Ψ_k Newsletter

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

Number 40 August 2000

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Contents

1 Editorial

A large part of this newsletter is devoted to the Psi-k 2000 conference. It contains both the schematic and detailed programmes of the conference. Also the lists of contributed talks and posters are published for quick reference. Please do check the **General News** section for details. Apart from the conference material this newsletter contains also reports on workshops/conferences and collaborative visits, abstracts in the usual section but also in some reports on workshops, workshop/conference announcements, as well as the announcements of available positions at Ph.D. and post-doctoral level. Note that there are also position announcements in the new section, concerned with the RTN network on **"Computational Magnetoelectronics"**. In this newsletter we also publish the contents of the book on **"The use of the LMTO method"**, based on the TMR1 workshop organized in Mont Sainte Odile (France) in October 1998, and dedicated to the *"Electronic structure and physical properties of Solids"*. The scientific highlight of the month is by I.I. Oleinik, E.Yu. Tsymbal, and D.G. Pettifor (Oxford) on **"First-principles modelling of magnetic tunnel junctions"**. For further details please see the table of contents.

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

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

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

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

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

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

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

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

2 General News

2.1 Distribution of Psi-k Newsletters

The time for change has arrived for the way the Psi-k Newsletter is distributed.

It seems that more and more of our readers prefer to download the newsletters from the web and want just to be informed by electronic mail of the day when a newsletter becomes available on our web site. Moreover, the newsletters are getting bigger and bigger and many servers simply fall over when such bulky newsletters arrive at their destinations. Another matter is ever more complex figures of the scientific highlights, which cannot be simply produced in the LaTeX format for an easy distribution. And emailing encapsulated postscript files in large quantities is not the best solution either. Of course, one could think of zipping all ingredients etc., but not on all platforms such files can be easily decoded or processed. So, we have come to conclusion that the best solution is just to place the pdf- and postscript files on our web site and simply inform you electronicly that the newsletter is there to be collected, downloaded, read, etc. Concerning the LaTeX file of the newsletter, we shall also place it on the web site, but in case of encapsulated figure files these will be kept at a specified directory to be picked up if necessary. Of course, if anyone of our readers would still like to receive electronically the LaTeX version of the newsletter then please do contact us about it and we shall try to do our best in providing you with whatever is requested.

Please do not hesitate to contact us in case of any problems. We would be happy to hear from you whether this way of distribution of the newsletter is satisfactory or perhaps even a better solution could be found. Thank you.

2.2 Psi-k 2000 Conference

"Ab initio (from electronic structure) calculations of complex proceses in materials"

Congress Centre (Stadtgarten), Schwäbisch Gmünd, 22-26 August, 2000

2.2.1 Web Site

Please note that both schematic and full programmes of the conference, and the lists of contributed talks and posters can be be found on our web site:

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

Please do check whether your name appears either in the list of contributed talks or posters, and whether your abstract is the one you wanted. Some of you have submitted more than one contribution and we had to make a selection, since only one contribution per participant is allowed. At the moment we have 422 registrations and the confernce programme is rather full. There are 4 plenary talks, 103 invited talks, 111 contributed talks and 154 posters. Some of the participants have chosen not to give a contribution, but we are still missing over 20 abstracts that some of you declared to contribute but have not delivered. Because of that, please do keep on checking the above web pages for any changes in the number of new posters. There may also be some further refinements to the programme and please do check them regularly before the conference.

Please see below for the current versions of the schematic and full programmes, lists of contributed talks and posters, and details on how to get to Schwäbisch Gmünd.

2.2.2 Book of abstracts

The book of abstracts is rather large and can be downloaded from the above web site. Please note that it is however a dynamical object and may still be changed before the conference. The printed copies of the book of abstracts will be distributed to you at the registration desk, so you should not bring your own copy downloaded and printed from the web above.

2.2.3 Accommodation

Please note that all participants have to take care of their own accommodation. So, if you have not booked a hotel place yet, please do so as soon as possible. We are being told that the hotels available in the centre of Schwäbisch Gmünd are already rather full. We have noticed, however, from the lists provided to us by the Tourist Office in Schwäbisch Gmünd, that many people registered to the conference have not booked their accommodation yet.

2.2.4 How to get to Schwäbisch Gmünd

From the Stuttgart Airport: Follow the signs for the S-Bahn (a large S sign). The train station in the Airport is situated in the underground of the arrival building. There you need to buy a ticket to Schwäbisch Gmünd from the automatic ticket machine. The single ticket costs 20.20 DM. It is possible to use bank notes and the machine gives change in coins. There are two trains (S2, S3) that one can take. At the Bad Cannstatt stop, the first one after the Hauptbahnhof, the main railway station, leave the train and change to the train for Schwäbisch Gmünd (direction Aalen). The whole journey time from the airport to Schwäbisch Gmünd is just over an hour.

To travel from the Stuttgart Airport to the main railway station (Hauptbahnhof), one needs to take S-Bahn (trains S2 or S3). The price of the ticket is 4.80 DM. The journey takes 27 minutes. The frequency of trains is at least three per hour from 5:00 until 24:00. You will arrive at the underground level of the 'Hauptbahnhof'.

If you are starting your journey from the Stuttgart main railway station or you want to break your journey to visit the town and then follow to Schwäbisch Gmünd, you can buy tickets for the train to Schwäbisch Gmünd at the street level, on the right hand side of the train station (facing the station building in the street outside). The price is 15.40 DM (return ticket 30.80 DM) for a second class ticket. Tickets are also available on the train but purchasing them on the train you will pay an extra 10 DM or so for convenience. The platforms for Schwäbisch Gmünd are one level above the street level. The track (=Gleis, in German) number from which the train leaves can be found on the timetables in the station. There are two timetable posters: Abfahrt (= departure) and Ankunft (= arrival). There is at least one train per hour from 5:51 until 23:22. The journey takes about 40mins.

