

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

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1 Editorial

We have just learned that **Volker Heine**, the driving force behind the Psi-k network, has been awarded 2001 Max Born medal and prize "*For his pioneering theoretical and computational studies of the electronic structure of solids and their application to physical properties, including his recent contributions to the development of a new field of "mineral physics"*". More details on the award and the medallist will be published in the February issue of the newsletter.

In this *Newsletter* in the **General News** section we write about the 2001 TMS Bardeen and Hume-Rothery awards won by **Alex Zunger** and **Balazs Gyorffy**, respectively, and about 2001 APS Rahman award won by **Alex Zunger**. In the **TMR1** section we publish the annual report of the 'Interface Magnetism' network. The **RTN** section contains announcements of a few post-doctoral positions available within the RTN network. A joint TMR2/ESF workshop on @Nonlollinear Magnetism is announced in the **TMR2** section. In the **ESF** section we have two reports on conference/workshops, five announcements of workshops and conferences, plus a whole list of Psi-k workshops for 2001. General position announcements, namely those not linked to any of the networks, can be found in the General Job Announcements section. Additionally, after the **General Job Announcements**, we advertise call for nominations for '**Michelson Postdoctoral Prize**'. Abstracts of newly submitted papers are placed in the usual **Abstracts** section. The newsletter is finished with the scientific highlight of the month by Niels E. Christensen (*Aarhus*) and D.L. Novikov (*Cambridge, MA*) on "**High-pressure phases of the alkali metals**". Please see the table of contents for further details.

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

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

The above contains 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
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psik-network@daresbury.ac.uk	messages to the whole Ψ_k community

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2 General News

2.1 Bardeen, Hume-Rothery, and Rahman Awards for 2001

Balazs Gyorffy and Alex Zunger receive 2001 TMS and APS awards

The Minerals, Metals and Material Society (TMS) named **Alex Zunger**, research fellow of the National Renewal Energy Laboratory, USA, as the recipient of its 2001 John Bardeen Award, and **Balazs Gyorffy**, professor of physics at the University of Bristol, UK, as the receipient of its 2001 William Hume-Rothery Award. **Alex Zunger** has also been declared by the American Physical Society (APS) as the winner of the 2001 Rahman prize.

The TMS John Bardeen Award was established in 1994 and recognizes an individual who has made outstanding contributions and is a leader in the field of electronic materials. This prize is named in honor of the two-time Physics Nobel Prize Laureate John Bardeen (in 1956, with Shockley and Brattain for the invention of the transistor; and in 1972 with Cooper and Schrieffer for the BCS theory of superconductivity).

The TMS William Hume-Rothery Award was established in 1972 by the Institute of Metals Division of TMS and recognizes outstanding scholarly contributions to the science of alloys. The award includes an invitation to the recipient to be the honored lecturer at the William Hume-Rothery Memorial Symposium during the TMS Annual Meeting.

The APS Rahman prize is given annualy to a single person "to recognize outstanding achievement in computational physics research".

Alex Zunger receives the John Bardeen Award "*For his seminal contributions to the theoretical understanding and prediction of "spontaneous ordering", phase-stability, and electronic properties of semiconductor alloys; for the impact that this work has had on experimental studies of electronic materials, and for his continued leadership in the field*".

Bulk semiconductor alloys such as $(\text{GaP})_x(\text{InP})_{1-x}$ are known to exhibit a repulsion between the constituents, so they were never expected to order crystallographically. Indeed, they were known to form random structures at high temperatures and phase-separation at low temperatures. Theory has shown, however, that "*surface reconstruction*" - an almost universal feature of covalent surfaces - can lead to an ordered atomic arrangement in alloys since the alternative (random configuration), is highly strained by surface dimers. Thus, strain-minimizing surface-stable ordered structures are frozen in-by the growth process. The lower symmetry of ordered structures relative to random alloys leads to profound changes in band gaps, optical selection rules, effective-masses, pressure dependence and transport properties, predicted by Zunger and his group starting in 1984. Ordering has since been discovered in virtually all covalent semiconductor alloys. For more details see:

http://www.sst.nrel.gov/topics/alloy_order.html.

These effects, plus the fact that control of ordering creates new, technologically significant materials properties has led to > 1000 experimental publications in this field.

Zunger emphasizes that his work on this theoretical problem was done in collaboration with his post-doctoral fellows since 1983: J. Bernard, D. Laks, K. Mader, R. Magri, J.L. Martins, T. Mattila, A. Mbaye, R. Osorio, V. Ozolins, G.P. Srivastava, and D. Wood, as well as with his NREL associates L. Ferreira, S. Froyen, S.H. Wei and S.B. Zhang. This project was funded by the U.S. Department of Energy (DOE) Photovoltaic Program (1983-1991) and since 1991 by DOE's Office of Science, Basic Energy Science, Division of Materials Science. Zunger's other areas of interest include Photovoltaic materials, the theory of semiconductor quantum-dots, and the theoretical design and predictions of stable crystal structures and phase-diagrams.

This award will be presented formally to Alex Zunger at the 130th Annual TMS meeting on February 13, 2001, in New Orleans.

Previous recipients of this award include M. Panish (1994); N. Holonyak (1995); L.G. van Uitert (1996); J.B. Goodenough (1997); S. Mahajan (1998); L. Kimerling (1999) and A. Chang (2000).

Biography: Alex Zunger is an Institute Research Fellow and leader of the Solid State Theory at the U. S. Department of Energy's National Renewable Energy Laboratory (NREL). He received his B. Sc, M.Sc and Ph.D education at the Tel Aviv University, Israel (PhD: 1976 in chemical physics), and did his post-doctoral training at Northwestern University, Evanston, Ill. (1975-1977) and (as IBM Fellow) University of California, Berkeley (1977-1978). He joined the newly founded NREL in 1978 where he established the Solid State Theory group and trained and collaborated, since, with 35 post-doctoral fellows. He is an author of 400 journal publications, including over 85 in Physical Review Letters and Rapid Communication. According to recent research done by the Institute of Scientific Information (ISI), he is the 39th most cited physicist out of more than 500,000 physicists examined, based on publications in 1981-1997 in all branches of physics (his work was cited-8, 000 times). His work centers on development and application of "First-Principles" electronic structure theory of "real materials". It includes the development of "first-principles pseudopotentials; accurate exchange-correlation functionals; the momentum-space total energy formalism; simultaneous relaxation of atomic positions and electronic wave functions; "order N" electronic structure approaches, and "cluster expansions" for alloy thermodynamics. These techniques were applied by him to metal alloys, quantum semiconductor nanostructures, points defects and surfaces.

Balazs Gyorffy receives the Hume-Rothery Award "*For the invention [1] and, with his collaborators, the pioneering use [2,3] of the KKR-CPA*"

By the mid 1930-ies the impact of Quantum Mechanics on Condensed Matter Physics has called for books to rewrite the subject. The first monographs were "The Theory of the Properties of Metals and Alloys" by N.F. Mott and H. Jones (1936), and "The Structure of Metals and Alloys" by William Hume-Rothery (1936). The award which bears his name has been established by the American Minerals-Metals-Materials Society (TMS) to celebrate Hume-Rothery's early recognition that the structure of metals and alloys is determined by the quantum mechanical states of the electron glue that holds the positively charged nuclei together. In particular, the famous 'Hume-Rothery Rules' called attention to the correlation of electron per atom ratio, e/a , and crystal structure in metallic alloys Thus, it is

not surprising that a few years ago the prize was awarded to David Pettifor for the introduction of the Mendeleev number to explain structure maps. Similarly, it is appropriate that the 2001 award went to Balazs L. Gyorffy for the invention [1] and, with his collaborators, the pioneering use [2,3] of the KKR-CPA.

Random solid solutions are a scientifically interesting and technologically important class of materials but due to the fact that disorder is an essential feature of the problem none of the standard first-principles methods, like LAPW, Pseudopotentials, etc., could deal with the problem. In the hands of B.L. Gyorffy, G.M. Stocks, J.S. Faulkner, W.M. Temmerman, J.B. Staunton, J. Wadsworth, Z. Szotek, S. Lovatt, P. Weinberger, A. Pindor, P.J. Durham, D.D. Johnson, F.J. Pinski, A. Gonis, H. Winter, H. Ebert, B. Ginatempo, and D.M. Nicholson, the KKR-CPA became a fully self-consistent, spin-polarized and relativistic first principles method firmly based on LDA of Density Functional Theory in the late 1980-ies [4]. From then on it has been used to make progress with many important problems such as: Copositional Short Range Order [5], Evolution of the Fermi Surfaces Alloys with Concentration [6], Electrical Transport in Metallic Alloys [7], The Invar Problem [8], Surface Alloys [9], Local Moments and Magnetic fluctuations in Metallic Paramagnets [10] and Oscillatory Magnetic Exchange Coupling Across Alloy Spacers [11] to mention but the highlights. Recently, encouraged by the successes of KKR-CPA, an LMTO version of the CPA has been developed. The impact of LMTO-CPA has been recorded in a very readable book of Turek, Drchal, Kudrnovsky, Sob, and Weinberger [12].

Balazs Gyorffy will present his Hume-Rothery Award lecture at the '2001 William Hume-Rothery Symposium' at the 2001 TMS Annual Meeting in New Orleans on Monday, February 12, 2001. The title of the lecture is: "On the quasiparticle spectra of superconducting random alloys".

Biography: Balazs L. Gyorffy received his B. Sc. and Ph. D. from Yale University. He has held the following positions at the University of Bristol: 1970-1980 Lecturer, 1980-1987 Reader, 1987-present Professor of Theoretical Physics. He has held visiting positions at Oak Ridge National Laboratory, Brookhaven National Laboratory, Institute Laue-Langevin, Grenoble, University of Toronto, and Technical University of Vienna. In collaboration with many, but particularly with G.M. Stocks and J.S. Faulkner, he invented and pioneered the application of the Korringa-Kohn-Rostoker-Coherent Potential Approximation, a first-principles method for calculating the electronic structure of metallic alloys. Advances made using the KKR-CPA are summarized in Ref. [5]. Balazs Gyorffy has been elected an external member of the Hungarian Academy of Sciences (1995), Fellow of the Institute of Physics (1998), and was co-recipient of the Gordon Bell Prize (1998). He has authored or co-authored 220 publications.

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The APS Rahman prize **Alex Zunger** receives "*For his pioneering work on the computational basis for first-principles electronic structure theory of solids*". This award, centering on a different aspect of Zunger's work than the one depicted by the John Bardeen Award, focuses on Zunger's development of first-principles methodologies for predicting properties of solids. These include: (i) The early development of first-principles LDA atomic pseudopotentials [Topiol, Zunger, Rutner, Chem. Phys. Lett. **49**, 367 (1977), and Zunger and Cohen, Phys. Rev. B**18**, 5449 (1978)]; (ii) the pseudopotential total energy and force methods [Ihm, Zunger and Cohen, J. Phys. C**12**, 4409 (1979); (iii) the strategy of simultaneous relaxation of atomic positions and electronic charge densities, a precursor to Car-Parrinello [Bendt and Zunger, Phys. Rev. Lett. **50**, 1684 (1983)]; (iv) accurate exchange-correlation functional; (v) the self-interaction correction (Perdew and Zunger, Phys. Rev. B**23**, 5048 (1981)], and; (vi) mixed-basis cluster expansion for prediction of ground state crystal structures and the temperature-composition phase-diagram of alloys. Other areas of interest of A. Zunger include photovoltaic materials, spontaneous ordering in solids (the subject of the year 2001 Bardeen Award) and quantum nanostructures.

Previous recipients of this award include Ken Wilson (1993), John Dawson (1994), Roberto Car and Michele Parrinello (1995), Steve Louie (1996), Donald Weingarten (1997), David Ceperley (1998), Michael Klein (1999) and Michael Creutz (2000).

This award will be presented to Alex Zunger at the annual APS meeting in Boston, MA, on June 25, 2001. The announcement will appear in the March 2001 issues of the APS News.

3 News from the TMR1 Network

"Interface Magnetism"

3.1 Annual Report of TMR1-Network

Report of TMR-Network: "Interface Magnetism"

This Network is concerned with ab initio calculations of magnetic properties of surfaces, interfaces and multilayers. The Network is structured around 6 projects with 6 partners in the UK, Germany, France, Austria, the Netherlands and Sweden contributing. This report covers the fourth year of operation (1999-2000) and we can see that this Network has employed up to 10 young researchers during the reporting period. Our Network had an extremely successful year leading to wide international recognition of its work. Firstly, a Network member shares Europe's Most Prestigious Physics Prize, the "Agilent Technologies Europhysics Award for the Discovery of Magnetic X-ray Dichroism". Paolo Carra (ESRF, Grenoble, France), Gerrit van der Laan (Daresbury Laboratory, Warrington, UK) and Gisela Schutz (Institute of Physics, Wuerzburg, Germany) have won the Europhysics Award for the year 2000 for their "Pioneering work in establishing the field of magnetic X-ray dichroism, ... leading to advances in the fields of electronic, electrical and materials engineering which represents scientific excellence". The award ceremony took place on March 17th, 2000 during the EPS Condensed Matter General Conference in Montreux, Switzerland. Secondly, Network members have published two articles in Nature and one in Science, in addition to many publications in Physical Review Letters. A short report on each of the articles in Science and Nature appears in the Highlights further below.

The status of the different projects is as follows:

Interlayer Coupling At the beginning of this Network, the study of interlayer exchange coupling represented one of the strongest activities within the Network, activities to which all nodes contributed strongly. Now at the end of the regular period, these efforts are slowly fading out and instead we observe a strong shift to spinindependent transport, i.e. giant magnetoresistance and tunneling magnetoresistance. The reason for this is twofold. Firstly, this follows the realisation of the importance of spin-dependent transport for future magnetoelectronics. Secondly this is a consequence of the fact that interlayer coupling is now to a large extent well understood. That such a good understanding could be achieved, can be considered as big success of our Network. Without exaggeration we can claim, that the most important theory contributions came from our Network. Here we just list a few highlights: (i) the pioneering paper of Patrick Bruno showing the connection of the oscillation periods with the Fermi surface of the spacer, (ii) the enormous amount of calculations by the Austrian-Czech group about the effects of interdiffusion at the interface and of alloying in both the spacer and the ferromagnetic layer, (iii) the detailed studies of the Swedish, British and French groups for the understanding of the complex Fe/Cr systems, (iv) the calculations of the spin dependent reflection and transmission coefficients of the Dutch and German groups, etc. Very many of these papers have been published in Physical Review Letters and are widely

recognised.

Nevertheless, during the current reporting period Dr N Lathiotakis, the TMR research assistant of the UK node, has completed the study of Oscillatory Exchange Coupling (OEC) of magnetic layers across a metallic alloy, $\text{Cu}_c\text{Ni}_{1-c}$, spacer. In this work the amplitude and phase as well as the frequency of the OEC was calculated on the bases of an asymptotic analysis in the context of a first-principles (KKR) framework for the first time. In addition to satisfactory agreement with experiment he found a new periodicity, determined by a new external spanning vector of the Fermi Surface, as the Ni concentration approach $c \sim 11\%$. This discovery has been reported on a poster at the Psik 2000 Conference and a paper about it appears in the Physical Review B (September 2000). As we have forecast in our previous report we have investigated the bi-quadratic coupling by the same first-principles asymptotic analysis as the one we have developed for the study of the quadratic OEC. This work has now been completed and a paper about it is in preparation. On the matter of staff supported by this grant we are happy to report that the post-doc, Dr N Lathiotakis, was offered and accepted another post-doctoral position at the University of Würzburg in the group of Professor E A K Gross.

This work was supplemented by a review of the AT node, together with the DE node, on the theory of interlayer coupling (in the LMTO-book of H. Dreysse) and by work of the Dresden group on interlayer coupling in the Fe/Au system.

Magnetic Anisotropy and Surface Structure This project has had a post-doc based with the Swedish team, first J.Henk from DE and after Dr. Henk left the group for a research position in Halle, Dr.O.Le Bacq joined the group (in June 1999). The Swedish node has established good contact with world leading experimental groups on thin film magnetism (lead by Prof. K.Baberschke in Berlin and by Prof.R.Wäppling in Uppsala). After a learning period, Dr.Le Bacq has studied the magnetic properties (spin and orbital magnetic moments and magneto crystalline anisotropy-MAE) of Fe_n/V_m multilayers for various values of n and m. Experimental data show that when n=2 and m=5 the MAE gives the out of plane direction as the easy axis, whereas for n=4 and m=4 the MAE gives a moment in plane. The experimental data have successfully been reproduced using a highly accurate first principles full potential electronic structure method. The microscopical reason for this spin reorientation transition has been analysed in detail, and it has been established that both structural effects (lattice distortion and lattice expansion) in combination with the Fe-V interaction (hybridization) are crucial for the MAE. In addition a novel method, based on elasticity theory, for calculating the in-plane and out-of-plane lattice constant of any multilayer has been developed and shown to agree with experiments with good accuracy.

A large effort of the activities of the Vienna Node was devoted to the magnetic anisotropy and perpendicular magnetism, in particular for layered systems with tetragonal distortions, and has resulted among others in two joint publications. This work was supplemented by a similar strong activity of the Bluegel group at Juelich centered at the anisotropy energy of 3d layers on the surface of W.

