)$ surface structure – on the comparison of theory and experiment

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Abstract

We examine the reasons for the poor quantitative agreement between the structures predicted from the minimum energy configuration of first principles calculations and those deduced from surface x-ray diffraction experiments for the structure properties of the $TiO_2(110)$ surface. In order to confine all numerical approximations very large scale all-electron first principles calculations are used. We find a very soft, anisotropic and anharmonic surface rigid-unit vibrational mode which involves displacements of the surface ions of approximately 0.15 Å for thermal vibrations corresponding to room temperature. It is concluded that in order to perform an accurate comparison between theory and experiment for this and perhaps other oxide surfaces it will be necessary to take account of such anisotropic vibrations in models used to interpret experimental data. In addition the contribution of the vibrational entropy to the surface free energy is likely to be significant and must be taken into account when computing surface energies and structures.

Faraday Discussion **114** (in print)
Manuscripts available from: n.m.harrison@dl.ac.uk

Size, shape and stability of InAs quantum dots on the GaAs(100) substrate

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Abstract

We study the energetics of island formation in Stranski-Krastanow growth of highly mismatched heteroepitaxy within a parameter-free approach. It is shown that the (frequently found) rather narrow size distribution of the self-assembled coherent islands can be understood as the result of the system being trapped in a *constrained* equilibrium state. Moreover, we investigate the dependence of island size on the island density and coverage. Our approach reproduces well the experimental island size dependence on coverages. Our study also indicates that the island shape depends on the island size, i.e., an island with larger volume has a higher value of the height-to-base ratio. The calculated energy gains show that larger islands corresponding to lower island density are more stable, this implies that Ostwald ripening will occur when time scales are sufficiently long so that different islands are allowed to exchange atoms.

(submitted to: Phys. Rev. B)
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Indium induced changes in GaN(0001) surface morphology

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Abstract

First-principles calculations of the energetics of the In-terminated GaN(0001), (0001), (1011) and (1011) surfaces indicate that In has a substantial effect on the relative energies of formation of these surfaces. Indium induced changes in the surface energetics enable the formation of inverted hexagonal pyramid defects having (1011) facets at the termination of threading defects on the (0001) surface of pseudomorphic InGaN films. For dislocations terminating on the InGaN(0001) surface, the calculations predict that large (1011) facetted defects are not energetically favorable.

(submitted to: Phys. Rev. B)
Manuscripts available from: neugebauer@fhi-berlin.mpg.de

9 Presenting Other Initiatives

HPC Users/Colleagues:

I am soliciting input from colleagues and users of HPC technology about holding a conference in year 2000 on computational science and engineering. We held a session on this topic during the HPCU '99 conference this year and it seems like this field warrants even a larger meeting and more time to thrilly discuss issues around both educational and research aspects of the field.

Please visit our web site at http://www.cps.brockport.edu to learn more about our computational science program.

The HPCU '99 program (including session on computational science education) can be reached at http://www.hpcu.org or http://hpcu.cybeready.com.

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Senior Consultant, Lockheed Martin, http://www.ornl.gov
Founder/Chairman, OYSOFT, http://www.oysoft.com
Founder/Chairman, HPCU, http://www.hpcu.org

10 SCIENTIFIC HIGHLIGHT OF THE MONTH

Crystal Field Excitations as Quasi-Particles

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The splitting of localised atomic energy levels by the crystalline electric field in solids affects many areas of physics and chemistry. The crystal field energy levels of rare earth atoms are particularly important in intermetallic compounds containing Fe, Co and Ni which have both high Curie temperatures and large magnetic anisotropy. The strong magnetic coupling governing the Curie temperature is provided by the 3d element whereas the strong orientational dependence of the magnetism is due to the energy differences between the crystal field levels of the rare earth. Models which attempt to explain the crystal field energy level differences in terms of electrostatic interactions between the $4f$ and conduction electrons exist but computed values for the energies have been poor. The measured crystal field excitation energies with which theory has been compared have been assumed to be bare $4f$ excitations in the static electric field of the ions and conduction electrons. We show here that crystal field excitations in metals are quasi-particles composed of a $4f$ excitation plus an associated cloud of shielding conduction electrons.