Please note that detailed information on the train connections to Schwäbisch Gmünd can be found on the web pages of the Deutsche Bahn. Note that the Psi-k web site provides a link to the Deutsche Bahn web site.

A taxi from the Stuttgart Airport to Schwäbisch Gmünd costs about 130 DM, although one could try to negotiate a fixed price which might then be somewhat lower.

2.2.5 Schematic programme of the conference

Symposia

Title	Abbreviation
Bandstructure Methods	BSM
Correlated Systems	CORR-SYS
Density Functional Theory	DFT
Excited States/Quasiparticles	EXC/QP
F-electron Systems	F-EL
Interfaces	INTERF
Large Systems/O(N)	LARGE-SYS
Magnetism	MAGNET
Magneto-Electronics	MAGNET-EL
Materials	MATER
Molecular and Biological Materials	MOL/BIOL
Nanostructures and Quantum Dots	NANO/QD
Optimized Effective Potential	OEP
Polymers and Optoelectronics	POLYM
Quantum Monte Carlo	QMC
Semiconductors	SEMIC
Spectroscopies	SPECTR
Superconductivity	SUPERC
Surfaces	SURF

TUESDAY, August 22

15:00-20:00	Registration

WEDNESDAY, August 23

8:00 - 8:35	Registration		
Room:	*Baldung*	*Parler*	*Ratgeb*
8.40 - 8.55		Welcome	
		PLENARY	
		Chair: *R. Nieminen*	
9:00 - 9:50		**M. Scheffler**	
	CORR-SYS	SEMIC	POLYM
Chair:	*B.L. Gyorffy*	*R. Nieminen*	*M. Springborg*
10:00-10:30	**Pickett**	*Coffee*	**Weiss**
10:30-11:00	*Coffee*	**Hierlemann**	Bobbert, Katan
11:00-11:30	**Georges**	**Lindefelt**	*Coffee*
11:30-12:00	Fleck, Drchal	Bockstedte, Pollmann	**Cote**
12:00-12:30	Terakura, Fujiwara	**Blöchl**	**Frank**
12:30-14:00	**Lunch break**		
	MATER	SURF	BSM
Chair:	*J.L. Martins*	*J. Hafner*	*R. Zeller*
14:00-14:30	Pentcheva, Winkler	**Stampfl**	**Andersen**
14:30-15:00	**Bihlmayer**	A.Gross, Gandulia-P	**Saha-Dasgupta**
15:00-15:30	**Fichthorn**	Bernasconi, Rantala	**Skriver**
15:30-16:00	**Fang**	**Bogicevic**	Eschrig, Sjöstedt
16:00-16:30	*Coffee*	*Coffee*	*Coffee*
	NANO/QD	SURF	BSM
Chair:	*A. Rubio*	*A. Kiejna*	*G.M. Stocks*
16:30-17:00	**Williamson**	Rosa, Gottschalck	**Dederichs**
17:00-17:30	Martins, Nayak	**Alavi**	**Marzari**
17:30-18:00	**Todorov**	Soler, Neugebauer	**Krasovskii**
18:00-18:30	**Sanchez-Portal**	**Fiorentini**	Mavromaras, Hytha
18:30-19:00	**B-Nardelli**	**Morikawa**	Šimunek, Theurich
19:00-23:00	**Food and Posters**		

THURSDAY, August 24

Room:	*Baldung*	*Parler*	*Ratgeb*
		PLENARY	
		Chair: *B. Johansson*	
8:30 - 9:20		**N. Lang**	
	MATER	MAGNET	INTERF
Chair:	*M. Gillan*	*B. Johansson*	*M. Finnis*
9:30-10:00	**Martonak**	**Abrikosov**	**Köstelmeir**
10:00-10:30	**Colombo**	*Coffee*	Elsässer, Scheerschmidt
10:30-11:00	*Coffee*	**Staunton**	**Pasquarello**
11:00-11:30	Perez, Mannstadt	**Udvardi**	*Coffee*
11:30-12:00	**Kresse**	Ebert, Zabloudil	Lindan, Kohyama
12:00-12:30	Ikeda, Meyer	Frota-Pessoa, Enkovaara	**Sigle**
12:30-14:00	**Lunch break**		
	CORR-SYS	SURF	SPECTR
Chair:	*K. Terakura*	*E. Wimmer*	*H. Ebert*
14:00-14:30	Blaha, Tyer	**Nørskov**	**Redinger**
14:30-15:00	**Solovyev**	**Toulhoat**	Maca, Strange
15:00-15:30	**Lichtenstein**	S. Lorenz, Heid	**Paxton**
15:30-16:00	Manghi, Patterson	**Kollar**	**Lorente**
16:00-16:30	*Coffee*	*Coffee*	*Coffee*
	MAGNET	SEMIC	LARGE-SYS
Chair:	*J. Kübler*	*P. Kratzer*	*J.M. Soler*
16:30-17:00	K. Schwarz, Turek	**Ortega**	**Pettifor**
17:00-17:30	**Pederson**	Alippi, Hakala	Hoshi, Canning
17:30-18:00	**Blügel**	Brocks, G. Schwarz	**Ordejon**
18:00-18:30	Heinze, Ledentu	**Schröder**	**Goedecker**
18:30-19:00	**Baroni**	Seifert-L, Bernardini	**Bowler**
19:00-23:00	**Food and Posters**		