Giant Magneto Resistance (GMR) Theoretical research on magnetic structures and devices continued with emphasis on the mesoscopic and nanoscopic regimes. On the one hand, we considered how metallic ferromagnets in contact with conductors inject a spin-polarised current into a variety of other materials such as simple normal metals, semiconductors and superconductors. On the other hand, we studied how transport in mesoscopic devices could be used to test basic concepts of quantum mechanics such as charge and conductance quantization. The behaviour of a collection of electron spins in small

structures combines these two fields. We focused our attention on transport in hybrids of normal and ferromagnetic metals as well as ferromagnets and superconductors, our aim being to develop novel or improved theoretical methods for understanding transport and other phenomena in such systems. The main applications of this phenomenological theory were to: single-electron tunnelling in magnetic systems; ferromagnetic/superconducting devices; non-collinear diffuse transport.

The microscopic scattering matrices used in the phenomenological theory discussed above were calculated using a newly developed formalism based on the TB-LMTO basis and applied to the study of the interface resistance of a variety of magnetic/non-magnetic interfaces including disorder. The disorder was modelled by means of large lateral supercells. Interface disorder was found to *reduce* the majority-spin interface resistance for a Fe/Cr (100) interface by a factor of three. The calculational framework is currently being extended: to calculate spin-mixing matrices which arise when transport in non-collinear magnetic systems is formulated in the circuit theory developed above; to study the influence of disorder on spin-dependent transport in tunneling systems; to study transport through interfaces between magnetic and superconducting materials.

The Giant MagnetoResistance postdoc based with the Dutch team, A. Brataas, left at the beginning of the reporting period for a position in Harvard and has not yet been replaced.

The efforts of the Dutch team were accompanied by many strong activities in other nodes. Here in particular the Austrian node excelled with many results for the current-in-plane (CIP) GMR. Moreover they have calculated for the first time also the current-perpendicular-to-plane (CPP) GMR which shows many characteristic differences. In addition the Dresden group continued the discussion of the GMR by the Boltzmann approach resulting in a simple understanding of the different trends and characteristics of CIP and CPP conductances.

Spin-Polarised Spectroscopies Project The main research interest of the Daresbury based post-doc (M. Lueders from DE, since January 1999) are photoemission calculations for quantum-well multilayer systems. During the past year M. Lueders has tested and validated a newly developed photoemission code especially adapted for the study of layered systems. Calculations for Co/Cu quantum well states are now in progress. Furthermore, the Daresbury based Network post-docs have performed calculations in support of synchrotron experiments on magnetic multilayers which resulted in two publications.

The Munich group has studied, partly in collaboration with the Strasbourg team, the magnetic circular X-ray dichroism of ordered and disordered alloys with the 3d and 4d elements. The calculations employ the fully relativistic KKR-CPA method for disordered alloys. Particular emphasis is put on the local moments of the 4d-atoms, being induced by the 3d alloy partners. The results are in good agreement with available MXCD data for ordered FePd alloys and show, that by combining such calculations with MXCD data for partially disordered tetragonal layered systems, a direct information about the chemical ordering of the films can be obtained.

One publication of the AT node dealt with spectroscopy and was based on an exchange of data and discussions with the group of H. Ebert in Munich of the DE node. This in particular was a very good example of the use of the network!!

Tight-Binding KKR-Green's Function Methods The intensive and successful activities of the Network in constructing highly accurate KKR-programs were also pursued in the fourth year. In particular, this concerns the tight-binding or screened KKR method, which was jointly invented by the Vienna and

Juelich teams of the Network. During the last year an efficient '*Full-Potential-Screened KKR-2000 Code*' was developed which can be applied to both three-dimensional complex lattices and supercells as well as to systems with complex two-dimensional periodicity, i.e. finite slabs, semi-infinite crystals, interfaces, two coupled halfspaces etc. This program can be used in both the ASA- and the full-potential-mode, the latter one allowing force calculations and structural optimizations. Of course, most important are the N-scaling properties achieved by the short range of the 'screened' structure constants. In addition, also the other KKR activities went on as planned. For instance the Munich efforts in constructing spin-polarised and fully relativistic Dirac KKR-codes, which now exist for bulk systems, surfaces, impurities in the bulk and at surfaces, layered systems and so on. Another strong effort has been devoted to linear response calculations within the KKR scheme, with special emphasis on spectroscopy and transport problems. Thus several groups of the Network are performing already KKR-transport calculations based on either the Kubo-Greenwood or Landauer-Büttiker formalism and are thus well prepared for the challenges of the future RT-Network '*Computational Magnetoelectronics*'.

FP-LMTO-Method **FP-LMTO-Method** In the last years the French node has concentrated its efforts in the study of the x-ray magnetic circular dichroism (XMCD) and its correlation to the magnetic properties of solids and mainly the spin and orbital magnetic moments and the magnetic anisotropy energy (MAE). XMCD is the difference in the absorption coefficients between left and right circularly polarized x-rays. Its popularity is due to the development of synchrotron radiation that allowed for high quality experiments and the development of sum rules which allow to extract from the experimental spectra the spin and orbital moments for any atom. Bruno has also developed a relation that connects the orbital moment anisotropy to the MAE for ferromagnetic systems, so XMCD is also indirectly correlated to the MAE. To investigate these phenomena, the relativistic full-potential linear muffin-tin orbital (FP-LMTO) method has been used. This latter method is capable of dealing with the non-spherical part of the potential in a crystal and it treats in the same footing all space. The method is computationally very demanding but its use is necessary to calculate with big accuracy physical quantities sensitive to approximations during calculations, like the orbital moment and the MAE. Several systems have been studied, going from the high uniaxial systems (FePt, FePd and CoPt) that present high MAE values, to systems with holes (Heusler alloys) that are potential candidates for spin-filters, and finally the case of ultra thin Fe films on top of a W(110) substrate. In all cases the correlation between the different quantities in question was found to be straightforward. Finally in collaboration with the Swedish node, the VAu₄ compound was studied and there was found evidence for the influence of ligand states (Au) on the magnetic properties of the 3d atom (V) and mainly on the orbital magnetic moment of the latter. It was shown that the large spin-orbit parameter of gold is responsible for the break-down of Hund's third rule for the vanadium atom and there was proposed a way to construct an alloy with vanishing orbital moment and MAE that could be used in applications like the AC/DC converter.

Highlight 1: The INVAR Effect- after 100 years finally understood

In 1897 the Swiss physicist Charles Edouard Guillaume discovered that fcc Fe-Ni alloys with a Ni concentration around 35 atomic % exhibit anomalously low, almost zero, thermal expansion over a considerable temperature range. This effect is now known as the Invar effect. Guillaume's discovery immediately found widespread application in the construction of calibrated, high-precision mechanical instruments,

such as seismographs and hair springs in watches. Today, Invar alloys are used in many temperature-sensitive devices, such as surveying tapes and shadow masks for television and computer screens. In 1920 Guillaume was awarded the Nobel Prize in Physics for the discovery of these Fe-Ni alloys.

The Invar effect has now been found in various ordered structures, random alloys or even in amorphous materials. Other physical properties of Invar systems, such as atomic volume, elastic modulus, heat capacity, magnetization, Curie (or Néel) temperature, also show anomalous behavior. It was realized early on that the explanation of the Invar effect is related to magnetism. Yet, though it has been 100 years since this effect was discovered, it was not understood. In a recent article published in Nature "Origin of the Invar effect in iron-nickel alloys" (**Nature 400, 46 (1999)**), I. Abrikosov and B. Johansson from Uppsala node of the Network, in collaboration with Mark van Schilfgaarde from Sandia National Laboratories, Livermore, USA, presented results of *ab initio* calculations of volume dependences of magnetic and thermodynamic properties for the most typical Invar system, a random fcc Fe-Ni Invar alloy, where they allowed for noncollinear spin alignments, i.e. where the spins may be canted with respect to the average magnetization direction. They have found that the evolution of the magnetic structure already at zero temperature is characterized principally by a continuous transition from the ferromagnetic state at high volumes to a disordered noncollinear configuration at low volumes, and that there is an additional, comparable contribution to the net magnetization from the changes in the amplitudes of the local magnetic moments. The noncollinearity gave rise to an anomalous volume dependence of the binding energy curve, and this allowed Mark van Schilfgaarde, I. Abrikosov and B. Johansson to explain the well-known peculiarities of Invar systems.

Highlight 2: A Highly Sensitive GMR-Device

The sensor devices being based on the Giant Magnetoresistivity (GMR) effect, which was discovered by the pioneering work by Peter Grünberg and Albert Fert in the late 80's, have in ten years developed into a billion dollar industry. These devices are typically consisting of artificially grown magnetic multilayers, with the main ingredient being two magnetic layers with an intermediate non-magnetic spacer layer, as for instance a Co/Cu/Co combination, where cobalt is the magnetic layer and copper the non-magnetic one. The GMR effect then utilizes the fact that the resistance is very different whether the magnetic moments of the two magnetic layers are parallel or anti-parallel. In the device the magnetic stray field of the stored magnetic bits on the magnetic hard disk flips, in case of a stored "1", the moment of one of the magnetic layers in the device which then give rise to a detectable change in the resistance through the device. It is the fact that these devices can be made very small, that has permitted the recent large improvements in storage density of magnetic hard disks.

Although the GMR effect has been very successful, there is still an ongoing strive to optimize these magnetic multilayers, both regarding efficiency and production costs. In a recent article in Nature "Non-collinear states in magnetic sensors" (**Nature 406, 280-282, (2000)**) Adrian Taga, Lars Nordström, Peter James, Börje Johansson, and Olle Eriksson, of the Uppsala node of the Network, presented results of ab-initio calculations for an asymmetric magnetic trilayer of the type Fe/V/Co. In such an asymmetric combination the local magnetic anisotropy may favor different easy axes. In the vicinity of the non-magnetic vanadium layer the iron magnetic moment prefer a direction in the plane of the layer while the moment of the cobalt prefer a perpendicular direction, out of the plane. When these moments are combined in a trilayer they will interact, through the so-called interlayer exchange coupling, resulting in

a non-collinear ordering, which depending on the vanadium thickness vary from close to collinear to almost perpendicular. These calculations suggest that by tuning the anisotropy and the interlayer exchange interaction independently, trilayers can be manufactured that are very sensitive to the stray field, which in principle may make more efficient sensor devices possible. The actual chemical composition as well as spacer layer thickness which will give the most optimized asymmetric trilayer has to be decided by future experimental studies.

Highlight 3: A Very Close Look at Magnetic Nanostructures

The invention of scanning tunneling microscopy (STM) has revolutionised our knowledge about surfaces. Suddenly being able to see the atomic structure of surfaces in all details with atomic resolution has been like making a blind man see and has lead to strong advances in fields like molecular beam epitaxy or catalysis. Yet for the magnetic structures of surfaces and ultrathin magnetic films STM has remained blind, since only the chemical structure, but not the magnetic structure, could be resolved atomistically. Thus despite many efforts, no spin-polarised STM images with atomic resolution could be obtained in the past.

In a recent article in Science "Real-space imaging of two-dimensional antiferromagnetism at the atomic scale" (**Science 288, 1805-1808 (2000)**) an experimental group at the University of Hamburg and Blügel's group of the Jülich node of our Network have demonstrated that spin-polarised STM is possible on the atomic scale and that the resulting magnetic contrast is much larger than expected. More than 10 years ago Blügel et al. had predicted by ab-initio calculations that Mn or Cr monolayers on noble metal surfaces form ideal two-dimensional antiferromagnets. However, until now these predictions remained unconfirmed, basically because the available bulk techniques like neutron scattering cannot detect such minute amounts of magnetic materials. With a spin-polarised tip the Hamburg group was now able to confirm the magnetic superstructure for an antiferromagnetic Mn-monolayer on W(110). In advance the Jülich group had calculated the expected spin polarised STM intensity and predicted an unusually strong superstructure intensity. This was indeed observed, i.e. the magnetic contrast measured with the spin-polarised Fe-tip, produced by coating a W-tip with a thin Fe-layer, suppressed the chemical contrast obtained with a non-magnetic W-tip. Blügel et al. gave a very clear explanation of the strong magnetic contrast. The measured corrugation of the STM current is determined by the Fourier components of the smallest reciprocal lattice vectors, since these components decay most slowly into the vacuum region where the tip is located. The magnetic superstructure introduces new reciprocal lattice vectors, being smaller than the ones of the chemical structure, so than the related spin-current decays more slowly than the charge current.

The availability of the spin-polarised STM offers a bright outlook for surface magnetism. It allows the direct observation of antiferro- and ferrimagnetism on surfaces, non-collinear structures, magnetism at steps, nanostructures etc. All we could only calculate in the past, will now be accessible to the experiment. A true test for theory (and the theorists)

Workshops and Conferences: After five workshops in the third and previous 12 month's period, the Network had not scheduled any official TMR-workshop for the fourth year. Nevertheless communications and cooperations continued on the, now already normal, high level which is indicated by the three TMR-Miniworkshops organized more or less spontaneously by members of the Network. A Mini-

workshop "**Tunneling Magnetoresistance**" took place on Jan. 13-14, 2000 in Orsay/Paris, which was also attended by the group of Albert Fert (Unite Mixte CNRS-Thomson) and by Peter Levy (New York University). Both will be our partners in the future RT-Network "Computational Magnetoelectronics". The Czech colleagues, being members of the Vienna Node, organized a TMR-Miniworkshop on "**Giant and Tunneling Magnetoresistance**" in Prague, April 13-14, 2000. In addition a "**KKR**" TMR-Miniworkshop was organized in Daresbury on November 17, 1999 dedicated to the recent experiences and application of the screened KKR. Our Network-member Patrick Bruno was co-organizer of the "**Symposium on Spin-Electronics**", which was held at Halle (Germany) on July 3-6, 2000. It was the first international conference of this kind, being attended by more than 300 persons. It clearly showed that the field of Magnetoelectronics is growing fast and strongly moving into semiconductor research. Twenty seven members of our Network attended the symposium, presenting 33 contributions.

As a substitute for the 4th Annual Meeting the Network co-organised the " **Ψ_k – 2000 Conference**" in Schwaebisch Gmuend, Aug 22-26, 2000. This was the second international conference only dedicated to electronic structure calculations and it was attended by 424 participants, an increase of 33% over the participation of the first Ψ_k -Conference four years ago. 80% of the participants came from EU-countries. Our Network strongly participated in the meeting, presenting in total 70 contributed talks and posters. In addition ten members of the Network gave invited talks. The TMR young researchers were exposed to a wide range of topics ranging from physics, chemistry, materials, mineralogy and even biological systems which all had in common the application of the same methodology of ab initio Density Functional Theory quantum mechanical calculations which our Network applies to the study of magnetic and electronic properties at magnetic interfaces. Our TMR young researchers had the opportunity to meet many other young researchers: 40% of the attendees were young researchers of which several came from other TMR Networks such as Psi-k. Finally, the Conference was a vibrant event from early in the morning until the late hours with excellent talks, lively discussions in or outside the lecture halls and in this atmosphere our Network was playing a prominent role and was well noticed. A detailed account of the Ψ_k -Conference and reports on the three Miniworkshops and on the "**Symposium on Spin-Electronics**" can be found in the Appendix 1.

Ψ_k -Newsletter etc: The Network publishes the announcements of workshops and vacant positions in its dedicated section in the **Ψ_k -Newsletter** which is published every two months and which is distributed to over more than 800 e-mail addresses worldwide, of which most are in Europe. This Newsletter is also used to disseminate abstracts of our scientific papers to the community concerned with electronic structure computations of solids and as a consequence has led to the high profile of our Network in the electronic structure community. In this respect, it is rather disheartening that the small contribution that the Daresbury node charges for the publication and dissemination of this Newsletter by e-mail and on the web is according to the Brussels appointed auditors not an allowed Networking cost. This is in flagrant contradiction with the contract which allows the costs of the Newsletter to be charged.

The Network has a home page on the psi-k www-server:

(<http://psi-k.dl.ac.uk/TMR1/default.html>),

where also all the Newsletters can be found:

(<http://psi-k.dl.ac.uk/psi-k/newsletters.html>).

The web page of the general Psi-k Network which includes pointers to our Network was recently redesigned (<http://psi-k.dl.ac.uk>).

The Philips cost statements have been consistently very low. The main reason for this is not a lack of activity of the Dutch node. On the contrary, Philips has been one of the main movers and shakers of this Network in the direction of transport studies. However Philips has not been charging the full costs of the TMR young researcher to the Network. This unexpected windfall is now being redistributed over all the nodes of the Network giving rise to a very healthy budget for all the nodes for our fifth and final year.

At end of the fourth year, the regular lifetime of the Network, we are proud about the performance and successes of our Network. We have achieved a high scientific level with many publications in the most prestigious journals. We have established many successful collaborations in the Network, resulting alone in the last year in a staggering number of 24 joint publications(see Appendix 3). We could meet all milestones and deliver in total 367 man months of training, 31 more than promised in the contract. Our Network as a whole had a strong impact on the field of surface and interface magnetism and is unique worldwide. Recently the EU has approved our application for an extension of the Network by one year without additional funding. Our proposal for a Research Training Network "Computational Magnetoelectronics" within the V. Framework has also been approved and this new and exciting Network will start at Oct. 1, 2000.

3.2 Reports on Visits to Conferences/Workshops

Report on a Conference Participation:

16th ICMFS (International Conference on Magnetic Films and Surfaces), Natal, August, 13-18, 2000

The ICMFS meeting was attended by about 130 people from Europe, Japan, Latin America and the USA. The conference was very exciting and gave a representative aspect of the international activities in Nanoscale Magnetism. In a lively atmosphere numerous exchanges have strengthened the cohesion of this community.