The ability to calculate the $4f$ crystal field energies accurately from first principles is not only a prerequisite for the computation of low temperature thermal and magnetic properties, but would also be a considerable aid to the development of rare earth transition metal permanent magnets and other magnetic devices. It is therefore desirable to have a theoretical framework from which the energies of the crystal field levels in solids may be calculated accurately from first principles. Such a framework must, however, combine the merits of the two very successful, but apparently incompatible, models that have been used to describe the localized atomic $4f$ electrons and the metallic conduction electrons, respectively. The standard model [1] for the $4f$

states is based upon the theory of the free atom and properly includes the effects of electron-electron interactions within the $4f$ shell, leading to Russell-Saunders coupling of the individual electronic angular momenta to a conserved value of the total angular momentum of the atom. A direct consequence of Russell-Saunders coupling, which is preserved in the solid since the $4f$ states are localized is that the $4f$ levels are degenerate in a spherical environment. The energy differences between the crystal field states are then entirely due to the non-spherical environment in the crystal [2]. Calculations based upon this model attribute these energy differences to the average interaction between the non-spherical $4f$ and conduction electron densities [3, 4, 5, 6, 7]. The strengths of the model are that the internal dynamics of the $4f$ shell are handled very well and that only the crystal field energies, which are of the order of meV, enter the calculation. Its weakness is the assumption that the conduction electron density remains unchanged when the $4f$ electron density changes in a transition from one crystal field state to another.

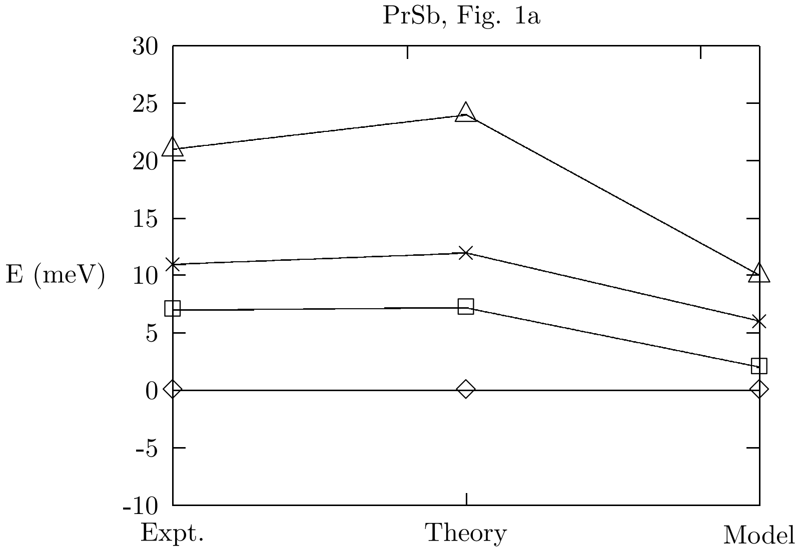
In other areas of physics and chemistry energy differences in solids are obtained from the local density approximation [8] to density functional theory [9] as the difference in the *total* energy, typically of the order of 10^5eV, of the solid in different states. The strength of this method, which has become the standard model for first principle calculations of ground state properties of metals, is that the entire electron density is allowed to relax since it is calculated self-consistently by iteration. It should in principle be possible to calculate crystal field excitation energies as total energy differences in the same way, removing any assumptions concerning relaxation of the conduction electron density, but adding the requirement that the calculation of the total energy be numerically accurate to at least 10^{-2}meV in 10^5eV.

However, we have found that such an approach fails in calculations of crystal field excitations and the ultimate evidence for its breakdown is that it does not yield degenerate $4f$ energy levels for the free atom. Density functional theory is based upon a variational principle for the total energy of the entire electron density (which is why the entire electron density is allowed to relax iteratively) and the total energy is a functional [9, 8] of the total electron density, n,

$$E[n] = T_s[n] + E_N[n] + E_H[n] + E_{xc}[n], \tag{1}$$

where the contributions are the kinetic energy, $T_s[n]$, electron-nuclei interaction energy, $E_N[n]$, Hartree electron-electron interaction energy, $E_H[n]$, and exchange-correlation energy, $E_{xc}[n]$. In the limit of the free atom the Hartree contribution differs for different $4f$ charge densities corresponding to different crystal field states. If the exchange-correlation functional were known exactly its contribution for the different 4f densities would cancel the corresponding energy differences from the Hartree contribution and the Russell-Saunders degeneracy would be reproduced. However the exchange correlation functional for such highly correlated localized $4f$ states is not known and the one used in practice is more appropriate for itinerant conduction electrons in metals. This lack of exact cancellation leads to finite energy differences between crystal field levels even in the atomic limit. Since direct application of the local density approximation to localized $4f$ states is flawed but we require it to calculate the total energy of the solid, we have explicity removed the pertinant $4f-4f$ interactions in both $E_H[n]$ and $E_{xc}[n]$. The total energy of the solid is then slightly incorrect, but by the same amount for each crystal field level and the errors in the transition energies cancel rigorously.

We have imposed a control on the applicability and numerical integrity of the method by verifying



that the calculated crystal field levels become degenerate in the atomic limit for some selected rare earth compounds. This criterion was found to be satisfied for all of the calculations reported here. We have made self-consistent calculations[10] for two experimentally well studied rare earth compounds, PrSb and TmSb [11, 12] with no shape restriction on either the valence electron density or potential. The $4f$ occupation number was constrained 2 and 12 for PrSb and TmSb, respectively. The shape of the $4f$ density was constrained to correspond to the symmetry of each crystal field level whereas the rest of the electron density was obtained self-consistently, being allowed to relax to shield the change in $4f$ density.