FRIDAY, August 25

Room:	*Baldung*	*Parler*	*Ratgeb*
		PLENARY	
		Chair: *K. Schwarz*	
8:30 - 9:20		**E.K.U. Gross**	
	SPECTR	DFT	MOL/BIOL
Chair:	*P. Strange*	*K. Schwarz*	*F. Seno*
9:30-10:00	**Alouani**	**Resta**	**Lesyng**
10:00-10:30	*Coffee*	Garcia-Gonzales, Kurth	Ireta, Petrilli
10:30-11:00	**Karlsson**	**Vitos**	*Coffee*
11:00-11:30	**van der Laan**	*Coffee*	**Röthlisberger**
11:30-12:00	Lambrecht, Van den Brink	**Snijders**	**Carloni**
12:00-12:30	**Crampin**	Ullrich, Nesbet	**Segall**
12:30-14:00	**Lunch break**		
	CORR-SYS	SEMIC	OEP
Chair:	*R. Martin*	*M. Scheffler*	*E.K.U. Gross*
14:00-14:30	Koch, Rosner	**Kratzer**	**Görling**
14:30-15:00	**Gunnarsson**	**Pesola**	Fleszar, Kim
15:00-15:30	**Mookerjee**	Wahnón, Fall	**Engel**
15:30-16:00	**Ezhov**	**Van de Walle**	**Seidl**
16:00-16:30	*Coffee*	*Coffee*	*Coffee*
	MAGNET-EL	MATER	EXC/QP
Chair:	*H. Dreysse*	*J. Kollar*	*O. Gunnarsson*
16:30-17:00	**Barthelemy**	Simak, Hirschl	**Louie**
17:00-17:30	**Butler**	**Gillan**	Schindlmayr, Yamasaki
17:30-18:00	**Papanikolaou**	Wahnström, Alatalo	**Wolf**
18:00-18:30	Blaas, Akai	**Christensen**	Fuchs, Van Gelderen
18:30-19:00	**Tsymbal**	Montanari, Lechermann	**Del Sole**
19:45-20:15	**Organ concert, Münster**		

SATURDAY, August 26

Room:	*Baldung*	*Parler*	*Ratgeb*
		PLENARY	
		Chair: *P. Dederichs*	
8:30 - 9:20		**P. Levy**	
	MOL/BIOL & POLYM	MAGNET-EL	SUPERC
Chair:	*C. Koenig*	*P. Dederichs*	*O.K. Andersen*
9:30-10:00	**Rovira**	**Mertig**	**Annett**
10:00-10:30	**Artacho**	*Coffee*	**Szotek**
10:30-11:00	*Coffee*	**Kudrnovsky**	Lüders, Maksimov
11:00-11:30	**Molinari**	Riedel, Zahn	*Coffee*
11:30-12:00	**Delley**	Oleinik, Xia	**Singh**
12:00-12:30	Seno, Springborg	**Mazin**	**Capelle**
12:30-14:00	**Lunch break**		
	F-EL	EXC/QP	SUPERC
Chair:	*L. Sandratskii*	*R. Del Sole*	*E. Maksimov*
14:00-14:30	**Svane**	**Reining**	**Pavarini**
14:30-15:00	**Svane**, Petit	Rohlfing, Kuzmin	Ambrosch-D, Massidda
15:00-15:30	Penicaud, Pickard	**Rubio**	Klein, Süle
15:30-16:00	*Coffee*	*Coffee*	*Coffee*
	F-EL & MAGNET	MATER	QMC
Chair:	*O. Eriksson*	*B. Winkler*	*E. Koch*
16:00-16:30	**Brooks**	Postnikov, Šob	**Needs**
16:30-17:00	Oppeneer, Sandratski	**Jepsen**	**Filippi**
17:00-17:30	**Nordström**	Crisan, Eglitis	**Caffarel**
17:30-18:00	Steinbeck, Cottenier	Münch, Parlinski	**Sorella**
		SUMMARY	
		Chair: *O.K. Andersen*	
18:05-18.35		**Heine**	
		Summary of the conference	
18:35-18:45		**Durham**	
		Closing of the conference	

2.2.6 Full programme of the conference

Conference Program: Authors, Titles and Schedules

Tuesday, 22 August 2000

15:00–20:00 Registration

Wednesday, 23 August 2000

08:00–08:35 Registration

Wednesday Morning Session, Parler room: Opening and Plenary
Chair: R.M. Nieminen

08:40–08:55 Welcome

09:00–09:50 M. Scheffler
The cutting edge: Surfaces and their role in materials' properties

Wednesday Morning Session, Baldung room: CORR-SYS
Chair: B.L. Gyorffy

10:00–10:30 W.E. Pickett, A. B. Shick, R. Weht
Coexistence of high temperature superconductivity and magnetism: $RuSr_2GdCu_2O_8$

10:30–11:00 Coffee

11:00–11:30 Antoine Georges
Introduction to dynamical mean field theory and prospects for electronic structure calculations of correlated materials

11:30–11:45 M. Fleck, E. Pavarini, and O. K. Andersen
Electronic Structure of the striped phase in $La_{2-x-y}Nd_ySr_xCuO_4$

11:45–12:00 V. Drchal, J. Kudrnovský, and V. Janiš
Dynamical electron correlations in transition metals and their alloys

12:00–12:15 K. Terakura, Z. Fang, K. Miura, J. Kanamori
Ferromagnetism and antiferromagnetism in double perovskites:
La_2FeCrO_6, Sr_2FeMoO_6 and Sr_2FeWO_6

12:15–12:30 Takeo Fujiwara, Michael Korotin, and Vladimir Anisimov
Long period orbital order with hole stripes in $La_{7/8}Sr_{1/8}MnO_3$

Wednesday Morning Session, Parler room: SEMIC

Chair: R.M. Nieminen

10:00–10:30 Coffee

10:30–11:00 M. Hierlemann
Quantum chemical calculation in an industrial environment

11:00–11:30 U. Lindenfelt
Electronic structure of intrinsic and doped SiC

11:30–11:45 M. Bockstedte, A. Mattausch, and O. Pankratov
Boron diffusion in SiC: the role of intrinsic point defects

11:45–12:00 J. Pollmann, P. Krüger, W. Lu, and M. Rohlfing
Theory of structural and electronic properties of SiC surfaces