Let us here shortly sketch some highlights: the mesoscopic magnets elaborated by self-organization (J. Kirschner), the last developments in the micromagnetism approach (J. Miltat), the magnetoresistance in ballistic and nonballistic nanocontacts (N. Garcia), the magnetization reversal by spin injection (A. Fert), the irradiation-fabricated nanostructures (T. Devolder), the single electron tunneling in granular system (S. Mitani), and the hot-electron spin-transport (R. Jansen).

Activities of the TMR network "Interface Magnetism" have also been presented: Magnetic anisotropy properties of VAu₄ (Strasbourg-Uppsala collaboration), Influence of the interdiffusion at the Fe/Cr (Strasbourg-Vienna collaboration) and XMCD properties of different alloys.

Hugues Dreyssé

4 News from the Research Training Network (RTN)

COMPUTATIONAL MAGNETOELECTRONICS

4.1 Young Researcher Positions

**Daresbury - Bristol - Juelich - Muenchen - Halle - Paris - Vienna - Twente - Uppsala -
Brno - Budapest - New York**

We have positions for several Young Researchers to work on an EU funded Network to model, understand and predict the electronic, magnetic and transport properties of materials and material systems relevant to magnetoelectronics. These positions have been available from 1st October 2000.

The scientific projects are:

- **Ferromagnet/ Semiconductor Interface.** For more detail please contact Susanne Mirbt (susanne@fysik.uu.se)
- **Ferromagnet/ Oxide Interface.** For more detail please contact Patrick Bruno (bruno@mpihalle.de)
- **Ferromagnet/ Superconductor Interface,** post-doc position already filled. Contact Balazs Gyorffy (b.gyorffy@bristol.ac.uk).
- **Magnetic Nanostructures.** For more detail please contact Laszlo Szunyogh (szunyogh@dirac.phy.bme.hu)
- **Magneto optics.** For more detail please contact Mebarek Alouani (mea@Taranis.u-strasbg.fr)
- **Magnetic X-ray Scattering.** For more detail please contact Walter Temmerman (w.m.temmerman@dl.ac.uk)
- **Giant Magnetoresistance.** For more detail please contact Peter Weinberger (pw@cms.tuwien.ac.at)
- **Tunneling Magnetoresistance.** For more detail please contact Peter Dederichs (l.gerken@fz-juelich.de)
- **Spin Mesoscopics.** For more detail please contact Paul Kelly (p.j.kelly@tn.utwente.nl)
- **Experiment.** For more detail please contact Albert Fert (fert@lps.u-psud.fr)

A copy of the proposal including the scientific projects can be found on
<http://psi-k.dl.ac.uk/Magnetoelectronics/default.html>.

The Network actively encourages the application of female researchers. Nine senior researchers in the Network are female.

If you wish to find out more detail please contact Walter Temmerman (w.m.temmerman@dl.ac.uk) or Peter Dederichs (l.gerken@fz-juelich.de).

The EC Rules for Young Researchers are that the Researcher must be:

1. aged 35 years or less at the time of appointment by a participant. An allowance to this age limit may be made for the actual time spent in compulsory military or civil service or child care (a maximum of two years per child for the actual time spent off work);
2. a holder of a doctoral degree or enrol on a Ph.D. course;
3. a national of a Member State of the Community or of an Associated State or have resided in the Community for at least five years prior to appointment by a participant in the frame of this contract;

and must not be:

1. a national of the state in which the participant's research appointing team is located and must not have carried out their normal activities in that state for more than 12 of the 24 months prior to appointment.

Details of the those countries which are defined as "Associated States" (such as Bulgaria, Czech Republic, Estonia, Hungary, Latvia, Lithuania, Poland, Romania, Slovakia, Slovenia) may be found at:

<http://www.cordis.lu/fp5/src/3rdcountries.htm>

5 News from the TMR2 Network

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

5.1 Workshop Announcements

5.1.1 Workshop on Noncollinear Magnetism

Joint ESF/TMR workshop on **NONCOLLINEAR MAGNETISM**

Wien, March 8-10,2001

**Organized by the Institut für Materialphysik, Universität Wien and the Center for
Computational Materials Science, Wien**

J. Hafner, R. Lorenz, D. Spišák, T. Branis

Objective: The objective of the meeting is to review the status of first-principles approaches to non-collinear magnetism, discussion of the current implementation of noncollinear capabilities in the major electronic structure codes and perspectives for achieving an ab-initio treatment of spin-dynamics. Applications to intermetallic compounds, disordered crystalline and amorphous alloys, thin films and multilayers will be discussed.

Format:

A small meeting with about 30 participants, recruited mainly from the participants of the TMR2 network and the ESF- Ψ_k community. There will be review talks, short presentations and ample time for discussion, including short (one overhead) contributions to specific topics.

Invited participants : I. Abrikosov (Uppsala), G. Bihlmayer (Jülich), S. Blügel (Jülich), P. Bruno (Halle), H. Dreyssé (Strasbourg), H. Ebert (München), H. Eschrig (Dresden), M. Fähnle (Stuttgart), M. Freyss (Jülich), B. Györffy (Bristol), G. Kresse (Wien), J. Kübler (Darmstadt), J. Kudrnovsky (Praha), I. Mertig (Dresden), L. Nordström (Uppsala), P. Oppeneer (Dresden), A. Pasquarello (Lau-

sanne), L. Sandratskii (Darmstadt), D. Singh (Washington), J. Staunton (Warwick), A. Svane (Aarhus), L. Szunyogh (Budapest), W. Temmerman (Daresbury), I. Turek (Brno), P. Weinberger (Wien).

The list of participants should be completed by students and younger scientist to be nominated by their group leaders.

Funding:

ESF- Ψ_k Network

TMR2-Network "Electronic structure calculations"

Center for Computational Materials Science (CMS), Wien

Institut fuer Materialphysik (IMP), Univ. Wien

Persons interested in attending the workshop should contact via email the workshop secretary (Tina Branis, email: tina.branis@univie.ac.at). Abstracts of contributions should also be sent via email (preferably in LATEX format, max. one page) to the same address.

6 News from the ESF Programme

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

6.1 Reports on Workshops/Conferences

6.1.1 Report on MML2000 Workshop

MML2000

International Workshop on Materials Modelling

**18-20 September 2000
Oxford, United Kingdom**

Conference Organisers:

Prof. D. G. Pettifor, FRS (Oxford), Prof. A. P. Sutton (Oxford)

Dr. R. E. Rudd (LLNL), Dr. S. D. Kenny (Oxford)

Web Site:

<http://users.ox.ac.uk/~mml2000>

Conference Sponsors:

Psi-k Network (ESF), ONR-IFO, EOARD, ARL-ERO, SIMU

Abstract:

The International Workshop on Materials Modelling: Applications in Materials Processing (MML2000) was held in Oxford, UK, on 18-20 September 2000. The workshop centered on 4 keynote talks and an additional 9 invited talks. These were given by experts in computer modelling of polymers, surfaces and metal processing who have addressed the issue of the multiple scales inherent in these systems. The workshop focused on materials modelling over a range of physical scales: electronic to atomistic to microstructural to macroscopic. The talks were pedagogical in style, making them well-suited for the diverse audience of graduate students and more senior scientists from a variety of fields. The informal atmosphere of the workshop and the outstanding talks on this cutting-edge topic made MML2000 a great success.

Comprehensive Report:

On 18-20 September 2000 a workshop was held in Oxford, UK, on the computer modelling of materials and materials processing, "The International Workshop on Materials Modelling: Applications in Materials Processing (MML2000)." According to the workshop announcement, "The focus of the workshop will be materials modelling over a range of physical scales: electronic to atomistic to microstructural

to macroscopic. The workshop will be divided into applications of multiscale modelling to polymers, to surfaces and interfaces and to metal processing. Quite a range of state-of-the-art materials modelling will be covered, but the talks will be given at a level accessible to non-experts and young scientists.” The format of the workshop proved to be very effective. In all 13 invited talks were given, each lasting 75 minutes. This gave the speakers time to give background material, before launching into their own research. This was particularly crucial due to the multidisciplinary nature of the workshop. It allowed polymer experts to get up to speed on metal processing, and vice-versa. The invited speakers were Pettifor (Oxford), Windle (Cambridge), Kremer (Max-Planck), Theodorou (Patras), Paul (Mainz), Gilmer (Bell Labs-Lucent), Willis (Cambridge), Rudd (LLNL), Gyure (HRL), Farrugia (CORUS), Evans (Swansea), Phillips (Brown) and Grant (Oxford). There were no contributed talks beyond the invited talks, but there was a poster session in which most of the participants gave presentations. In addition to the scientific programme, participants in the workshop also had the opportunity to discuss their work in an informal setting over the conference meals and banquet in the college and during the tour of Oxford University on Sunday afternoon before the start of the workshop. The focus of MML2000 on multiscale techniques is very timely. This is one of the key issues in materials modeling which is being faced at universities, national laboratories, industrial research facilities and indeed throughout the materials community. There are many length and time scales that are relevant to materials systems, ranging from the Angstrom scale where the physics and chemistry of electronic bonding resides, to the nanoscale where the next generation of electronic, electro-optical and even electro-mechanical devices must be fabricated and where polymer and liquid crystal molecules reside, to the many intermediate scales or mesoscales at which metallic microstructures develop and protein folding takes place, to the continuum where materials exhibit their macroscopic properties. It has long been appreciated that phenomena at each scale are based on the physics of the smaller scales, and it has been a major goal to understand exactly how this occurs—in particular, whether it is possible to start with an ab initio model of chemical bonding and produce a complete understanding of the materials physics at larger scales. Of course, even now we are very far from this goal, and without the recent boom in computer power, the situation would have been nearly intractable. The broad array of results in many subfields presented at the MML2000 workshop may be summarized in two sweeping statements. Firstly, the advent of fast computers including supercomputers has revolutionized the theoretical basis of materials science and great progress has been made in making the link between the microscopic and macroscopic physics. Secondly, the further increase in speed in computers in the next decade will have relatively little impact on the field. The first statement is fairly orthodox at this point, but the second is not. Nevertheless, the point was first raised by Windle, and echoed throughout the workshop. Indeed, it seemed to be the consensus among a group of the leading practitioners of computational materials science from around the world, that while fast computers have opened the door to new avenues of theoretical research, computer speed alone will not advance the field significantly further. That is not to say that faster computers are not wanted, rather that they will not have the qualitative impact that has been seen in the past two decades. Now we need better algorithms, more powerful methodologies and in general more incisive insight in order to bridge the gap between the scales and achieve truly predictive models. This has been seen across the broad range of modeling presented at the workshop. In the keynote talks, Pettifor emphasized the need to simplify models as much as possible, but no more. His work has made analytic connections between the efficient interatomic potentials and the quantum mechanical models that underpin them in a way that reproduces BCC structural stability at fourth order and distinguishes FCC and HCP structures at sixth order. Windle emphasized

the need for new approaches to polymer modelling that are necessary to treat the vast array of polymer and liquid crystal systems. Gilmer described models that have been developed for surface science associated with the semiconductor industry, and Farrugia related the efforts to develop models across the scales to describe the processing of steel. In the focussed sessions, the polymer modelers Kremer, Paul and Theodorou spoke of the barrier to direct simulation of polymers systems imposed by the time scale during which large polymers deform. This has begun to be addressed through techniques which start at the scale of individual atoms, link the atoms into clusters governed by effective potentials, evolve the coarse-grained system and then use a relaxation procedure to refine back to the atomic scale. Such techniques would be very powerful in general, but they are still in their infancy. The surface modelers, Gilmer, Rudd and Gyure, described coarsening phenomena in which self-assembled structures appear at the nanoscale governed by surface energies and bulk elastic energies that are essentially determined at the atomic scale. In one of those coincidences that serve to highlight the multidisciplinary aspect of multiscale modeling, level set methods were used to solve the same problem in two systems separated not only by the type of material but by 7 orders of magnitude in the size! Gilmer presented a level set model of deposition of material in the microscopic interconnects on computer chips, while Grant presented an almost identical model to describe the deposition of material in a spray-formed steel ingot several meters in length. The shadowing instability due, as Gilmer showed, to the microscopic granularity of the material was an essential part of both systems. In another link both Phillips and Rudd addressed the question of how material plasticity is governed by the nucleation and dynamics of dislocations. In both cases the key question involved how the mesoscopic physics emerged out of the underlying atomistic interactions. New techniques were presented that made this link more apparent. This in turn leads to a new understanding of phenomena like scab formation on the surface of deformed metals, a process that was described at two vastly different time and length scales by Farrugia and Rudd. This connection was echoed in somewhat different terms by Willis. He has used analytic methods to extract continuum physics of elastic deformation about crystal defects from microscopic lattice models. In all, the workshop was most successful at bringing out these themes common throughout what outwardly appear to be very different fields of study. From the Angstrom scale of Pettifor's electronic models to the meter scale and beyond discussed by Farrugia, Evans and Grant, the challenge in building models has been to balance the accuracy necessary to get meaningful results with the efficiency required to be able to carry out the computer simulation. Already many important insights have been gleaned and many models are available, but clearly this is just the beginning. The hope is that the advances made in one field may be transplanted into another, with the same great benefits. Workshops such as MML2000 are an excellent way to help make this happen.

MML2000 Conference Participant List:

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MML2000 Speaker List:

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6.1.2 Report on CECAM Meeting

“Future developments in the study of structure-property relations by computational crystallography and experiments”

This workshop (held in Lyon at CECAM, from October 23 to 27, 2000) was planned in order to provide the opportunity to discuss recent advances in theoretical and experimental approaches of interest to crystallographers. It was intended to continue the sequence of workshops on similar topics funded by CECAM (1997) and the ESF (1998). The present workshop would not have been possible without the generous funding provided by CECAM and ESF, the latter coming from the STRUC Psik program.

The format of the workshop was a small and extremely informal meeting (about 20 participants), in the approximate ratio theory/experiment=1/1. All speakers were given a one hour slot, and all participants made extended presentations of their research. Long discussions of points of interest were a typical feature of each presentation. There was also ample time for even less formal discussions during the breaks. An interesting (and unusual) feature of the workshop was the publication of a book of extended abstracts before the workshop. This really helped participants to get up to speed with everyone's recent research.

Huge progress has been made in the last few years with respect to the modelling of structures and properties of complex inorganic structures. Examples that were discussed during the workshop include the calculation of phonon dispersion curves, NMR chemical shifts, compression mechanisms, solid state and surface reactions, optical properties, etc. Similarly, significant progress has been made in the experimental determination of structures and their properties, for example, by using synchrotron radiation from a 3rd generation source in combination with position-sensitive detectors and modern diamond anvil cells for very high pressure studies. The main motivation for the workshop was to assess the current state-of-the-art since we need to understand the capabilities and limitations of both theoretical and experimental approaches. This is an important consideration when interpreting experimental results, validating a theory by comparing with experimental data, or predicting outcomes of experiments that are difficult to perform. We therefore hope that the contributions to the workshop advanced the mutual understanding of theoreticians, code developers, users of quantum-mechanical programs, and experimentalists, and also provided an outlook of progress to be expected in the next few years.

The organisation of the workshop was an activity of the 'Computational crystallography' group of the German Crystallographic Society, DGK. The proceedings of the meeting are already available in the series 'Berichte aus Arbeitskreisen' published by the DGK (vol. 10; contact Prof. Dr. H. Küppers, Mineralogisches Institut, Univ. Kiel, D-24098 Kiel, Germany). We are all enormously grateful to Karsten Knorr, one of the organisers of the meeting, for all the efforts that made this publication possible, and to the DGK for an amazingly speedy response.

The meeting's web page:

<http://www.min.uni-kiel.de/kristallographie/cecam2000/>

gives the information about the workshop program and a list of participants. It is gratifying to note that even after a number of last minute cancellations the meeting had a truly international and interdisciplinary character.

The organisers would like to thank again the host organisation, CECAM, in particular Michel Mareschal and Emmanuelle Crespeau for their competent, efficient, and friendly help. I think it is fair to say that the meeting was successful and enjoyable for participants. A brief description of the contributions follows.

Various aspects of lattice dynamics studies were discussed by Markus Braden (KFZ, Germany and LLB, France) and Stefano de Gironcoli (SISSA, Italy). Markus Braden described recent advances in lattice dynamics measurements at high pressure. For a long time the maximum attainable pressure for neutron scattering experiments was 2-3 GPa, the main limitation being the sample volume needed for reliable phonon measurements. Recent advances in spectrometer and high-pressure cell design allow the limit to be pushed to 10-12 GPa. This opens the way for the search for soft phonon modes in pressure-induced phase transitions, to measure mode Gruneisen parameters (and thus infer a number of thermodynamical properties), and to study pressure dependence of magnetic excitations. Particular results that were presented include the phonon dispersion of Ge up to 10 GPa, phonon and magnon spectra of iron up to 10 GPa (the first ever study of any magnetic excitation under high pressure), etc. It is rather reassuring that existing ab initio predictions of the mode Gruneisen parameter in germanium agree extremely well with the latest reported measurements.

Stefano de Gironcoli presented a review of the developments in the area of density functional perturbation theory followed by an impressive results on geophysical applications with the main emphasis on thermoelasticity of minerals (MgO and perovskite MgSiO_3). Ab initio study of elastic constants at high temperature and pressure is now sufficiently accurate that the results of ab initio calculations can be reliably used to make conclusions on applicability of various phenomenological models of the Earth's core, for example.