In Figs. 1a and 1b we compare the results with measurements.Typically the calculated levels differ from the measurements by less than a few meV, with the largest error being some 30% for the Γ_5 level of PrSb. This level of agreement is much better than that obtained by earlier theories. Whereas previously the crystal field excitation energy was assumed to be the change in energy due to a change in $4f$ density in an unchanged conduction electron density - a bare excitation - we find that there is an important change in conduction electron density in response to the bare crystal field excitation of the $4f$ shell. Therefore the crystal field excitations in metals are composed of the change of density within the $4f$ shell plus the concomitant screening charge of the conduction electrons. The combination is a quasi-particle involving the degrees of freedom of many electrons. The interaction between the 4f charge density and the conduction electrons is strong but the interactions between the quasi-particles should be relatively week.

The importance of the change in valence electron screening is illustrated in Fig.2 by the difference between the valence electron densities of PrSb for the Γ_1 and the Γ_3 crystal field levels. The lobes elongated vertically and horizontally represent a surplus of electron charge whereas the lobes which are rotated by 45 degrees represent a charge deficiency. Therefore rearrangements and relaxation effects of the valence electron states are seen to be substantial in crystal field excitations. The change in valence electron density for the free atom is much larger than for the solid and in this case the shielding is complete because the crystal field levels remain degenerate. The valence electrons in the solid are subject to crystalline boundary conditions which reduce their ability to redistribute to shield a change in the $4f$ density and it is precisely this restriction

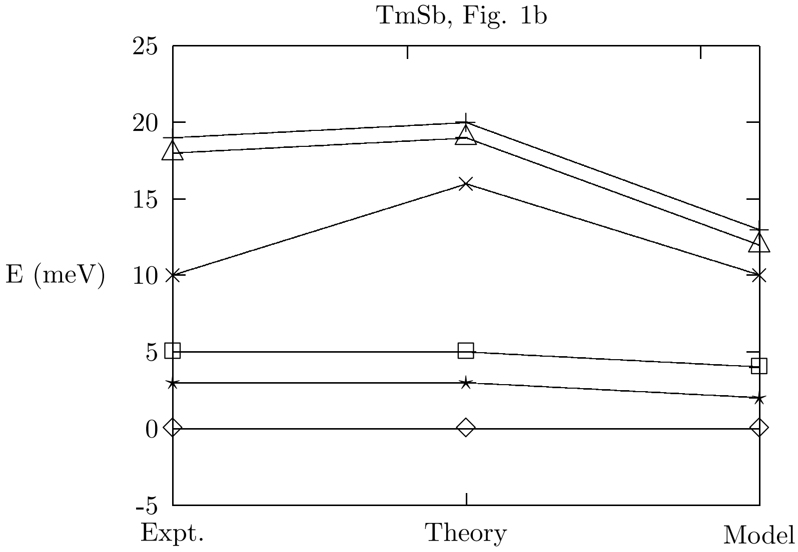


Figure 1: Measured and calculated crystal field energy levels of PrSb and TmSb. For PrSb the diamonds correspond to Γ_1 level, the squares to Γ_4, the x's refer to Γ_3, and the triangles correspond to Γ_5. For TmSb the stars correspond to Γ_4 level, the squares and triangles to Γ_5, and all the others to Γ.

which splits the crystals field energy levels.

The conventional view that crystal field excitation energies in metals are due to an electrostatic field of the ligands alone is useful for pedagogical purposes but is much too simple to enable computational accuracy. We have shown, however, that it is possible to modify the local density approximation to calculate crystal field excitation energies from first principles and include the effects of relaxation of the conduction electrons. Since shielding by the conduction electrons is strong the crystal field excitations should be viewed as quasi-particle excitations where the change of the localized 4f density is intimately connected with a corresponding change of the valence electron charge.

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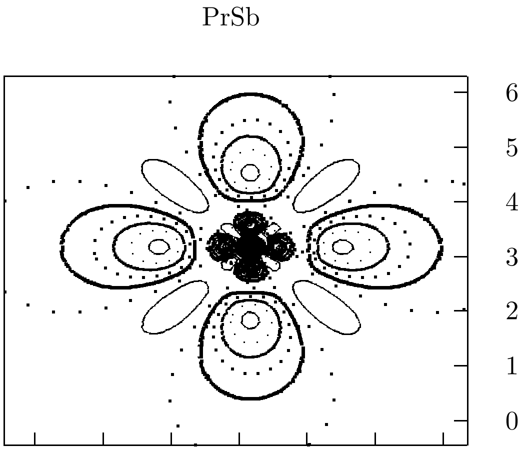

Figure 2: Charge density contour in the 001 plane of the difference in shielding valence electron density of PrSb when there is a transition from the Γ_1 to the Γ_3 crystal field state.

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