12:00–12:30 P. Blöchl
Hydrogen electrochemistry in SiO_2 related to breakdown
of gate oxides

Wednesday Morning Session, Ratgeb room: POLYM

Chair: M. Springborg

10:00–10:30 H. Weiss, M. Boero, and M. Parrinello
DFT as a versatile tool in industrial catalysis research

10:30–10:45 J.-W. van der Horst, P.A. Bobbert, M.A.J. Michels, G. Brocks, P.J. Kelly
Electronic and optical properties of conjugated polymers from first principles

10:45–11:00 C. Katan, P. Rabiller, M. Souhassou
Charge density analysis in molecular charge transfer complexes:
a comparison between experiment and PAW calculations

11:00–11:30 Coffee

11:30–12:00 M. Côté, Peter D. Haynes, and Carla Molteni
New polymers for optoelectronic applications

12:00–12:30 I. Frank

Chemical reactions induced by mechanical stress: ab-initio simulation

12:30–14:00 Lunch

Wednesday Afternoon Session, Baldung room: MATER

Chair: J.L. Martins

14:00–14:15 Rossitza Pentcheva, Matthias Scheffler, and K. Fichthorn

Influence of substitutional adsorption on the initial growth of Co on Cu(001): a DFT-kMC study

14:15–14:30 B. Winkler, C. J. Pickard, V. Milman, G. Thimm

Systematic prediction of crystal structures and its application to sp^2-carbon polymorphs

14:30–15:00 G. Bihlmayer, Ph. Kurz, F. Förster, and S. Blügel

The FLAPW method applied to complex magnetic systems

15:00–15:30 Kristen A. Fichthorn

Island nucleation in thin-film epitaxy: a multi-scale study

15:30–16:00 Zhong Fang

Applications of ultrasoft pseudopotentials to 3d and 4d transition metal oxides

16:00–16:30 Coffee

Wednesday Afternoon Session, Parler room: SURF

Chair: J. Hafner

14:00–14:30 Catherine Stampfl

Ab initio modelling of temperature-programmed desorption of molecules from metallic surfaces

14:30–14:45 A. Groß, A. Eichler, J. Hafner, F. Kirchhoff, M.J. Mehl, and D.A. Papaconstantopoulos

Ab initio derived tight-binding molecular dynamics simulation of O_2/Pt(111): new unified picture of the molecular adsorption process

14:45–15:00 M.V. Ganduglia-Pirovano, K. Reuter, M. Scheffler

Surface core-level shifts as a probe of the local overlayer structure: O on Rh(111) and Ru(0001)–a DFT study

15:00–15:15 D. Ceresoli, M. Bernasconi, S. Iarlori, M. Parrinello, E. Tosatti
Two-membered silicon rings on a dehydroxylated surface of silica

15:15–15:30 T. T. Rantala,T. S. Rantala, and V. Lantto
Surface relaxation and electronic structure of SnO_2 (110) surface

15:30–16:00 Alexander Bogicevic
Atomistic concepts in epitaxial growth

16:00–16:30 Coffee

Wednesday Afternoon Session, Ratgeb room: BSM

Chair: R. Zeller

14:00–14:30 O.K. Andersen and T. Saha-Dasgupta
Muffin tin orbitals of arbitrary order (NMTOs)

14:30–15:00 T. Saha-Dasgupta and O. K. Andersen
Tight-binding modeling and generation of first-principles Wannier-like orbitals using the new NMTO scheme

15:00–15:30 L. Vitos, H. L. Skriver, and J. Kollar
Application of the exact muffin-tin orbitals theory

15:30–15:45 Helmut Eschrig, Klaus Koepernik
Density functional theory of low temperature phase diagrams: magnetism in the $[Fe(Mn)]_{(1-x)}Al_x$ system

15:45–16:00 Elisabeth Sjöstedt and Lars Nordström
A cautious linearization of the full-potential APW method

16:00–16:30 Coffee

Wednesday Late Afternoon Session, Baldung room: NANO/QD

Chair: A. Rubio

16:30–17:00 A.J. Williamson, A. Franceschetti, and A. Zunger
Calulations of multiple excitons in InAs quantum dots

17:00–17:15 J. M. Pacheco, José Luís Martins
First principles Monte-Carlo optimization of geometries of large alkali clusters

17:15–17:30 Saroj K. Nayak
Exploring magnetism at the nanoscale with electronic structure calculations

17:30–18:00 T. N. Todorov, A. P. Sutton, and J. Hoekstra
Current-induced mechanical effects in atomic-scale conductors

18:00–18:30 D. Sánchez-Portal, E. Artacho, J. Junquera, J. M. Soler
P. Ordejón, A. García
Monatomic gold wires

18:30–19:00 Marco Buongiorno Nardelli
Theory of electronic and transport properties of carbon nanotubes

Wednesday Late Afternoon Session, Parler room: SURF

Chair: A. Kiejna

16:30–16:45 A. Rosa and J. Neugebauer
Silicon at (0001)GaN surfaces: surface structures and adatom kinetics

16:45–17:00 Z. Sljivančanin, J. Gottschalck, and B. Hammer
H_2 dissociation on defected Cu(111): role of steps, vacancies, kinks and adatoms

17:00–17:30 Ali Alavi
Chemistry at metal surfaces from density-functional theory

17:30–17:45 Jose M. Soler, Emilio Artacho, and Gabriel Fabricius
Structure of the liquid silicon surface

17:45–18:00 J. Neugebauer, T. K. Zywietz, M. Scheffler, J. E. Northrup
Adatom kinetics on and below the surface: The presence of a novel diffusion channel

18:00–18:30 Alessio Filippetti and Vincenzo Fiorentini
Theory and applications of the stress density

18:30–19:00 Yoshitada Morikawa and Kiyoyuki Terakura
Ab initio study of methanol synthesis over Zn-deposited Cu surfaces