A number of contributors addressed issues related to electronic transitions and optical properties. Eugene Krasovski (Kiel, Germany) gave an overview of the all-electron methods used to calculate optical properties of crystals within DFT. The experimental viewpoint was presented by Michael Andrus (Vienna, Austria) who gave an excellent introduction to state-of-the-art in infrared and optical absorption spectroscopy of minerals. Michael also described in detail the status of the semiempirical crystal field theory in geosciences. Petra Becker (Cologne, Germany) presented a field of materials for nonlinear optics. Attempts to rationally design new NLO materials are still quite rare, and modelling can help to advance the case of devising a new material that satisfies a number of imposed constraints and has desired nonlinear optical properties. Petra's examples of the recent work on a variety of promising materials (e.g., potassium rare-earth nitrates, bismuth triborate, potassium niobium triborate, alkaline-metal niobium borates) showed just how difficult the quest for an industrially-acceptable NLO material can be.

A large body of discussion was centered around a relatively new field of NMR chemical shifts as an analytical tool in solid state studies. Ian Farnan (Cambridge, UK) introduced the experimental field using ^{17}O studies of silicates as an example. One particular area of interest here is the application of NMR to study element-specific dynamics on a diffusive time scale. These temperature-dependent spectra can

become a very good test of molecular dynamics simulations in oxides.

Theoretical developments in the field of NMR calculations were presented in two separate talks by Francesco Mauri (Paris, France) and Chris Pickard (Cambridge, UK). Francesco Mauri introduced the method, which is based on density functional perturbation theory, and presented a number of new results relevant to studies of silicates. The most recent work on disorder in amorphous silica gives a hold on such fine structural details as Si-O-Si angular distribution based on the existing experimental NMR data. Chris Pickard continued the subject by investigating at greater depth the approximations that are made in the theoretical studies, and also by making connections with the NMR methods commonly used in quantum chemistry when studying nonperiodic systems. His set of examples included a number of medium-sized molecular complexes where NMR information is crucial for determining, for example, molecular conformations of porphyrins.

A session on high pressure studies was opened by Michael Hanfland (Grenoble, France) who presented a number of recent high-pressure studies carried out at the European Synchrotron Radiation Facility (ESRF). His examples included the study of phase transitions in solid molecular nitrogen where orientational ordering accompanies the structural changes; pairing of lithium atoms in metallic lithium under compression; and the structural properties of LaFeO₃ under pressure. The theoretical part of the high pressure discussions was presented by Bjoern Winkler (Kiel, Germany) in his opening notes and later by Victor Milman (Cambridge, UK). Bjoern Winkler presented the latest results of the DFT study of a mixed valence compound, CsAuCl₃, under pressure. DFT calculations for this system reproduce with great accuracy the 'signature' feature of the structure - the change from Au(I)Au(III) electronic configuration to Au(II) which is seen as a creation of a cubic structure with no charge ordering. This finding is encouraging for DFT practitioners in view of recent comments on the necessity of SIC corrections to reproduce mixed-valence compounds correctly. It appears that a straightforward DFT application is sufficiently accurate to describe the structural properties. Further examples of compression studies given by Victor Milman included a recent systematic study of the compressibility of cubic garnets and the study of the phase stability and compression of klockmannite, CuSe. The conclusion is that the DFT results are exceptionally reliable for a large number of compounds and that the bulk modulus is reproduced with an accuracy which is typically better than 10%.

A large section of the workshop was broadly classified as "Structure and Properties". Michele Catti (Milan, Italy) presented recent results on LCAO-HF calculations for silica polymorphs as compared to numerous DFT studies. The main practical conclusion of the long discussion that followed was that the need for analytically calculated gradients in the CRYSTAL code is very strong. Another direction of the discussion was towards clarifying the relative accuracy of LDA and GGA approaches in oxides and related systems. The current situation where GGA is more accurate for some systems and LDA for others, makes systematic studies very difficult.

Julian Gale (London, UK) presented a complete study of crystallisation problems relevant to the aluminium production process. This gave a very clear picture of a complex computational experiment that involves an ab initio study of a number of solid state phases of Al(OH)₃, and also a study of a number of molecular reactions in solvents, followed by an ab initio MD simulation of a Bayer liquor.

Marek Hytha (Kiel, Germany) presented a rarely used computational method that involves adaptive self-consistent pseudopotentials. The basic theory is very straightforward; the only difference with respect to standard pseudopotential DFT implementations is that the pseudopotentials are recalculated with the

boundary conditions that are appropriate for a given crystal rather than with the free atom boundary conditions. The resultant scheme preserves the advantages of the pseudopotential method, while giving access to a number of properties like core-level shifts that are not easily available in the standard pseudopotential approaches. The reliability of the scheme was illustrated by a number of examples including layered compounds and silicon (100) surface.

Nicolas Lorente (Toulouse, France) presented theoretical results that shed light on the recent experimental findings from inelastic electron tunneling spectroscopy of molecular adsorbates on metallic surfaces. Ab initio calculations followed by symmetry analysis allow one to interpret experimental results in terms of the vibrational properties of adsorbed species.

A very welcome contribution from Jurgen Schreuer (Zurich, Switzerland) gave a thorough introduction to the world of experimental measurement of elastic constants. A clear and logical description of various techniques was extremely helpful to anyone interested in evaluating the reliability of published experimental data. A subsequent discussion of the recent experimental work on temperature dependence of elastic constants near the phase transition was very interesting.

Karsten Knorr presented a scheme for reconstruction and interpretation of density distributions. It is based on optimal geometric embedding of the fragments into density distributions resulting from maximum entropy reconstructions. A number of examples showed convincingly that a rich variety of structural information can thus be extracted from diffraction data. One of the most impressive cases involves a qualitative representation of a dynamic disorder in the system.

A discussion of various aspects of structure and electronic properties of titanium dichalcogenides was given by Andrei Postnikov (Duisburg, Germany). FLAPW calculations were used to study perfect and doped structures and to relate changes in crystal and electronic structures with the experimental data on transport properties.

Georg Thimm (Singapore) caused a lot of interest in the audience by his talk on topology of crystal structures. The bottom line of the method is that one can generate in a systematic way full sets of all possible structures with given topological constraints. This approach is increasingly used in crystallography for a number of reasons. Firstly, recent experimental findings of various new forms of well-known materials (e.g., carbon) suggest that even more polymorphs might be synthesised, and it is challenging to be able to predict where to look for them. Secondly, computational methods are now sufficiently advanced to be able to process the output of the graph theory methods and end up only with physically viable structures.

The thermodynamics of disorder in minerals was presented by Michele Warren (Manchester, UK). A variety of methods were used, ranging from ab initio simulations on 20-100 atoms to Monte Carlo studies of tens of thousands of cations. The conclusion is that the combination of techniques of different levels of sophistication is capable of describing order-disorder transitions quite accurately.

Björn Winkler, Karsten Knorr, Chris Pickard, Victor Milman
(November 2000)

6.1.3 Report on CMS2000

CMS2000 - 10th Computational Materials Science Workshop Villasimius, Sardinia, Italy, 7-12 September 2000

The tenth edition of the Computational Materials Science Workshop (CMS2000) has been held successfully in Villasimius, Sardinia, Italy on 7 to 12 September 2000. The workshop has been funded by the European Union under the *High-Level Scientific Conferences* programme, by the European Science Foundation under the program *Electronic structure calculations for elucidating the complex atomistic behaviour of solids and surfaces*, by the University of Cagliari, and the National Institute for the Physics of Matter.

A total of 89 participants took part in the event. Almost all of them (96%) were scientists active in EU countries or associated states. The number of participants (of any nationality) active in the various represented countries was as follows: Italy 31; Germany 17; U.K. 7; France 7; Sweden 5; Switzerland 4; Brasil 4; Finland 3; Belgium 3; Spain 3; Netherlands 2; Austria 1; Czekia 1; Ukraine 1, USA 1. The pleasant environment and reasonably good weather helped the integration among participants.

The scientific activities consisted of 8 oral sessions comprising 20 invited lectures (1 hours each), and of two distinct poster sessions, comprising 30 posters each. The (one-hour or three-hour) invited lectures were centered on both basic issues and applications of ab initio methods, prevailingly density-functional based. *A. Baldereschi* (EPF Lausanne, Switzerland) discussed recent advances in the understanding of electronic structure of adsorbates on metals. *S. Baroni*, (SISSA Trieste, Italy) reviewed the very successful linear response theory of dielectric and dynamical properties of solids, and a novel ab initio theory of magnons. *S. Fahy* (Cork University, Ireland) gave a compelling review of the present state of the art in Quantum MonteCarlo. *R. O. Jones* (KFK Jlich, Germany) addressed in detail the limits of different DFT exchange-correlation functionals in his talks on clusters, polymers and anomalous-thermal-expansion materials. *M. Parrinello* (MPI-FF Stuttgart, Germany) covered the recent work of his group on Ziegler-Natta catalysis and NMR shifts in organics. *R. Resta* (Università di Trieste, Italy) reinterpreted his own seminal work on dielectric polarization in the light of the generalized position operator, and presented applications to electronic localization in dielectrics. *M. Scheffler* (Fritz-Haber-Institut Berlin, Germany) covered several topics relevant to the growth of semiconductor nanostructures and catalytic activity on metal surfaces. Finally, two experimental talks completed the picture: *O. Ambacher* (WSI-TU Munich, Germany) reviewed very recent experimental evidences and effects of macroscopic polarization effects in nitride nanostructures, and *J. Frenken* (Leiden University, The Netherlands) discussed an intriguing case of in-surface diffusion mediated by vacancies, and the exciting prospects of nanotribology with the STM.

Last-minute changes to the oral invited program were fairly substantial. Quite unfortunately, A. Zunger (NREL) had to cancel his participation a week before the event. Even more regrettably, U. Landman (Georgia Tech) simply did not show up at the conference. M. Parrinello kindly agreed to cover part of

the time thus freed up.

The poster sessions collected about 60 distinct original contributions from participants. The titles of the contributions are collected on the web site of the conference, <http://www.dsf.unica.it/CMS2000>. Papers related to both contributed and invited talks will be published in a special issue of Computational Materials Science in 2001.

6.2 Workshop/Conference Announcements

6.2.1 EUROPEAN WINTER SCHOOL

**STATE OF THE ART SIMULATIONS
IN ELECTRONIC STRUCTURE AND TOTAL ENERGY
FOR SURFACE SCIENCE
Institut d'Etudes Scientifiques de Cargèse**

Cargèse, Corsica, France
February 19th - March 3rd 2001

PURPOSE

The aim of this school is to present the state of the art in electronic structure and total energy calculations in view of their applications to the physics of solid surfaces. The theoretical methods which will be treated will extend from *ab-initio* methods to empirical potentials. In each case their field of applications and their limitations will be discussed. Many practical examples will be given dealing with metal, semiconductor as well as oxyde surfaces. In addition, a number of lectures will be devoted to experimental techniques (photoemission, STM, magnetic dichroism...) the interpretation of which relies on these theoretical methods. The scheduled lectures will be organized into six main subjects:

- 1. Electronic structure: Methods**
- 2. Electronic structure: Applications and Experiments**
- 3. Empirical potentials and applications**
- 4. Surface Magnetism**
- 5. Excitations at surfaces**
- 6. Physisorption and Chemisorption**

The school is mainly intended for PhD students, post-docs and young researchers in the field and both for theoreticians and experimentalists.

MAIN ORGANIZERS:

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38054 Grenoble Cédex 9 , France

VENUE

The school will be held at the "Institut d'Etudes Scientifiques de Cargèse" which is affiliated to the Centre National de la Recherche Scientifique and the Universities of Corsica and Nice-Sophia-Antipolis. Cargèse is a small village of Corsica (France), it is located at the seaside, 50kms from Ajaccio on the west coast.

More information can be found at the Institute web-site:

<http://cargese.univ-corse.fr>

SCHEDEULE AND OTHER DETAILS

The programme will be organized in nine working days during which there will be four lectures (1H30

each, including 15' for discussions). Poster sessions are planned to enable the participants to present the results (also preliminary) of their current research.

Participants from any european country are invited. However the number of participants is limited to 60. The fees including registration, lodging and lunches should not exceed 750 Euros but may be lower depending on the funds collected by the organizers. A substantial reduction of these fees will be granted to PhD students. All necessary information on the school is available and will be continuously updated at the web-site:

http://www-drfmc.cea.fr/SP2M/L_Sim/Congres/Corse_2001/cargese.html

The interested persons are asked to visit this web-site in order to find a complete list of lecturers and titles of lectures, as well as a preregistration form to be sent as soon as possible.

6.2.2 2001 E-MRS Spring Meeting

**Symposium A – 2001 E-MRS Spring Meeting:
"Computational Materials Science Across Time and Length Scales ".
Strasbourg (France) June 5-8, 2001**

MOTIVATION

Processes and structures in materials science might easily involve variables that span ten or more orders of magnitude in time and space. Clearly, a detailed description of the overall phenomenon at the smallest level of resolution is out of the question and therefore schemes must be developed that allow for a seamless integration across the relevant scales. Thus, atomistic first-principles calculations may have to be matched with classical molecular dynamics simulations, which may in turn have to be joined onto a continuum description. Likewise, acceleration techniques must be developed to cross the gap in time-scales. Both problems benefit from the sustained upward trends in computer speed and memory, but they also necessitate the development of new algorithmic tools. Recent years have seen much activity in this area and it is the aim of this symposium to bring together researchers working on these multi-resolution, multi-scale methods, to review progress, to address common concerns, and to integrate the findings with experimental techniques.

SCOPE

Papers are solicited that fall in the general subject matter of the symposium, with specific attention to the following areas:

1. mechanical properties, including fracture, fatigue, lattice mismatch, defect structures, dislocations, etc.;
2. growth and evolution of surfaces, thin films, and interfaces;
3. semiconductor structures, from the atomic to the device level.

Papers announcing new methodologies are also within the scope of the symposium as long as they are applied to real materials problems.

Financial support through the ESF programme ψ_k is possible, especially for young scientists. Request should be sent to H. Dreyssé by e-mail (hugues@lugh.u-strasbg.fr) with the abstract and the following informations

Name:

Position:

Full address:

For PhD student please add a letter from your thesis supervisor

DEADLINE FOR ABSTRACT SUBMISSION: January 10, 2001 !!!!

Form for abstract and all informations are available at:

E-MRS 2001 Spring Meeting

BP 20

67037 Strasbourg Cedex 2, France

e-mail: emrs@phase.c-strasbourg.fr

<http://www-emrs.c-strasbourg.fr>

Abstract should also be sent to this same address **before jan. 10, 2001**

ORGANIZERS:

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6.2.3 Workshop in Exeter

DOPING ISSUES IN WIDE BAND-GAP SEMICONDUCTORS

Exeter, United Kingdom

21-23 March 2001

<http://newton.ex.ac.uk/widegap2001/>

Supported by the European Science Foundation through the Psi-k network.

The aim of the workshop is to bring together experimentalists—interested in optimising and characterising the electrical activity of dopants in wide band-gap materials—and theoreticians who carry out calculations in this area. The workshop will focus mainly on defects and impurities in GaN, SiC, and diamond.

There is a great deal of interest in overcoming problems relating to shallow dopants in these materials. For example, boron is a shallow acceptor in diamond but there are problems relating to shallow donors. Phosphorus and sulphur are key candidates at the moment and there is intense interest in optimising their activity.

In GaN, oxygen and silicon are known to be shallow donors but there are difficulties in finding efficient shallow p-type dopants - Mg and Be are favoured but have low activities. In SiC, nitrogen and boron on the Si site are the best donors available. Nevertheless all these dopants suffer problems relating to solubility and the formation of complexes.

Experimentalists are well aware that ab initio modelling is a very effective way in which dopant activity can be predicted. It is significant that the oxygen donor in GaN was first suggested from ab initio theoretical results.

There is current interest in co-doping where the electrical activity can be increased when two or more impurities (sometimes both donors and acceptors) are involved and this will be one of the topics at the workshop. Other topics will involve growth and characterisation.

This workshop will feature extended invited talks, contributed talks, and poster sessions. Ample time for informal discussions will also be provided. Proceedings will be published in a special issue of Journal of Physics: Condensed Matter. The workshop venue will be the campus of the University of Exeter, in the south-west of England. Accommodation will be provided on site in the University halls of residence.

Confirmed invited speakers include:

Friedhelm Bechstedt, Universität Jena, Germany

Bernard Clerjaud, Université Pierre et Marie Curie, Paris 6, France

Peter Deak, Budapest University of Technology, Hungary
Hiroshi Katayama-Yoshida, Osaka University, Japan
Joerg Neugebauer, Fritz-Haber-Institut, Berlin-Dahlem, Germany
Risto Nieminen, Helsinki University of Technology, Finland
Bo Monemar, Linköping University, Sweden
Juergen Ristein, University of Erlangen, Germany
John Robertson, University of Cambridge, UK
Bengt Svensson, Royal Institute of Technology, Stockholm, Sweden
Kimmo Saarinen, Helsinki University of Technology, Finland
Chris Van de Walle, Xerox PARC, Palo Alto, USA
Christian Wetzel, Uniroyal Optoelectronics, USA

Contributed papers:

The call for contributions is now open. Please submit contributions via the form provided on our web site: <http://newton.ex.ac.uk/widegap2001/>. Registration is now also possible on the web site.

Please submit abstracts of your contributions by: 28 February 2001
Notification of acceptance will be before: 5 March 2001
Early registration possible until: 28 February 2001

Organisers:

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School of Physics Secretary: +44 1392 264151
University of Exeter Fax: +44 1392 264111
Exeter EX4 4QL Email: widegap2001@excc.ex.ac.uk
United Kingdom

6.2.4 International Conference on DFT

FIRST ANNOUNCEMENT
9th International Conference
on the Applications of the Density Functional Theory
in Chemistry and Physics

September, 10-14, 2001

San Lorenzo del Escorial, Madrid, SPAIN

<http://www.uam.es/dft2001>

We are pleased to announce herein the 9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics and look forward to your participation. The purpose of this Conference is to offer a forum where the recent developments in Density Functional Theory and their applications to the Chemistry and Physics of increasingly complex materials can be presented and discussed. This is the 9th in a Series of successful Conferences, and follows recent ones that took place in Paris (1995), Wien (1997) and Roma (1999).

To achieve maximal representation in this Meeting, please forward this circular to interested colleagues in and outside your institution.

SCIENTIFIC COMMITTEE:

E.J. Baerends (Amsterdam)

R. Car (Princeton)

P. Fantucci (Milano)

P. Geerlings (Brussels)

E.K. Gross (Wurzburg)

N.C. Handy (Cambridge)

S.G. Louie (Berkeley)

B.I. Lundqvist (Goteborg)

R.G. Parr (North Carolina)

D. Salahub (Ottawa)

J. Weber (Geneve)

ORGANIZING COMMITTEE:

J.A. Alonso (Universidad de Valladolid)

J.M. Garcia de la Vega (Universidad Autonoma de Madrid)

M. Moreno (Universidad de Cantabria)
P. Wahnon (Universidad Politecnica de Madrid)

LOCAL ORGANIZING COMMITTEE:

R. Lopez (Universidad Autonoma de Madrid)
B. Miguel (Universidad Autonoma de Madrid)
A. Zarzo (Univerisdad Politecnica de Madrid)

INVITED SPEAKERS:

E. Artacho (Madrid)	U. Landman (Atlanta)
V. Barone (Napoli)	D. Langreth (Rutgers)
A.D. Becke (Queen's)	P. Madden (Oxford)
E.A. Carter (Los Angeles)	J.L. Martins (Lisboa)
M.E. Casida (Montreal)	R.F. Nalewajski (Krakow)
C.A. Daul (Fribourg)	J. Perdew (Tulane)
R. Godby (York)	U. Rothlisberger (Zurich)
A. Goerling (Munchen)	A. Rubio (Valladolid)
O.V. Gritsenko (Amsterdam)	A. Savin (Paris)
E.K. Gross (Wurzburg)	M. Scheffler (Berlin)
F. Illas (Barcelona)	J. Schofield (Toronto)
W. Kohn (Santa Barbara)	M. Teter (Cornell)

This list will be expanded after confirmation of several invited speakers.

SCOPE OF THE CONFERENCE:

The Conference will be devoted to a broad and balanced overview of new results, emerging trends and perspectives pertaining to the applications of Density Functional Theory to Chemistry and Physics. The main topics covered by the Conference will be new and recent advances on: -Methodological developments. New exchange-correlation and kinetic energy functionals. Excited states.

- Computational advances. New codes.
- Isolated systems: molecules, reactivity, dynamics, small clusters.
- Condensed phases: mesoscopic systems, solids, assembled materials.
- Complex molecular systems: biomolecules, molecular materials.
- Electric and magnetic properties.

FORMAT:

The scientific Program will consist of thematic sessions where plenary talks, invited lectures and some oral contributions (selected from the submitted Abstracts) will be presented. In addition there will be poster sessions, scheduled for optimal viewing and discussion.

LOCATION:

Colegio Universitario Maria Cristina, in San Lorenzo del Escorial, 50 Km from Madrid. San Lorenzo

del Escorial is a picturesque village near the mountains of Sierra de Guadarrama, easily accesible from Madrid. It is also an important historical site, with its famous Monastery.

ACCOMODATION:

It is expected that most participants will be lodged in single rooms at the Colegio Universitario Maria Cristina and Residencia Sagrados Corazones. They provide confortable and modern installations and we have negociated very reasonable prices for full board accomodation from the evening of September 9th Sunday until 14th Friday, after lunch. No fractions of this special global package can be offered. Alternative accomodations can be found in several hotels in town.

REGISTRATION AND CONFERENCE FEES:

Details will be provided in the second circular. It is expected that the Registration will be around 50.000 Pesetas (300 euros). This would include attendance at all scientific sessions, the book of abstracts, coffee breaks, excursion and the Conference Banquet.

GRANTS:

We expect that a number of grants will be available. These grants are mainly intended for people coming from countries with short resources and for young scientists.

SPONSORSHIP:

The Conference is sponsored by:

ESF Psi-k Programme EC COST Action D9

PRE-REGISTRATION:

Pre-registration form is available on web site.

Updates and pertinent details will be placed periodically on the web site:

<http://www.uam.es/dft2001>

6.2.5 Euroconference Announcement

Electronic Structure of Solids and Surfaces

EuroConference on Computer Simulation of Complex Interfaces:

Out of the Vacuum Into the Real World

Giens, near Toulon, France, 7-12 September 2001

Chairpersons: Philip Lindan (CLRC Daresbury Lab., UK) & Claudine Noguera (Univ. Paris II, F)

Deadline for applications: April 2001

Preliminary programme and application form at:

<http://www.esf.org/euresco/01/pc01138a.htm>

6.3 Psi-k Workshops in 2001

The following 15 workshops, to take place in 2001, are being partially supported by the Psi-k ESF Programme:

1. European Winter School: State of the art simulations in electronic structure and total energy for surface science. February 19 - March 3, 2001 in Institut d'Etudes Scientifiques de Cargese (Corse), France.
http://www-drfmc.cea.fr/SP2M/L_Sim/Congres/Corse_2001/cargese.html
2. Workshop on Application of Density-Functional Theory in Physics and Biochemistry. Hands-on workshop organized by organised by Arno Schindlmayr, Peter Kratzer, Jrg Neugebauer and Matthias Scheffler. 23 July- 1 August; Fritz-Haber-Institut, Berlin.
3. Euresco Conference: Out of the Vacuum into the Real World. Organizers: Philip Lindan and Claudine Noguera. 7-12 September; Giens, France.
<http://www.esf.org/euresco/01/pc01138a.htm>
4. 2001 E-MRS Spring Meeting: "Computational Materials Science Across Time and Length Scales ". Organizers: H. Dreyssse, R. Nieminen and L.T. Wille June-5-8; Strasbourg, France.
5. Psi-K – CECAM Workshop on “Application of Ab-Initio Methods to Geophysical Problems”. Organizers: Sandro Scandolo, Francois Guyot, Francesco Mauri and G. David Price.
6. 'Physics of Magnetic Multilayers - Theory and Experiment' Prague, June 9-16, 2001.
http://195.113.32.128/EGSCM_Prague.htm
7. Oxide-metal interfaces – Progress and challenges. Jointly with CECAM. Organizer: Mike Finnis. Three days in early to mid October (Thursday, Friday, Saturday), with arrivals on Wednesday.
8. Doping Problems in Wide Band-gap Semiconductors. Easter 2001 at Exeter.
9. Density Functional Theory for the Study of Complex Oxides. Royal Institution of Great Britain, between the 14-18 of May 2001.
<http://www.ri.ac.uk/DFT2001/>
10. Biological jointly with CECAM. Organizer: Matthew Segall.
11. 9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics September, 10-14, 2001 San Lorenzo del Escorial, Madrid, SPAIN.
12. "Local orbitals and linear-scaling ab initio calculations" to be held at CECAM in 2001. Organizers: Peter Haynes, David Bowler, Emilio Artacho.
13. Non-collinear Magnetism, Organizer: Juegen Hafner. March, Vienna, Austria.

14. UK Plane-Wave Pseudopotential Tutorial Workshop. Organizers: Philip Lindan, Stewart Clark and Walter Temmerman. 5-12 December, Durham, UK.
15. The Physics of f-electron systems. Organizers: Olle Eriksson, Walter Temmerman and Axel Svane. April, Daresbury, UK.

7 General Job Announcements

Postdoctoral/Research Associate Positions

in Electronic Structure Theory

National Renewable Energy Laboratory (NREL)

<http://www.sst.nrel.gov>

NREL's Solid State Theory Group is looking to fill a postdoctoral or research associate position in the area of Electronic Structure Theory of nanostructures and alloys, as well as method development. This position is with Dr. Alex Zunger and is for 2-3 years starting July-October 2001. Applicants are expected to have a background in solid-state theory. Depending on experience and qualifications, the position could be at the rank of post-doctoral fellow (40,000–53,000 per year) or Research Associate (52,000–65,000 per year). More details about ongoing work in the group, computer facilities, personnel, publications are included in <http://www.sst.nrel.gov>. Clarification or further details can be obtained via e-mail to azunger@nrel.gov.

Interested candidates should send immediately a curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two references addressed to:

Dr. Alex Zunger
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401

The search will continue until the position is filled, but will not extend beyond 1 January 2001.

NREL is an equal opportunity employer and proud of its commitment to diversity. Women and minorities are encouraged to apply.

Postdoctoral Position
Condensed Matter Sector (INFM)
Department of Physics, University of Padua, Italy

We invite applications for a post-doc position, starting approximately between the end of 2000-beginning of 2001, in our group (Condensed Matter sector (INFM), Department of Physics at the University of Padua, Italy). The successful candidate is expected to have experience in ab initio techniques and his/her research project will mainly concern first principles applications to the study of chemisorption of organic molecules on the surface of semiconductors.

The duration of the position is 2 years and the salary will be 34,000,000 Italian Lire per annum.

For further information please contact:

P.L. Silvestrelli or F. Ancilotto
Istituto Nazionale per la Fisica della Materia and
Dipartimento di Fisica G. Galilei
Via Marzolo 8
I-35131 Padova, Italy
fax +39-049-8277102
tel. +39-049-8277170
e-mail: psil@padova.infn.it, franc@padova.infn.it

Postdoctoral and PhD Positions
Computational Design and Research of Molecules and Materials
(CDROM2)
University of Antwerp, Belgium

The CDROM2 group of the University of Antwerp, Belgium, has several positions available. The group, led by Profs. C. Van Alsenoy, V.E. Van Doren and visiting professor N.H. March (Oxford), works on the electronic and structural properties of materials and molecules by using first-principles calculations, semi-empirical and analytical techniques. We are looking for the following people :

1. A postdoc (or PhD student) to study the thermodynamical and rheological properties of amorphous polymers by means of MC/MD simulation techniques. The candidate should have experience with computer simulation techniques and a good knowledge of statistical mechanics and polymer physics.
2. A PhD student to work on the electronic and optical properties of dyes by means of ab-initio calculations and tight-binding methods. The applicant should have a good knowledge of solid state physics.
3. A postdoc or PhD student to work on the theory of new exchange-correlation potentials for the description of non-bonded interactions in polymers and biomolecules. The candidate should have a profound knowledge of condensed matter theory and /or theoretical chemistry and preferably also a good knowledge of programming.
4. A postdoc or PhD student to work on the reaction mechanism of HIV protease using quantum mechanical and molecular mechanical methods. The candidate should preferably have experience with molecular dynamics and visualization of biomolecules.

These positions are starting from January 2001. The appointment will be for four years for the PhD positions. The postdoc positions will be for two years, with a possible extension of another two years. The gross salary for the PhD-student positions is between 2200-2550 euro/month (depending on age and experience) which results after taxes, health and social insurance in a net salary of 1250-1450 euro/month. The gross income of the postdoc is within the range of 3060-3520 euro/month , resulting in a net salary of 1600-1900 euro/month, depending on age and experience.

Informal inquiries to :

Dr. D. Lamoen. Email : lamoen@ruca.ua.ac.be
tel : 32-(0)3-2180316

To apply, please forward a letter specifying for which position(s) you are applying and a full CV with the names and addresses of two referees to

Dr. D. Lamoen
Department of Physics
University of Antwerp
Groenenborgerlaan 171
B-2020 Antwerpen
Belgium

Two Junior Faculty Positions
(at the Assistant Professor level (tenure track))
Institute for Theoretical Physics
Karl-Franzens University Graz, Austria

Minimum Requirement: Graduate Degree in Physics

Desired Qualifications: Ph.D. (or equivalent) in theoretical physics; several years of demonstrated research activities (publications in scientific journals, scientific talks, etc.) in one or more of the following areas of theoretical physics: quantum-optical and mesoscopic phenomena in solids, optical properties of semiconductors, quantum transport in semiconductors, statistical mechanics and/or many-body physics in condensed matter physics; fluency in German and/or English.

In addition to the documents listed in the Merkblatt, complete applications must contain a list of publications, a short description of research interests, as well as three letters of recommendation, which must be solicited by the applicant.

For further details, see:

<http://physik.kfunigraz.ac.at/itp/aprof-ann.html>

Application Deadline: December 15, 2000 (Kennzahl: 23/49/99 or 23/50/99)

For questions consult with: walter.poetz@kfunigraz.ac.at

Applications must be mailed to:

Zentrale Verwaltung-Personalabteilung

Kennzahl: 23/49/99 or 23/50/99

Karl-Franzens Universitt Graz

Universittsplatz 5

A-8010 Graz

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e-mail: walter.poetz@kfunigraz.ac.at

homepage: <http://physik.kfunigraz.ac.at/~wap>

Post-Doctoral Fellowship

Applied Mathematics Team
Industrial Research Ltd
New Zealand

A post-doctoral fellowship in computational physics is available at Industrial Research Ltd in Wellington, New Zealand (<http://www.irl.cri.nz>). The fellow is expected to work with members of the Applied Mathematics Team and Materials Physics Team on first principles and classical molecular dynamics simulations of metal oxide surfaces and/or transparent glass ceramics. The fellowship would last for one year with the possibility of an extension for a further year. The salary is NZ\$44,000 with air-fares to and from New Zealand to be provided where appropriate. Applicants should have a PhD in either theoretical or computational physics, applied mathematics or similar field. Previous experience with computational many-body simulations is desirable.

Please contact:

Dr Shaun Hendy
IRL Applied Maths
PO Box 31-310
Lower Hutt
New Zealand
fax: 64 4 569 0003
email: s.hendy@irl.cri.nz

Two Postdoctoral Positions in Modeling of Nanostructures

**Rensselaer Polytechnic Institute
Troy, NY 12180-8554**

Interdisciplinary nanoscience research program at Rensselaer Polytechnic Institute seeks two postdoctoral candidates to work in the area of nanostructured materials modeling. Successful candidates will be a part of industrially supported experiment/theory collaborative effort on carbon-based nanostructures. One postdoctoral researcher will be focused on first principle calculations of electronic structure, bonding, and reactivity of nanoscale carbon systems. The second researcher will address larger-scale dynamical behavior of nanoscale systems with semiempirical and empirical modeling approaches, such as tight binding and/or classical molecular dynamics simulations.

Those interested should send a resume, statement of research interest, list of publications and list of references to:

Prof. Pawel Kebinski
Materials Sc. & Eng. Department
Physics Department
Phone: (518) 276 6858
FAX: (518) 276-8554
E-mail: keblip@rpi.edu
(Large scale atomistic simulations)

or

Prof. Saroj Nayak
Phone: (518) 276 2932
FAX: (518) 276-6680
E-mail: nayaks@rpi.edu
(First principle calculations)

8 Nominations for Michelson Postdoctoral Prize

**Michelson Postdoctoral Prize Lectureship
Department of Physics
Case Western Reserve University
Cleveland, Ohio**

Nominations are invited for the fifth annual Michelson Postdoctoral Prize Lectureship, to be held Spring 2000 in the Dept of Physics, Case Western Reserve University. This prize will be awarded to a junior scholar active in any field of physics. The winner will spend one week in residence at CWRU and deliver 3 technical lectures and a colloquium. The lectureship carries an honorarium of \$1000 plus travel expenses.

Eligibility: Nominees must have been awarded a PhD between 8/01/1993 and 8/31/2000, and as of 11/30/2000 may not hold or have accepted any tenured, tenure-track or equivalent position.

Requirements: One letter of nomination and two letters of support from ineligible scientists, at least one employed at an institution other than the nominee's. The letters should address the nominee's scientific accomplishments and promise and ability to communicate effectively. Nominee should submit a CV and an outline of his/her talks. Please send hard copies of all materials to:

Michelson Postdoctoral Prize Lectureship Dept of Physics Case Western Reserve University Cleveland,
OH 44106-7079

Inquiries may also be made by FAX: 216-368-4671 or email: mppl@theory1.phys.cwru.edu

Deadline for receipt of all materials: Nov. 30, 2000

9 Abstracts

Chemical Effect in Rare Gas Adsorption

Sean Clarke, Gustav Bihlmayer, and Stefan Blügel

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D-52425 Jülich, Germany*

Abstract

In order to investigate postulated chemical effects in adsorption of heavy rare gas atoms, we investigate the Ag(001)c(2×2)-Xe system using the Full-Potential Linearized Augmented Plane-Wave (FLAPW) method. Adsorption in the on-top site is found to be favored by 8.6 meV – adsorption in this site suggests that there is a chemical contribution to the bonding. The topology of the charge density associated with the Xe 5p states clearly shows that these states are involved in a bonding interaction with the substrate states. We also show that the extra splitting of the $5p_{3/2}$ orbitals arises from adsorbate-adsorbate interactions. It is observed that the spin-orbit interaction drastically alters the electronic but not geometric properties of the system.