Wednesday Late Afternoon Session, Ratgeb room: BSM

Chair: G.M. Stocks

16:30–17:00 P. H. Dederichs, N. Papanikolaou, and R. Zeller
Conceptional improvements of the KKR method

17:00–17:30 Nicola Marzari and David Vanderbilt
Localized Wannier functions in extended systems: theory and applications

17:30–18:00 E. E. Krasovskii and W. Schattke
Electronic structure of bulk and semi-infinite crystals by the extended LAPW-kp method

18:00–18:15 A. Mavromaras, A. Ponceau, I. Lado Touriño, F. Tsobnang, J. Sticht, and E. Wimmer
Optimized basis sets in a full potential LMTO method

18:15–18:30 Marek Hytha, Jiří Vackář, and Antonin Šimůnek
Core-level shifts within pseudopotential framework

18:30–18:45 Antonín Šimůnek and Jiří Vackář
Semicore states in all electron pseudopotentials: ground state properties of NaCl

18:45–19:00 G. Theurich, N. A. Hill
General local spin density approximation for plane wave pseudopotential calculations

Wednesday Evening Session

19:00–23:00 Food and Posters

Thursday, 24 August 2000

Thursday Morning Session, Parler room: Plenary
Chair: B. Johansson

08:30–09:25 N. Lang
DFT studies in molecular electronics

Thursday Morning Session, Baldung room: MATER
Chair: M. Gillan

09:30–10:00 R. Martoňák, C. Molteni, L. Colombo, M. Parrinello
Molecular dynamics with a classical pressure reservoir: simulation of pressure-induced transformations in silicon clusters

10:00–10:30 Luciano Colombo

Science-based engineering of defects in silicon by tight-binding molecular dynamics DFT studies in molecular electronics

10:30–11:00 Coffee

11:00–11:15 Rubén Pérez, Peter Gumbsch

Directional anisotropy in the cleavage fracture of silicon

11:15–11:30 W.Mannstadt, A.Canning, A.J. Freeman

Large scale computing and complex materials with the massive parallel FLAPW method

11:30–12:00 G. Kresse

Fast all-electron ab-initio molecular dynamics

12:00–12:15 M. Ikeda, G. Kresse, and J. Hafner

First principles study of bi-layered ferroelectric perovskite materials

12:15–12:30 Na Sai, B. Meyer, and David Vanderbilt

Design of novel ferroelectric materials via compositional inversion symmetry breaking

Thursday Morning Session, Parler room: MAGNET

Chair: B. Johansson

09:30–10:00 I. A. Abrikosov, B. Johansson, Mark van Schilfgaarde

Understanding the INVAR effect in Fe-Ni alloys

10:00–10:30 Coffee

10:30–11:00 J.B. Staunton, J. Poulter, B. Ginatempo, E. Bruno, D.D. Johnson

Spin fluctuations in nearly magnetic metals from ab-initio dynamical spin susceptibility calculations

11:00–11:30 László Udvardi, László Szunyogh, Peter Weinberger

Ab–initio determination of the width of Bloch–wall in Fe

11:30–11:45 H. Ebert, M. Deng, and H. Freyer

Relativistic calculation of magnetic linear response functions using the KKR-Green's function method

11:45–12:00 J. Zabloudil, R. Hammerling, P. Weinberger, C. Uiberacker

Magnetic anisotropy of Co on Cu(111) including relaxation effects

12:00–12:15 Sonia Frota-Pessôa

Exchange coupling from first principles in nonperiodi systems

12:15–12:30 J. Enkovaara, A. Ayuela, R.M. Nieminen, L. Nordström

Magnetic and orbital anisotropy in Ni_2MnGa from first principles

Thursday Morning Session, Ratgeb room: INTERF

Chair: M. Finnis

09:30–10:00 S. Köstlmeier and C. Elsässer

Ab-initio investigation of metal/ceramic bonding: metal/spinel interfaces

10:00–10:15 C. Elsässer, S. Nufer, A. G. Marinopoulos, T. Gemming, W. Kurtz, S. Köstlmeier, and M. Rühle

Microscopic analysis of the rhombohedral twin grain boundary in alumina

10:15–10:30 Kurt Scheerschmidt and Detlef Conrad

Modified empirical potentials for molecular dynamics modelling of bonded interfaces

10:30–11:00 Alfredo Pasquarello

Atomic structure at the interface between silicon and its oxide

11:00–11:30 Coffee

11:30–11:45 Philip Lindan

Interfaces between oxides and aqueous solutions

11:45–12:00 Masanori Kohyama

Strength and fracture of SiC grain boundaries: Ab Initio tensile tests

12:00–12:30 Wielfried Sigle

Electron microscopy studies of grain boundary and interface structures

12:30–14:00 Lunch

Thursday Afternoon Session, Baldung room: CORR-SYS

Chair: K. Terakura

14:00–14:15 P.Blaha, K. Schwarz, P.Novak

Charge distribution and EFGs in cuprates using LDA+U within the LAPW method

14:15–14:30 R. Tyer, W.M.Temmerman, Z. Szotek, H. Winter, and G.A.Gehring
Application of the self-interaction correction to $LaMnO_3$ and $CaMnO_3$

14:30–15:00 I. V. Solovyev
Aspects of charge, spin, and orbital ordering in manganites

15:00–15:30 A. Lichtenstein
Electronic structure of correlated systems: beyond LDA

15:30–15:45 Franca Manghi, Stefano Monastra, Catia Arcangeli
On-site correlation in the photoemission of transition metals

15:45–16:00 C.H. Patterson and M. Nicastro
Exchange coupling in manganites and cuprates

16:00–16:30 Coffee

Thursday Afternoon Session, Parler room: SURF

Chair: E. Wimmer

14:00–14:30 J. Nørskov
Catalysis from first principles?