(Submitted to Phys. Rev. B)

Copy available from: s.clarke@fz-juelich.de

Two-dimensional surface ordered Mn-Co alloys on Co(001)

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Abstract

The spin-polarization of various surface alloys of manganese and cobalt on cobalt (001) is determined by the Tight-binding-linear-muffin-tin-orbitals method. An ordered surface alloy restricted to the surface plane *i.e.* $Mn_{0.5}Co_{0.5}/Co(001)$ is shown to be more stable as compared to large islands of Mn or Co in the surface plane. The coupling between Mn and Co is found to be antiferromagnetic in the ground state with a metastable ferromagnetic configuration a few mRy higher in energy. This ferromagnetic coupling between Mn and Co is in agreement with recent magneto-optical Kerr effect and X-ray magnetic circular dichroism results. The two-dimensional (and two-layers thick) surface ordered alloy $(Mn_{0.5}Co_{0.5})_2/Co(001)$ is more stable as compared to the perfect Mn monolayer on Co(001) and only solutions with antiferromagnetic couplings between Mn atoms are obtained. A ferromagnetic coupling between the Mn atoms at the surface and the Co atoms in the substrate is the ground state. A buried monolayer of Mn *i.e.* Co/Mn/Co(001) is also found more stable as compared to Mn/Co(001) so that a complete exchange between surface Mn monolayer and the Co subsurface layer is energetically favorable.

(Accepted, Physical Review B, February 1)

Manuscripts available from: Claude.Demangeat@ipcms.u-strasbg.fr

Substrate-Mediated Interaction on Ag(111) Surfaces from First Principles

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Matthias Scheffler

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

Abstract

When two or more atoms bind to a solid surface, the substrate can mediate an interaction between them. In this paper, we use density-functional theory to quantify the substrate-mediated pair interaction between two adatoms on a compressively strained Ag(111) surface and on unstrained Ag(111). On the strained surface, the elastic interaction is significant over the short range and leads to a net attraction between two adatoms. However, at the longest distances probed, the interaction is primarily electronic and repulsive. The repulsion can be as strong at 50 meV, and it forms a ring-like structure around an atom. On unstrained Ag(111), the interaction is primarily electronic in origin and it is weak relative to the interaction found on the strained surface. We calculate the energy barrier for an isolated atom to diffuse in each of these systems. For the strained surface, the magnitude of the diffusion barrier is comparable to that of the adsorbate interaction. We discuss the implications of our findings for growth at surfaces.

(submitted to: *Collective Diffusion on Surfaces: Collective Behaviour and the Role of Adatom Interactions*, edited by M. C. Tringides and Z. Chvoj (Kluwer Academic Publ., Dordrecht))

Contact person: Matthias Scheffler (scheffler@fhi-berlin.mpg.de)

Orbital and dipolar contributions to the hyperfine fields in bulk bcc Fe, hcp Co and at the Fe/Ag(100) interface: The inclusion of orbital polarization

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³*Institute of Physics, Academy of Physics, Cukrovarnická 10, 16253 Praha 6,
Czech Republic*

Abstract

First principles calculations can make quantitative predictions of many properties of solids including magnetic hyperfine fields (B_{hf}). The inclusion of relativistic effects becomes important in this case. We have selected to study three systems in order to asses the importance of orbital and dipolar contributions to the B_{hf} and its anisotropies: bulk bcc Fe, hcp Co and the Fe/Ag(100) interface. For the last two, in-plane (parallel to the hexagonal planes and to the interface respectively) and perpendicular magnetizations were considered. The influence of different exchange correlation potentials (local density and generalized gradient approximation) and the inclusion of the orbital polarization term (known to improve the evaluation of orbital moments) in the Hamiltonian is reported. A comparison is made with other theoretical studies and to experiment when possible.

(submitted to: Phys. Rev. B)

Contact person: M. Veronica Ganduglia-Pirovano (pirovano@fhi-berlin.mpg.de)

Point defects on III-V semiconductor surfaces

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Abstract

The basic properties of point defects (atomic geometry, the position of charge-transfer levels, and formation energies) on the (110) surface of GaAs, GaP, and InP have been calculated employing density-functional theory. Based on these results we discuss the electronic properties of surface defects, defect segregation, and compensation.

(submitted to: Proceedings of the ICPS 25, Osaka (Springer, Berlin/Heidelberg, 2000))
Contact person: Günther Schwarz (schwarz@fhi-berlin.mpg.de)

Free energy and molecular dynamics calculations for the cubic-tetragonal phase transition in zirconia

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Queen's University, Belfast BT7 1NN, United Kingdom*

Abstract

The high-temperature cubic-tetragonal phase transition of pure stoichiometric zirconia is studied by molecular dynamics (MD) simulations and within the framework of the Landau theory of phase transformations. The interatomic forces are calculated using an empirical, self-consistent, orthogonal tight-binding (SC-TB) model, which includes atomic polarizabilities up to the quadrupolar level. A first set of standard MD calculations shows that, on increasing temperature, one particular vibrational frequency softens. The temperature evolution of the free energy surfaces around the phase transition is then studied with a second set of calculations. These combine the thermodynamic integration technique with constrained MD simulations. The results seem to support the thesis of a second-order phase transition but with unusual, very anharmonic behaviour above the transition temperature.

(To appear in Phys. Rev. B, February 15 2001)

Preprints available from <http://titus.phy.qub.ac>

Self-interaction corrected description of the electronic properties of americium monochalcogenides and monopnictides

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² *Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK*

Abstract

We calculate the electronic structure of the Am pnictides and the Am chalcogenides with the help of the *ab-initio* self-interaction corrected local spin-density approximation. This allows us to describe the Am ion with either a localized f^6 or f^7 shell, corresponding to a trivalent or divalent configuration respectively. From the calculation of the total energy versus lattice constant the valency configuration of the groundstate can thus be established. We find that the Am pnictides are well described by a trivalent Am configuration, whilst the chalcogenides might be described as intermediate valent.

(Submitted to Phys. Rev. Lett.)

Manuscripts available from: lpetit@ifa.au.dk

The inhomogeneous RPA and many-electron trial wave functions

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Prince Consort Road, London SW7 2BZ, England

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Abstract

The long-range electronic correlations in a uniform electron gas may be deduced from the random-phase approximation (RPA) of Bohm and Pines. Here we generalize the RPA to nonuniform systems and use it to derive many-electron Slater-Jastrow trial wave functions for quantum Monte Carlo simulations. The RPA theory fixes the long-range behavior of the inhomogeneous two-body terms in the Jastrow factor and provides an accurate analytic expression for the one-body terms. It also explains the success of Slater-Jastrow trial functions containing determinants of Hartree-Fock or density-functional orbitals, even though these theories do not include Jastrow factors. After adjusting the RPA Jastrow factor to incorporate the known short-range behavior, we test it using variational Monte Carlo. In the small inhomogeneous electron gas system we consider, the analytic RPA-based Jastrow factor slightly outperforms the standard numerically optimized form. The inhomogeneous RPA theory therefore enables us to reduce or even avoid the costly numerical optimization process.

(Submitted to Physical Review B)

Manuscripts available from R. Gaudoin: (r.gaudoin@ic.ac.uk)

* Present address: Centre for Computational Science, Department of Chemistry,
Westfield College, Mile End Road, London E1 4NS, England.

First principles relativistic theory of photoemission from magnetic surfaces

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^cMax-Planck-Institut für Mikrostukturphysik,

Weinberg 2, D-06120 Halle, Germany

Abstract

A first principles theory of spin- and angle-resolved photoemission has been developed. The theory is based on density functional theory and is fully relativistic. It is implemented using multiple scattering theory with a Green's function calculated using a real space cluster method. No lattice symmetry or periodicity is assumed and therefore our approach can be applied to low-dimensional systems. We illustrate the theory with a calculation of the photoemission spectra from Ni(100) and interpret the result in terms of the band structure. The effect of the polarisation of the photon on the spectra is emphasised.

(Accepted for Publication: Journal of Magnetism and Magnetic Materials)

Manuscripts available from: p.strange@phys.keele.ac.uk

X-rays exhibit large optical activity

Gerrit Van der Laan

*Synchrotron Radiation Department, Daresbury Laboratory,
Warrington WA4 4AD, United Kingdom*

Abstract

Optical activity was first observed almost two centuries ago on a quartz crystal using crossed polarizers and explained as being due to optical rotation, a rotation of the plane of the linear polarization, and optical rotatory dispersion, an unequal rotation of the plane of polarization of light of different wavelengths. With intensive research going on for so long one would not immediately expect any new discoveries in this field. However, using linearly polarized synchrotron radiation with an energy of around 5 keV, Jose Goulon at the European Synchrotron Radiation Facility (ESRF) in Grenoble and his coworkers have observed a strong non-reciprocal transverse anisotropy in the low temperature, antiferromagnetic, insulating phase of a Cr doped V₂O₃ crystal in which one single antiferromagnetic domain was grown by magnetoelectric annealing [Phys. Rev. Lett. 85, 4385 (2000)]. This effect, although theoretically predicted, has never been observed so clearly before.

(To be published in PhysicsWorld (December 2000))

Copies available from g.vanderlaan@dl.ac.uk

Ab initio calculation of phase boundaries in iron along the bcc-fcc transformation path and magnetism of iron overlayers

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²*Department of Solid State Physics, Faculty of Science, Masaryk University, Kotlářská 2, CZ-611 37 Brno, Czech Republic*

³*Department of Materials Science nad Engineering, University of Pennsylvania, 3231 Walnut St., Philadelphia, PA 19104-6272, U.S.A.*

Abstract

A detailed theoretical study of magnetic behavior of iron along the bcc-fcc (Bain's) transformation paths at various atomic volumes, using both the local spin density approximation (LSDA) and the generalized gradient approximation (GGA), is presented. The total energies are calculated by spin-polarized full-potential LAPW method and are displayed in contour plots as functions of tetragonal distortion c/a and volume; borderlines between various magnetic phases are shown. Stability of tetragonal magnetic phases of γ -Fe is discussed. The topology of phase boundaries between the ferromagnetic and antiferromagnetic phase is somewhat similar in LSDA and GGA, however, the LSDA fails to reproduce correctly the ferromagnetic bcc ground state and yields the ferromagnetic and antiferromagnetic tetragonal states at too low volume. The calculated phase boundaries are used to predict the lattice parameters and magnetic states of iron overlayers on various (001) substrates.

(Accepted for publication in Phys. Rev. B, Feb 1, 2001)

Latex-file or ps file available from : Martin Friák, mafri@ipm.cz

Magnetic circular dichroism in Co 2p photoemission of Co/Cu(1 1 13): Separation of the fundamental spectra

Giancarlo Panaccione,^{a,b} Gerrit van der Laan,^c H. A. Dürr,^c, and J. Vogel^d

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TASC Laboratory, I-34012, Trieste, Italy

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^d *Laboratoire de Magnétisme Louis Néel, CNRS,*

F-38043, Grenoble, France

Abstract

We measured high-quality Co 2p magnetic circular dichroism (MCD) spectra in photoemission for > 5 ML Co films grown on Cu(1 1 13) using a “complete” experiment, where the sample magnetization and the light helicity vector were reversed separately. We show how the four measured spectra, $M^\pm P^\pm$, can be used to make new linear combinations, which correspond to the circular dichroism in the angular dependence (CDAD), magnetic linear dichroism in the angular dependence (MLDAD) and MCD spectra. The integrated signals of the MLDAD and CDAD can be used to estimate the error caused by the difference in the degrees of magnetization and light polarization, respectively, in the opposite alignments. The MCD signal integrated over the entire 2p region does not average to zero, as one would have expected from the sum rule for photoemission to a non-interacting continuum state. There is a strong MCD signal in the entire region between the $2p_{3/2}$ and $2p_{1/2}$ main lines with pronounced satellite structure. The differences between the measured and calculated results for an independent-particle and an atomic model indicate the presence of interatomic electron correlation effects and configurational mixing.

(To be published in J. European Physical Journal B)

Preprints requests to: g.vanderlaan@dl.ac.uk

Three-dimensional spin-structure on a two-dimensional lattice: Mn/Cu(111)

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[†]Institut für Festkörperforschung, Forschungszentrum Jülich,
D-52425 Jülich, Germany

[¶]Department of Physics, Nara Medical University, Kashihara,
Nara 634-8521, Japan

Abstract

Based on first-principles vector spin-density total-energy calculations of the magnetic and electronic structure of Cr and Mn transition-metal monolayers on the triangular lattice of a (111) oriented Cu surface, we propose for Mn a three-dimensional non-collinear spin structure on a two-dimensional triangular lattice as magnetic ground state. This new spin-structure is a multiple spin-density wave of three row-wise antiferromagnetic spin states and comes about due to magnetic interactions beyond the nearest neighbors and due to higher order spin interactions (i.e. four-spin). The magnetic ground state of Cr is a coplanar non-collinear periodic 120° Néel structure.

(accepted at Phys. Rev. Lett.)

copy available from: s.bluegel@fz-juelich.de

Interdiffusion and exchange coupling in Cr overlayers on a Fe(001) substrate

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D. Stoeffler,^d and H. Dreyssé^d

^a Institute of Physics of Materials, Brno, Czech Republic

^b Center for Comput. Materials Science, TU Wien, Austria

^c Institut für Festkörperforschung, FZ Jülich, Germany

^d IPCMS, Strasbourg, France

Abstract

The influence of interfacial interdiffusion on the magnetic order in ultrathin epitaxial Cr films on a Fe(001) substrate was studied by means of electronic structure calculations. The total coverage of the films was assumed to be one, two, and six monolayers of Cr while the interdiffusion was simulated by two-dimensional Cr-Fe alloys in the two atomic layers forming the Cr/Fe interface. Two limiting cases were considered: (i) perfectly ordered alloys, described in terms of a semiempirical tight-binding method using the recursion technique, and (ii) substitutionally disordered alloys, whose electronic structure was determined ab initio using the tight-binding linear muffin-tin orbital method and the coherent-potential approximation. In both cases, the magnetic coupling of the Cr overlayer to the ferromagnetic Fe substrate exhibits similar transitions (π phase shifts) due to varying compositions at the interface. The calculated results provide additional support for recent interpretations of experiments on Fe/Cr/Fe(001) trilayers.

(submitted to: Phys. Rev. B – scheduled for January 1, 2001)

postscript file available from turek@ipm.cz

Nonuniqueness of the Potentials of Spin-Density-Functional Theory

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13560-970 SP, Brazil*

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

Abstract

It is shown that, contrary to widely held beliefs, the potentials of spin-density-functional theory (SDFT) are not unique functionals of the spin densities. Explicit examples of distinct sets of potentials with the same ground-state densities are constructed, and general arguments that uniqueness should not occur in SDFT and other generalized density-functional theories are given. As a consequence, various types of applications of SDFT must be critically reexamined.

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

Relativistic Fluctuations and Anomalous Darwin Terms in Superconductors

K. Capelle

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Universidade de São Paulo, Caixa Postal 369, São Carlos,
13560-970 SP, Brazil*

Abstract

The anomalous Darwin term, one of the recently derived relativistic corrections to the conventional theory of superconductivity, is analyzed in detail. This analysis leads to the prediction of unusual types of fluctuations, of relativistic origin, in superconductors. An alternative derivation of the anomalous Darwin term, much simpler than that given originally, is presented and used to clarify some puzzling features of the original derivation. The question of observability of the anomalous Darwin term and the resulting fluctuations is discussed, and its relation to the conventional Darwin term and to earlier proposed superconducting Darwin terms is clarified.

(To appear in Phys. Rev. B (scheduled for Feb 2001))

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

Density-functional investigation of the stability of spin-density waves

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² *Instituto de Física de São Carlos, Departamento de Física e Informática,
Universidade de São Paulo, Caixa Postal 369, São Carlos,
13560-970 SP, Brazil*

Abstract

Recent applications of and approximations to a novel density-functional approach to spin-density waves and antiferromagnetic systems are outlined. The nonlocal nature of the antiferromagnetic correlations and possible noncollinearity in spin space are described by a new fundamental variable, the staggered density, which supplements the spin densities of conventional density-functional theory.

(To appear in J. Magn. Magn. Mater. (proceedings of ICM 2000))

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

Spin-density waves and the Hubbard model: an exact numerical treatment

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² *Instituto de Química de São Carlos, Departamento de Química e Física Molecular,
Universidade de São Paulo, Caixa Postal 369, São Carlos,
13560-970 SP, Brazil*

Abstract

The formation of a spin-density wave in the one-dimensional Hubbard model with a small number N of sites is investigated. The numerical diagonalization of the model Hamiltonian shows that, for odd N , frustration gives rise to a spin-density wave in the ground state.

(To appear in J. Magn. Magn. Mater. (proceedings of ICM 2000))

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

Relativistic Theory of Superconductivity

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³ *Institut für Theoretische Physik
Universität Würzburg, D-97074 Würzburg, Germany*

Abstract

The relativistic formulation of the theory of superconductivity is reviewed with respect to its conceptual basis and first applications. The construction of relativistically covariant order parameters for superconductors is outlined, and the generalization of the Dirac equation for the superconducting state is presented. A weakly relativistic expansion of this equation leads to the Pauli equation for superconductors, which describes the lowest-order relativistic corrections to the conventional theory of superconductivity. The physics of these corrections is discussed, and the prospects for experimental detection of relativistic effects in superconductors are examined.

(To appear ‘*Condensed Matter Theories*’, Vol. 16. (Nova, New York, 2001))

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Intense-field double ionization of helium: Identifying the mechanism

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Abstract

We present quantum mechanical calculations of the electron and ion momentum distributions following double ionization of a one-dimensional helium atom by ultrashort laser pulses (780 nm) at various intensities. The two-electron momentum distributions exhibit a clear transition from non-sequential to sequential double ionization. We provide strong evidence that rescattering is responsible for non-sequential ionization by calculating the momentum spectrum of the He²⁺ recoil ions – which we find in excellent agreement with recent experiments – and by analysing the electronic center-of-mass motion via Wigner transforms.

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Discrete peaks in above-threshold double-ionization spectra

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Abstract

Quantum mechanical calculations of multiphoton double ionization by intense laser pulses show that the total-kinetic-energy spectrum of the photoelectrons consists of peaks separated by the photon energy, analogous to ordinary above-threshold ionization. Related structures appear in the two-electron and in the recoil-ion momentum distribution. We propose a method to extract the total-kinetic-energy spectrum from the experimental recoil-ion spectrum.

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Multicomponent Density-Functional Theory for Electrons and Nuclei

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Abstract

A multicomponent density-functional theory is developed for the combined system of electrons and nuclei. We construct approximate functionals for the electron-nuclear correlation energy and illustrate the theory by explicit calculations for the H_2^+ molecular ion.

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High-pressure phases of the alkali metals

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Abstract

A series of recent x-ray diffraction experiments carried out by scientists from the Max-Planck-Institut FKF in Stuttgart and the ESRF in Grenoble on elemental semiconductors and alkali metals under high pressure have provided new insight in pressure induced structural transformations. New structures have been identified, and some of these have surprising similarities, such as low coordination numbers. The new lithium phase, Li-cI16, which has a cubic structure with 16 atoms in the cubic cell, has not been found for any other element. Theoretical studies, some of which are described here, using *ab initio* methods to calculate electronic and structural properties provide theoretical support for the analysis of these experiments, and may also serve to predict new properties, such as superconductivity, of the materials when exposed to very high pressures.

Introduction

The alkali metals, earlier considered as *simple metals* with bandstructures that differ only slightly from those of free-electron systems, have attracted considerable [1] interest because application of external pressure changes the bonding properties fundamentally. For example lithium, the first monovalent metal in the Periodic Table, is sometimes expected to be a model system of hydrogen, where the atoms form diatomic molecules in insulating solid phases. The breaking of the bonds in hydrogen by applying very high pressures is a *Holy Grail* of physics[1], and it is important for the understanding of the metallic hydrogen in the interior of the heavy planets. In view of this it was remarkable that theoretical calculations by Neaton and Ashcroft[2] predicted that compressed Li might assume a structure (*oC8* with *iCmca*

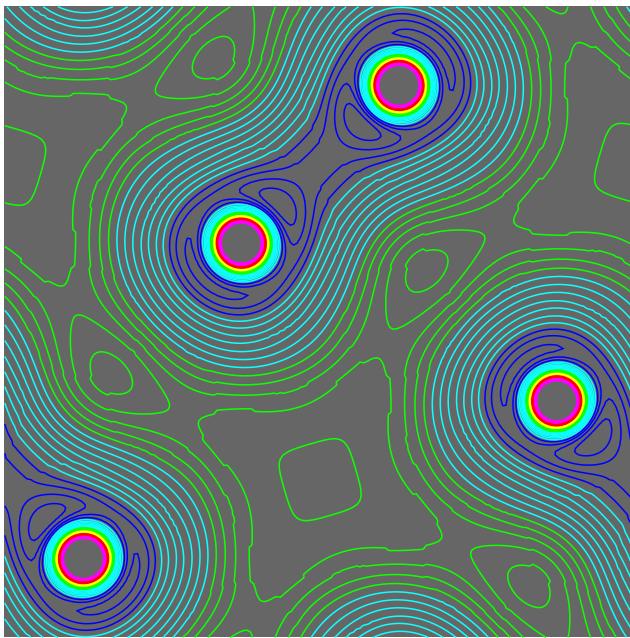


Figure 1: Contour plot of the calculated valence-electron density in lithium in the BC8 structure at 165 GPa ($V/V_0=0.23$). The colour coding is dark blue towards red/magenta for increasing density. The lowest contour value is 0.0472 \AA^{-3} , the increment is 0.0135 \AA^{-3} . Disregarding the innermost core oscillations, the highest valence density is found in the interstitial square-like green contour, $1.4 \times \rho_{av}$, where $\rho_{av}=0.204 \text{ \AA}^{-3}$ is the average density.

symmetry) where the atoms form *pairs*, and that this phase is semi-insulating. This is in sharp contrast to the intuitive expectation that application of hydrostatic pressure should favour highly coordinated metallic phases.

The compressibility of the alkali metals is very large, and the large volume reduction with application of pressure affects significantly the otherwise free-electron like electronic structure. As a consequence, these metals undergo several pressure-induced structural transformations. These have been studied experimentally (see for example Ref. [3, 4, 5, 6, 7, 8, 9]) as well as by theoretical methods (Ref. [2, 3, 9, 10, 11, 12, 13, 14] and references therein). Among several interesting results of this research, the most recent progress includes the observation[3] of new high-pressure phases of lithium, Li-*hR1* and Li-*cII6*, and the identification[6, 15] of the structure of Cs-V and Rb-VI as being the orthorhombic *Cmca* structure with 16 atoms in the orthorhombic unit cell (*oC16*). The same structure type, with very nearly the same relative atomic coordinates, is found in Si and Ge under pressure.[7, 12, 16, 17, 18] This *Cmca* structure contains two types of atoms, say Cs_1 and Cs_2 , with Cs_1 in planar arrangements separating Cs_2 double layers. The atoms in the single planes form a dense packing of *dimers*.[12] This has some similarity with the *Cmca* structure predicted for Li under pressure by Neaton and Ashcroft.[2] In that structure (*oC8*), however, the double layers of type-2 atoms are absent, i.e. the structure is similar to that of Ga at ambient pressure.

In Fig. 1 we show, as an example of such a "paired structure", the distribution of valence electrons in lithium at 165 GPa. The apparent formation of atom *pairs*, however, should not be overemphasized. It is true that there is a single, shortest interatomic distance, but the next-nearest neighbours in the *Cmca* structures are not much further away. Therefore the "effective" coordination number is rather ≈ 5 than

one. The interesting result, though, is that there is a tendency of formation of low-coordinated phases of highly compressed alkali metals. Further, as the results of the calculations will show, the bonding is very different from usual molecular (covalent) bonding. Already, the density plot, Fig. 1, demonstrates this.

The pressure-driven electronic $s \rightarrow d$ transition [19] plays a major role in the structural behavior of cesium,[11, 20] in particular the occurrence of the tetragonal CsIV phase which is only eightfold coordinated.[5] The unusual decrease of the coordination number with increasing pressure from 12 in *fcc* to 8 in CsIV has been interpreted in terms of a peculiar directional bonding induced by the $s-d$ transition.[20, 21] This leads to a softening and a dynamical instability in Cs-II (*fcc*).[13, 14] Also, the thermal expansion coefficients of Cs have been predicted to be negative at all temperatures in certain pressure ranges.[13, 14] The light alkali metals, Li and Na, are similarly strongly influenced by an $s \rightarrow p$ transition.

Structures and Method of Calculation

The *ab initio* simulation methods which we apply cannot be used to perform an ideal, molecular dynamical structural optimization. We must select a certain set of structure types, i.e. space groups and number of atoms in the cells. Some of the structures, however, will have parameters, like axial ratios and atomic site parameters, which must be optimized at each volume (pressure). We can then, among the structures included in the set, determine which one is stable, statically as well as dynamically, at a given volume. In that way one can never be sure to find the 'true' ground state structure, but the procedure will be given relevance in describing trends and binding properties to be expected if the structures to be examined are selected in a 'sensible manner'.

The simplest close-packed structures, *bcc*, *fcc*, *hcp dhcp*, body-centered cubic, face centered cubic, and hexagonal close packed are well-known. The *hcp* stacking sequence in the c-direction is ABA. Similarly, *fcc* and *bcc* can be built by stacking (111)-layers in the sequence ABCA. In this hexagonal representation, *fcc* has $c/a = \sqrt{6}$, and for *bcc* the axial ratio is $c/a = \frac{1}{2}\sqrt{3/2}$. The so-called ω -phase structure appears if the B and C layers in *bcc* are shifted so that they coalesce at $z=c/2$. The double-hexagonal close-packed structure (*dhcp*) has an ideal *c/a* ratio which is twice that of *hcp*, and the stacking is ABACA. The "samarium type structure", *9R*, is a nine-layer hexagonal structure, stacking ABABCBCACA. Calculations are most conveniently performed using the primitive rhombohedral cell which contains only 3 atoms. Also *A7* (space group 166 in the International Tables) has a rhombohedral primitive cell. It contains two atoms. For special parameters, *A7* becomes the simple cubic, *sc*, structure. The simple rhombohedral structure, *hR1*, is obtained by straining the *fcc* structure along a body diagonal. The structure which is called *cI16* belongs to the spacegroup *I $\bar{4}3d$* (number 220 in the International Tables). This was found experimentally for Li under pressure[3], and so far it has not been observed for any other elemental solid. The atoms are located in the *16c* Wyckoff positions. The primitive cell is *bcc*. The *oC8* structure is of *Cmca* symmetry, and it resembles that of α -gallium, but can also be viewed as that of black phosphorous compressed perpendicularly to its double layers.

Some of the high-pressure phases have structures similar to the cation sublattices of binaries,[3] and the structure of CsIV[5] is an example of this. CsIV forms in a tetragonal structure with *I4₁/amd* symmetry, SG 141, and the atoms are placed in

$$\mathbf{r}_1 = (0, 0, 0); \mathbf{r}_2 = \left(0, \frac{1}{2}, \frac{c}{2a}\right). \quad (1)$$

This is the structure of the Th sublattice in ThSi_2 .[22] The $cI16$ structure described above is in fact that of the cation sublattice in Eu_4As_3 and Yb_4As_3 , i.e. anti- Th_3P_4 structures.[23] As mentioned $cI16$ is a cubic structure with a bcc Bravais lattice and 8 atoms in the rhombohedral primitive cell. Several other cubic structures may be generated by distorting such a bcc supercell. As one example we consider the $BC8$ structure, mainly because it has been found, as also $R8$, in metastable Si phases. The $BC8$ structure[24] is also body-centered-cubic with 16 atoms in the unit cell (8 atoms in the primitive cell). The space group is $Ia\bar{3}$, and the atoms are in the $16c$ Wyckoff sites, (x_0, x_0, x_0) . It may also be viewed as a rhombohedral structure with an 8-atom primitive cell, SG $R\bar{3}$. This has 2 atoms in the $2c$, (u, u, u) and 6 in the $6f$, (x, y, z) , sites. These parameters are related to x_0 by $u=2x_0$, $x=1/2$, $y=0$, and $z=1/2-2x_0$. Thus, in $BC8$ there is one internal parameter (x_0) which must be optimized.

The $BC8$ structure can be considered as a special setting of the structural parameters of the $R8$ structure. Both have the SG $R\bar{3}$ (number 148). The 8 atoms in the $R8$ primitive cell are located at the $2c$, (u, u, u) , and the $6f$, (x, y, z) , Wyckoff sites. In $BC8$ all 8 sites are equivalent, but in $R8$ the $2c$ and the $6f$ sites are inequivalent. The Si- $BC8$ and - $R8$ phases are described in Ref. [25].

The total energy for a given choice of atomic coordinates is calculated within approximations to the density functional theory, the local approximation (LDA) as well as a generalized gradient approach (GGA). The results presented here are obtained with the GGA, and we used the Perdew-Burke-Ernzerhof scheme.[26] The solution of the effective one-electron equations is performed by means of the linear muffin-tin-orbital (LMTO) method [27] in the full-potential version. [28] The semi-core states, Li- $1s$, Na- $2s$, and Na- $2p$, are treated as *local orbitals*[29] in the same energy window as the valence states. The bandstructure calculations are scalar relativistic, i.e. all relativistic effects, except spin-orbit splittings, are included.

The structural optimization required in all cases except for the *bcc* and *fcc* structures is made at each of 21 volumes, V , in the range $0.10 \times V_0$ to $1.10 \times V_0$, where V_0 is the (experimental) equilibrium volume of *bcc*-Na at ambient pressure. (We use $V_0=21.2725 \text{ \AA}^3$ for Li and 37.7073 \AA^3 for Na). For some structures, like *hcp*, *dhcp*, and *hR1*, only a single, internal parameter needs to be varied, but other cases require more time consuming optimizations. A7 and 9R require optimization of two parameters, z and c/a . In the *Cmca* structures we need to vary the axial ratios, c/a and b/a , as well as 2 (in *oC8*) or 3 (in *oC16*) internal parameters. Also for $R8$ there are 5 parameters to be optimized simultaneously. This is done by means of a steepest-descent method.

Results

Having calculated the optimized total energies, E , vs. volume for all structures, and applying a least-squares fit to a power series in $X = (V/V_0)^{1/3}$ (positive as well as negative powers), we derive pressure, P , bulk modulus, B , and enthalpy, $H = E + PV$. The calculated $P-V$ relations are then used to calculate $H(P)$, and the results are summarized in Fig.2. The calculated pressures for some of the compressed Na phases are shown in Fig. 3.

The *dhcp* structure is not included since it is close in energy to *hcp*. Also, the calculations for *oC16*

have been omitted, since for Na (as for Li) it is above the other structures in energy. At low pressures (not visible on the scale of Fig.2) we find that the *bcc* structure is favoured in sodium. The calculation predicts that this remains the stable structure up to $P_{t1} \approx 80$ GPa, where it transforms to the *fcc*. It should be noted, however, that the maximum difference, $E(fcc) - E(bcc)$ is only 5 meV/atom. (We find the same differences using LDA). The fact that we find the energy difference to that small also implies that a substantial error bar is associated with the value of P_{t1} , and we there also made independent calculations using the FP-LAPW method as implemented in the WIEN97 code.[30] Very similar results were obtained.

The instability of Na-*bcc* is also reflected in the volume dependence of the elastic shear constants. As found by Katsnelson et al.[10] and also in the calculations[13, 14] for Cs, C' and C_{44} soften and tend to go negative under compression. Another distortion of the *bcc* structure of sodium could be possible, namely that to the ω -phase.[31] At high pressures, Fig.2 clearly shows that Na- ω cannot be a stable structure.

The (perfect) *fcc* (red-orange in Fig.2) structure remains stable up to ≈ 170 GPa, where it becomes unstable against a rhombohedral shear. The elastic constant C_{44} goes negative, and the *fcc*-lattice becomes dynamically unstable. This signals the transition to the distorted structure, *hR1* (orange). The *cII6* structure starts to be the favoured structure at $P_{t2} \approx 170$ GPa. The figure shows how a hypothetical *bcc* becomes unstable towards x -distortions around 130 GPa, and at P_{t2} the energy gain associated with these displacements has become so large that *cII6* enthalpy value is the same as that of *hR1*. However, in the very same pressure regime Na-*CsIV* rapidly lowers its free energy with pressure so much that it becomes the lowest among those examined up to $P_{t3} \approx 220$ GPa, where the *Cmca* structure, *oC8* takes over. The figure shows that with the error bars the onset of Na-*cII6* may be somewhere between 110 and 170 GPa if observed at all. The displacements, x , increase with compression, as in Li,[3], but in Na x seems to approach a limiting value of 0.065 at extreme compressions. This is different from Li, where a saturation value of 0.125 was found.[3]

Apart from the range around 170 GPa where several structures are close in energy, the hexagonal structures, *hcp* and *dhcp*, are not likely to be "good candidates" for Na at high pressure, and it is so although although substantial energy can be obtained by reducing c/a at small volumes.

The three *coexistence pressures* P_{t1} , P_{t2} , and P_{t3} are also marked in Fig.3 which shows the calculated $P - V$ relations for some selected structures of Na at small volumes. From low pressures (in fact from 0) up to 120 GPa we find that the pressures of the close-packed phases follow each other closely. The change of slope in $P(V)$ for *hcp*-Na structure around 270 GPa reflects a rapid change in c/a upon compression.