14:30–15:00 Hervé Toulhoat and Pascal Raybaud
Periodic trends and synergy effects in hydrodesulfurization catalysts: recent findings based on electronic structure calculations

15:00–15:15 Sönke Lorenz, Matthias Scheffler, Axel Groß
Reactions on surfaces with neural networks

15:15–15:30 R. Heid and K.-P. Bohnen
First principles investigations of the lattice dynamics of the Ru(0001) and O(1×1)/Ru(0001) surfaces

15:30–16:00 J. Kollár, L. Vitos, B. Johansson, H. L. Skriver
Stability of surfaces and small particles; surface, step, and kink formation energies

16:00–16:30 Coffee

Thursday Afternoon Session, Ratgeb: SPECTR

Chair: H. Ebert

14:00–14:30 Josef Redinger
First-principles simulation of scanning tunneling microscopy and spectroscopy

14:30–14:45 F. Máca, W.A. Hofer, J. Redinger

Comparison betwen ab-initio simulation and STM-images for Co/Pt(110) surfaces

14:45–15:00 M. Woods, P. Strange, A. Ernst, and W. M. Temmerman

Relativistic theory of photoemission from magnetic surfaces

15:00–15:30 A T Paxton

Near edge structure in energy-loss spectroscopy of transition metal nitrides: some many electron and magnetic effects using density functional theory

15:30–16:00 N. Lorente and M. Persson

First principles calculations of single molecule vibrational spectroscopy and microscopy

16:00–16:30 Coffee

Thursday Late Afternoon Session, Baldung room: MAGNET

Chair: J. Kübler

16:30–16:45 K. Schwarz, G. K. H. Madsen, and P. Blaha

Unusual magnetism in sodium or potassium electro sodalite (SES or PES)

16:45–17:00 I. Turek

Exchange interactions in itinerant magnets

17:00–17:30 Mark R. Pederson

Molecular magnets: anisotropy energies and resonant tunneling fields within DFT

17:30–18:00 S. Blügel, X. Nie, and G. Bihlmayer

Magnetic anisotropy in low dimensional systems

18:00–18:15 S. Heinze, Ph. Kurz, G. Bihlmayer, D. Wortmann, X. Nie, S. Blügel, M. Bode, A. Kubetzka, O. Pietzsch, R. Wiesendanger

Resolving complex atomic-scale spin-structures by spin-polarized STM

18:15–18:30 V. Ledentu, D. Spisak, J. Hafner

Structure and magnetism of Fe/Ge multilayers

18:30–19:00 Stefano Baroni

Magnons in real materials from density functional theory

Thursday Late Afternoon Session, Parler room: SEMIC

Chair: P. Kratzer

16:30–17:00 J. Ortega, R. Pérez, and F. Flores
Electron correlation effects and dynamical fluctuations at semiconductor surfaces: Sn/Si(111) and Sn/Ge(111)

17:00–17:15 P. Alippi, L. Colombo, A. Sieck, G. Seifert, T. Frauenheim
Boron related defects in silicon by density functional based tight-binding simulations

17:15–17:30 M. Hakala, M. J. Puska, and R. M. Nieminen
First-principles calculations of interstitial B in Si

17:30–17:45 G. Brocks, J.H. Snoeier, P. J. Kelly, E. Zoethout, H. J. W. Zandvliet, and B. Poelseman
The initial stages of growth on the Ge(001) surface: a joint theoretical and experimental study

17:45–18:00 G. Schwarz, J. Neugebauer, and M. Scheffler
Point defects in supercells: convergence with respect to cell size and charge compensation

18:00–18:30 Kurt Schroeder, Armin Antons, Ralf Berger, Stefan Blügel
Theory of surfactant-mediated growth

18:30–18:45 K. Seifert-Lorenz, J. Hafner, G. Kresse
Ab-initio MD of liquid Te and telluriumrich K-Te alloys

18:45–19:00 Fabio Bernardini and Vincenzo Fiorentini
Non-linear behavior of spontaneous polarization in III-V nitrides alloys

Thursday Late Afternoon Session, Ratgeb room: LARGE-SYS

Chair: J. M. Soler

16:30–17:00 D.G. Pettifor, I.I. Oleinik, and D. Nguyen-Manh
Bond-order potentials: bridging the electronic to atomistic modelling hierarchies

17:00–17:15 Takeo Hoshi and Takeo Fujiwara
Theory of Wannier states and order-N electronic structure calculations

17:15–17:30 A. Canning, W. Mannstadt, Wen-tong Geng, and A.J. Freeman
Parallelization of the FLAPW method and applications to large systems

17:30–18:00 Pablo Ordejón
Numerical-atomic-orbitals DFT approach for large systems: applications of SIESTA

18:00–18:30 Stefan Goedecker
Linear scaling methods for electronic structure calculations

18:30–19:00 D.R. Bowler, T.Miyazaki, and M.J.Gillan
Conquest: principles and applications of a linear scaling DFT code

Thursday Evening Session

19:00–23:00 Food and Posters

Friday, 25 August 2000

Friday Morning Session, Parler room: Plenary
Chair: K. Schwarz

08:30–09:25 E.K.U. Gross
New directions in density functional theory

Friday Morning Session, Baldung room: SPECTR
Chair: P. Strange

09:30–10:00 I. Galanakis, M. Alouani, H. Dreyssé
Calculated X-ray magnetic circular dichroism of binary alloys and surfaces

10:00–10:30 Coffee

10:30–11:00 Krister Karlsson, O. Gunnarsson, and O. Jepsen
Cuprate core-level line shapes for different Cu-O networks

11:00–11:30 Gerrit van der Laan
Configuration interaction effects in core-level dichroism of magnetic materials

11:30–11:45 Walter R. L. Lambrecht and Sergey N. Rashkeev
Nonlinear optical response calculations in chalcopyrite semiconductors and the relation to their band structures