For Li it was demonstrated that the distortion (finite x value in Fig. 2 of Ref. [3]) of the *bcc* structure into *cII6* causes the formation of a pseudo-gap, and thus to a downshift in an appreciable amount of filled electron states. The one-electron energy sum is similarly reduced in Na-*cII6* as x becomes non-zero. A similar effect is found in the *CsIV* and the *BC8* structures. Again the formation of a pseudogap near E_F tends to stabilize the structure. In all cases the increasing occupation of p states with pressure is essential for the formation of the new structures, and this is most spectacular in Na-*oC8*, the phase which is clearly the lowest in energy among those examined in the high-end of the pressure range of Fig. 2. The pseudogap which is present even at $V/V_0=0.45$ becomes rapidly deeper as the lattice is compressed, and at the smallest volume examined for Na, $V/V_0=0.10$, its DOS at E_F vanishes, Fig. 4. In fact a very small, finite gap has formed. In Li-*oC8* it was also found[2, 3] that DOS(E_F) vanishes at a very high pressure, but the energy-optimized structure did not exhibit a finite gap. The $s \rightarrow p$ transition responsible for this

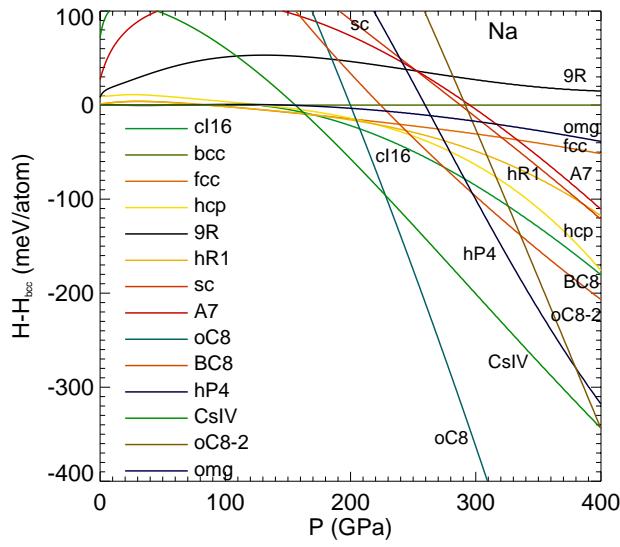


Figure 2: Enthalpies of 10 Na phases vs. pressure (P). The enthalpy of the bcc structure is used as a reference.

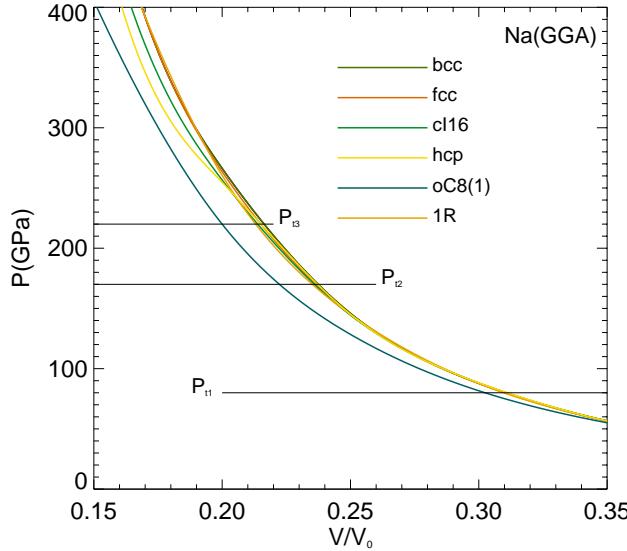


Figure 3: Calculated pressures vs. volume for Na in selected structures (only the range between 0.15 and $0.35 V_0$ is shown). The pressures P_{t1} , P_{t2} , and P_{t3} are the calculated pressures of transition from bcc to fcc/hR1, hR1 to "CsIV", and "CsIV" to Na-oC8, respectively.

behavior is further illustrated in Fig. 5.

A similar strong increase in the ratio between p - and s electron counts at large compressions was found for Li. At first, such a behavior might be explained for Li as an effect of orthogonality; the Li atom has a full s core, and the $2s$ valence states are kept away from the core regime, even at small volumes due to their orthogonality to the $1s$ states. Orthogonality does not impose a similar *radial* constraint on the Li- $2p$ states, and consequently the $2p$ canonical band[27] can increase its overlap with the Li- $2s$ band when Li is compressed.

A similar argument cannot be applied to Na. In that case the core of the atom contains s - as well as

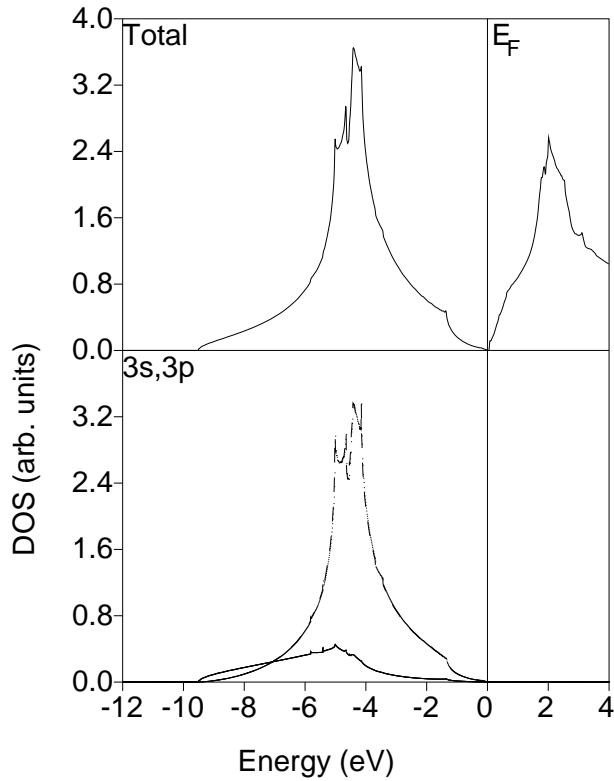


Figure 4: Density-of-states functions for Na in the *oC8* structure at $V/V_0=0.10$.

p-states ($2p$), and a weaker $s \rightarrow p$ transition should then be expected. But the behaviour in sodium is as that of lithium.

Hybridization is very strong in the compressed alkali metals. If we consider a hypothetical Na-*fcc* crystal at the smallest volume, $V=0.1V_0$, considered here, its interatomic distance is 1.73 Å. This is the same as the distance from the nucleus of the free Na atom to the outer maximum of the Na-3s wavefunction.[32] Consequently, a 3s wavefunction from a nearest neighbour atom in the compressed solid will, when expanded in around the local site, yield a very large *p* component. Only *s* states have non-vanishing amplitudes on the nucleus, and therefore the crystal structure adjusts so that there are interstitial regimes where the valence charge can pile up. This means that the coordination number is reduced to a lower value than in *fcc*, for example.

The valence electron distribution calculated for Na-*oC8*, see Fig. 6 is very similar to that found in the Li calculations. "Pairs" of atoms can be seen, but, as mentioned earlier, the next-nearest neighbour distances are close to the shortest interatomic distance, and it is not very meaningful to characterize this as a solid with coordination number 1. The density plot, Fig. 6, further shows that the structure has some similarity with *hP4*, that of graphite, and this is even more so in *oC8-2*, the Cmca structure derived from the Si sublattice in MoSi₂.

We have already at several places compared the Na results to experimental and theoretical results presented recently for lithium.[3, 2] Nevertheless, it is worthwhile to compare to a larger set of data than the one which was included in our calculations in Ref. [3]. Figure 7 summarizes enthalpy calculations for 14 out 16 examined structures.

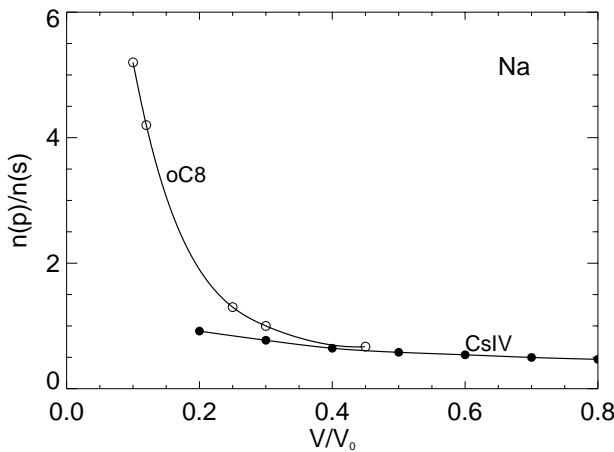


Figure 5: Ratios between the number of p - and s - valence electrons in two Na-phases vs volume.

Those not included are $oC16$ ("CsV") and $R8$. The former has energies which are well above the reference in Fig. 7, and Li- $R8$ was found to converge to Li- bcc at low pressures and to Li- $BC8$ at high pressures. Among the new results which are interesting, we mention those of Li- $hP4$ (graphite type) and Li- $CsIV$. Li- $hP4$ becomes a competitor to Li- $oC8$ at very high pressures, and the calculations show that it has the lowest enthalpy above ≈ 300 GPa. The $CsIV$ structure is even more interesting since its energy becomes very close to that of Li- $cII6$ in a pressure range which may be accessed experimentally. The upper pressure attained in the measurements of Hanfland and Syassen[3] is around 55 GPa, and the present calculations suggest that there could be a pressure window starting a bit higher where Li- $CsIV$ might be found. The smallest energy difference between Li- $CsIV$ and - $cII6$ in the calculation is 1-2 meV/atom, i.e. well below our error bars.

Comparing Fig. 1 to Fig. 8 we see that at high pressure the valence electrons in Na distributed similarly to those of Li. The shapes of the contours between the atoms in the "pair" resemble those of covalent bonds. But the nature of the bonding is far from being a conventional diatomic molecular bonding. The blue contours indicate *minimal* densities. The valence electrons are in the interstitial regimes, and the bonding may be considered as a multicenter bonding. The bonding in the high-pressure phases of Li and Na, for example in the $oC8$, is thus quite different from that in the SiVI phase ($oC16$, also Cmca), see for example Fig. 6 in Ref. [33]. In view of this, it is surprising how similar some of the high-pressure phases of the alkali metals are in structure to some of those found in Si and Ge. Apart from having different relative coordinates (x_0 is different) the $BC8$ structure of silicon resembles that of Li- $BC8$, but the bonding is quite different. Figure 9 shows our calculated density in Si- $BC8$. This may crudely be described as an "inverse" of the Li- and Na plots.

Conclusions

Sodium and lithium both assume several, rather complex structures under pressure. Examination of the band structures and orbital-projected density-of-states (DOS) functions show that the number of p -states is found to increase at the expense of s states under compression. The reason is that the interatomic distances become small compared to the range of the wavefunctions, and the high-pressure phases be-

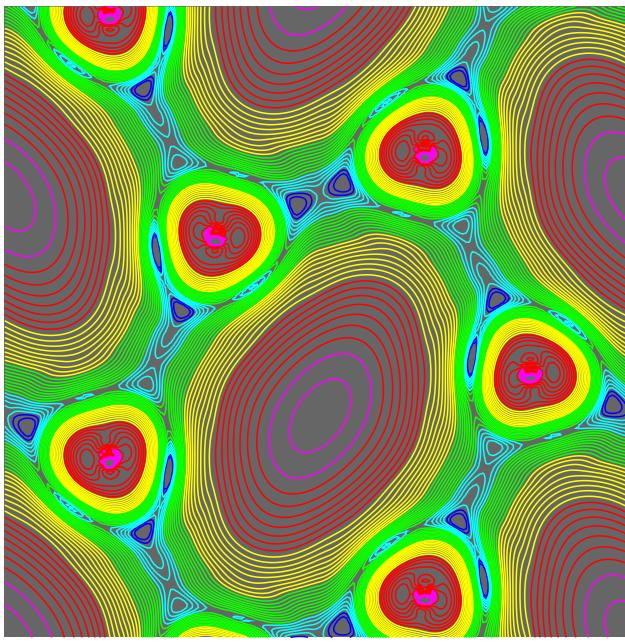


Figure 6: Density of valence electrons in Na-*oC8* at V/V_0 . Note that the lowest densities are shown in blue, whereas the red (magenta) correspond to high (highest) densities.

come rather open. Therefore, the structures found theoretically to be good candidates for sodium under very high pressures are characterized by having coordination numbers which are lower than those of the intermediate-pressure phases, *bcc* and *fcc*.

The structural energy differences calculated here do not include thermal effects, i.e. vibrational contributions to energy and entropy[13, 14] are neglected. This adds to the error bars of some of the tiny free energy differences. Within such limitations, the calculations cannot clearly distinguish between the *fcc*, *bcc* and the *R9* structures at zero pressure. At slightly elevated pressures, though, *bcc* is favoured, and a *bcc*→*fcc* transition is predicted near 80 GPa. The error bar is large, probably ± 20 GPa. Na-*fcc* undergoes a rhombohedral deformation, and close to 180 GPa several new structures become energetically possible. Among these the *cI16* is an interesting candidate, because this structure was experimentally observed[3] for Li under pressure. But also in this case the error bars, at best 5 meV/atom, on the energy difference calculations combined with the slow variation of enthalpy with P implies that a theoretical estimate of the stability range of Na-it *cI16* is difficult to give. If observed at all, the lower limit on the onset pressure would be around 110 GPa, and upper limit of its pressure range would be near 170 GPa. Among the structures examined here we find that Na-*CsIV* is lowest in enthalpy between 170 and 220 GPa. Above $P \approx 220$ GPa we find that the Na-*oC8*, *Cmca*, may be stable up to very high pressures. The structure of Na-*oC8* is similar to the Li-*oC8* phase, but the structural parameters, y , z , b/a , and c/a (not shown here) vary somewhat differently with volume.

Highly compressed Na contains even more $3p$ - than $3s$ states, and in the *oC8* the hybridization is so strong that the hybridization gap makes the DOS vanish at the Fermi level in the most compressed cases. (In that context, see also the discussion by Neaton and Ashcroft[2] of the Peirls distortion in Li). The metal-insulator transition occurs in Na only at extreme compression. At 88 % compression the *Cmca* phase is still metallic, but reduction of the volume to $0.10 \times V_0$ produces a tiny gap according to the calculations. The corresponding pressure is ≈ 950 GPa, roughly 3 times the pressure at the center of the

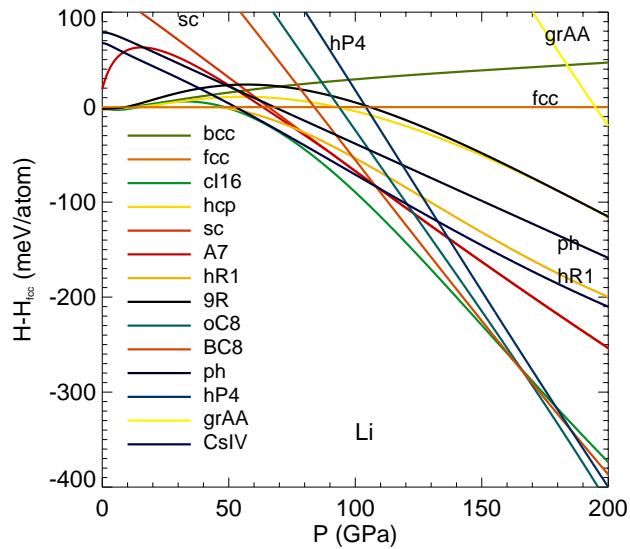


Figure 7: Calculated enthalpies for various Li phases vs. pressure relative to Li-*fcc*. (Note that the *bcc* was used as a reference in the case of Na).

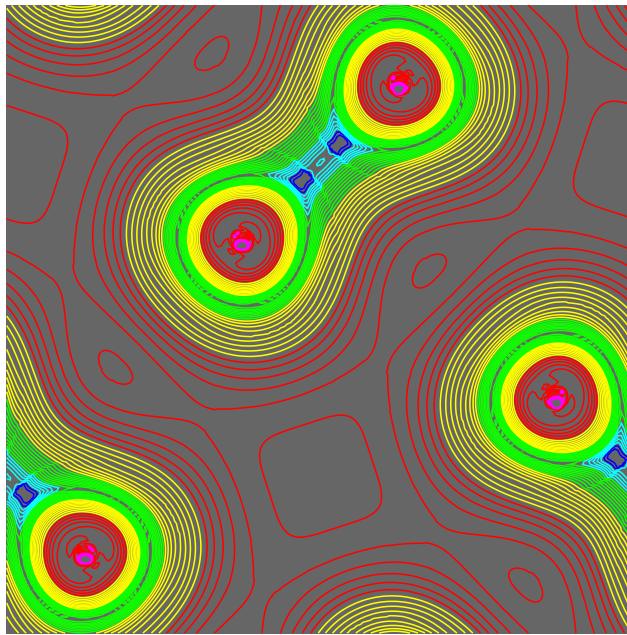


Figure 8: Contour plot of the calculated valence-electron density in sodium in the BC8 structure. Blue contours correspond to the lowest densities, red and magenta to the highest.

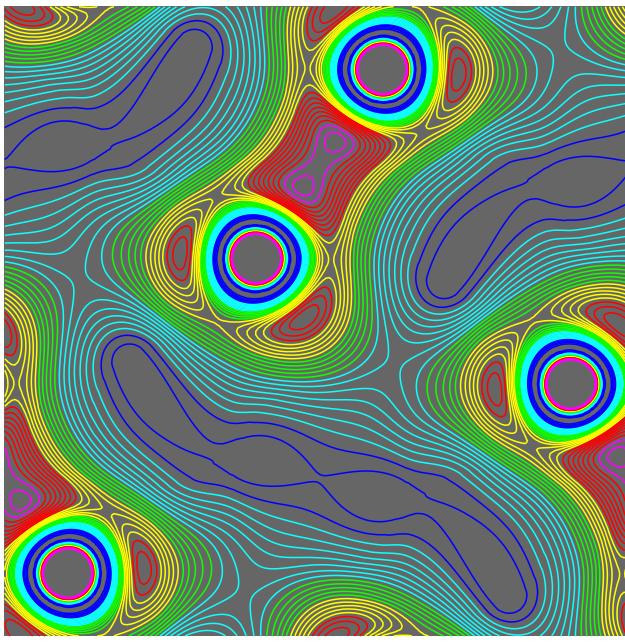


Figure 9: Contour plot of the calculated valence-electron density in silicon in the BC8 structure. Blue contours correspond to the lowest densities, red and magenta to the highest.

Earth. For comparison, *bcc*-Na would need ≈ 1500 GPa to be compressed to $V/V_0=0.10$.

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