11:45–12:00 Jeroen van den Brink, Eva Pavarini, Patrizia Benedetti, Assunta Vigliante, Peter Wochner
Ab initio calculation of resonant X-ray scattering in manganites

12:00–12:30 S. Crampin, E. Arola, M. James, L. Calmels, J.E. Inglesfield
Calculation of second harmonic generation from magnetic interfaces

Friday Morning Session, Parler room: DFT

Chair: K. Schwarz

09:30–10:00 Raffaele Resta
Macroscopic polarisation and electron localisation in extended systems

10:00–10:15 P. García-González, P. Sánchez-Friera, and R. W. Godby
Self-consistent calculations of the total energies of electron systems using many-body theory

10:15–10:30 Stefan Kurth, John P. Perdew, Aleš Zupan, Peter Blaha
Accurate density functional with correct formal properties: A step beyond the generalized gradient approximation

10:30–11:00 L. Vitos, B. Johansson, J. Kollár, H. L. Skriver
Kinetic and exchange functionals in the local Airy gas approximation

11:00–11:30 Coffee

11:30–12:00 J.G. Snijders, F. Kootstra, P.L. de Boeij
Time dependent density functional theory in extended systems

12:00–12:15 Carsten A. Ullrich and Giovanni Vignale
Linewidth of collective intersubband transitions in quantum wells

12:15–12:30 Robert K. Nesbet
Orbital-functional theory as an exact N-electron model

Friday Morning Session, Ratgeb room: MOL/BIOL

Chair: F. Seno

09:30–10:00 B. Lesyng

Mesoscopic Poisson-Boltzmann and quantum-classical studies of enzymatic-reaction

10:00–10:15 Joel Ireta, Jörg Neugebauer, Matthias Scheffler, Arturo Rojo, Marcelo Galván

Strain induced phase transition of an alpha-helix: the interplay between hydrogen bonds and peptide planarity

10:15–10:30 H. M. Petrilli, B. Ctortecka, W. Tröger, T. Butz

Electric field gradients in metal complexes with biological applications

10:30–11:00 Coffee

11:00–11:30 Ursula Röthlisberger

First-principles modeling of enzymes

11:30–12:00 Paolo Carloni

Drug-target interactions in anti-AIDS therapy: an ab initio approach

12:00–12:30 M.D. Segall, M.C. Payne, P.J. Eddershaw

An ab initio study of cytochrome P450 enzymes: understanding and predicting drug metabolism

12:30–14:00 Lunch

Friday Afternoon Session, Baldung room: CORR-SYS

Chair: R. Martin

14:00–14:15 E. Koch and Stefan Goedecker

Decay properties of the density matrix and Wannier functions for interacting systems

14:15–14:30 H. Rosner, S.-L. Drechsler, K. Koepernik, R. Hayn, and H. Eschrig

The electronic structure of $CuSiO_3$ - a possible candidate for a new inorganic spin-Peierls compound?

14:30–15:00 O. Gunnarsson and J. Han

Resistivity of alkali-doped fullerenes: Lack of saturation at high temperatures?

15:00–15:30 Abhijit Mookerjee, Tanusri Saha-Dasgupta

An augmented space recursive approach to the solution of the Hubbard model

15:30–16:00 S. Yu. Ezhov, V. I. Anisimov, D. I. Khomskii, G. A. Sawatzky

Orbital occupation, local spin and exchange interactions in V_2O_3

16:00–16:30 Coffee

Friday Afternoon Session, Parler room: SEMIC

Chair: M. Scheffler

14:00–14:30 P. Kratzer and M. Scheffler

From DFT studies to growth simulations: Modeling molecular beam epitaxy of arsenide compound semiconductors

14:30–15:00 M. Pesola, Y. J. Lee, R.M. Nieminen, J. von Boehm

Oxygen-related defects in Si and GaAs

15:00–15:15 P. Wahnón, J. Fernández, and C. Tablero

Electronic structure calculations for new photovoltaic materials

15:15–15:30 C.J. Fall, R. Jones, P. R. Briddon, S. Öberg

Electronic and vibrational properties of Mg- and O-related complexes in GaN

15:30–16:00 Chris G. Van de Walle and J. Neugebauer

Properties of GaN surfaces: the role of hydrogen

16:00–16:30 Coffee

Friday Afternoon Session, Ratgeb: OEP

Chair: E.K.U. Gross

14:00–14:30 Andreas Görling

Advances in DFT by treating exchange exactly

14:30–14:45 Andrzej Fleszar

Exact exchange (EXX) and GW calculations of the electronic structure of semiconductors

14:45–15:00 Y.-H. Kim

Exact-exchange-based hybrid-method investigations of small molecules

15:00–15:30 E. Engel, A. Höck, and R. M. Dreizler
Description of dispersion forces with implicit density functionals

15:30–16:00 Michael Seidl, John P. Perdew, Stefan Kurth
Strong-interaction limit of density functional theory: its simplicity and its relevance for electron systems

16:00–16:30 Coffee

Friday Late Afternoon Session, Baldung room: MAGNET-EL

Chair: H. Dreyssé

16:30–17:00 A. Barthélémy, J.M.De Teresa, A.Fert, J.P.Contour F.Pailloux, J.L.Maurice, M.Bowen, A.Vaures
Magnetic tunnel junctions : experimental results and open questions

17:00–17:30 W.H. Butler, X.-G. Zhang, T. C. Schulthess, J. M. MacLaren
Spin dependent tunneling in Fe|MgO|Fe

17:30–18:00 N. Papanikolaou, Ph. Mavropoulos, M. Freyss, R.Zeller, and P.H. Dederichs
Spin dependent transport in metal-insulator junctions

18:00–18:15 Claudia Blaas, Peter Weinberger, Laszlo Szunyogh, Peter M. Levy, and Charles Sommers
Theoretical evaluation of magnetotransport properties in Co/Cu/Co-based spin-valves

18:15–18:30 H. Akai, T. Kamatani, and S. Watanabe
Electronic structure and magnetism of diluted magnetic semiconductors

18:30–19:00 E.Y. Tsymbal
Spin polarization of conductance in magnetic tunnel junctions

Friday Late Afternoon Session, Parler room: MATER

Chair: J. Kollar

16:30–16:45 S. I. Simak, U. Häussermann, S. Lidin, R. Ahuja, and B. Johansson
Group-III metals under high pressure: a unified bonding picture

16:45–17:00 R. Hirschl, J. Hafner, Y. Jeanvoine
Ab initio phase diagram of palladium-vanadium alloys

17:00–17:30 Mike Gillan, Dario Alfè, and David Price
How to find the chemical composition of the Earth's core using DFT

17:30–17:45 K. Carling, G. Wahnström, T. R. Mattsson, A. E. Mattsson, N. Sandberg, G. Grimvall
Vacancies in metals: from ab-initio calculations to experimental data

17:45–18:00 M. Alatalo, M. Weinert
Defect–defect interactions in Al

18:00–18:30 Niels E. Christensen
New high-pressure phases of alkli metals and semiconductors

18:30–18:45 Barbara Montanari and Michael W. Finnis
Alumina: a tight-binding model with polarisable ions

18:45–19:00 F. Lechermann and M. Fähnle
Ab-initio statistical mechanics for ordering phenomena and phase diagrams of compounds including the effect of vacancies

Friday Late Afternoon Session, Ratgeb room: EXC/QP

Chair: O. Gunnarsson

16:30–17:00 Steven G. Louie
Ab initio optical absorption spectra

17:00–17:15 Arno Schindlmayr
Decay properties of the one-particle Green function in real space and imaginary time

17:15–17:30 Atsushi Yamasaki and Takeo Fujiwara
Quasiparticle properties of transition metals in the GW approximation

17:30–18:00 Walter Wolf, Sandro Massidda, Michele Posternak, Jürgen Sticht, and Erich Wimmer
Screened exchange FLAPW calculations of optical properties

18:00–18:15 M. Fuchs, X. Gonze, T. Klüner, and M. Scheffler
Potential energy surfaces of excited states from time-dependent density-functional theory

18:15–18:30 P. van Gelderen, P.A. Bobbert, P.J. Kelly, and G. Brocks
Parameter-free quasi-particle calculations for YH_3

18:30–19:00 R. Del Sole, G. Onida, P. Monachesi, M. Palummo
Ab-initio calculation of optical properties of surfaces

Friday Evening Session

19:45–20.15 Organ concert, Münster

Saturday, 26 August 2000

Saturday Morning Session, Parler room: Plenary
Chair: P.H. Dederichs

08:30–09:25 Peter M. Levy
Magnetotransport in multilayered structures

Saturday Morning Session, Baldung room: MOL/BIOL & POLYM
Chair: C. Koenig

09:30–10:00 Carme Rovira and Michele Parrinello
Ligand binding properties of myoglobin modeled by first principles molecular dynamics

10:00–10:30 Emilio Artacho
Large scale calculations on DNA and proteins

10:30–11:00 Coffee

11:00–11:30 A. Ruini, F. Rossi, E. Molinari, R.B. Capaz, and M.J. Caldas
Ab-initio study of Coulomb-correlated optical properties in conjugated polymers

11:30–12:00 Bernard Delley
Structural switching in condensed molecular complexes triggered by optical excitations

12:00–12:15 Flavio Seno
Learning effective energy functions for protein structure prediction

12:15–12:30 Michael Springborg
Modifying polyacetylene

Saturday Morning Session, Parler room: MAGNET-EL

Chair: P.H. Dederichs

09:30–10:00 I. Mertig, J. Binder, and P. Zahn
The phenomenon of giant magnetoresistance: an ab initio description

10:00–10:30 Coffee

10:30–11:00 J. Kudrnovský, V. Drchal, I. Turek, C. Blaas, P. Weinberger, and P. Bruno
Ab initio theory of perpendicular transport in layered magnetic systems

11:00–11:15 I. Riedel, P. Zahn, and I. Mertig
Transmission coefficients - a new formalism

11:15–11:30 Peter Zahn and Ingrid Mertig
Ab initio description of TMR electrodes Fe, Co, and Ni

11:30–11:45 I.I. Oleinik, E.Yu. Tsymbal, and D.G. Pettifor
Structural and electronic properties of $Co/Al_2O_3/Co$ magnetic tunnel junction from first-principles

11:45–12:00 K. Xia, P. J. Kelly, G. E. W. Bauer, I. Turek, J. Kudrnovský, and V. Drchal
Interface resistance of disordered magnetic multilayers

12:00–12:30 I.I. Mazin
Is spin polarization a measurable quantity?

Saturday Morning Session, Ratgeb room: SUPERC

Chair: O.K. Andersen

09:30–10:00 James F. Annett
Exotic superconductors

10:00–10:30 Z. Szotek, B. L. Gyorffy, W. M. Temmerman, O. K. Andersen, and O. Jepsen
Quasiparticles in d-wave superconductors

10:30–10:45 M. Lüders, M. Marques, L. Fast, E. K. U. Gross
Strong electron-phonon coupling in the density functional theory for superconductors

10:45–11:00 E.G. Maksimov and D.Yu. Savrasov
Dynamical stability, electron-phonon interaction and superconductivity in hydrogen at high pressure

11:00–11:30 Coffee

11:30–12:00 David J. Singh and Igor I. Mazin
Is singlet and triplet superconductivity incompatible?

12:00–12:30 Klaus Capelle
Relativistic effects and dichroism in superconductors

12:30–14:00 Lunch

Saturday Afternoon Session, Baldung room: F-EL

Chair: L. Sandratskii

14:00–14:45 A. Svane, L. Petit, W. Temmerman, Z. Szotek, P. Strange, and H. Winter
Self-interaction corrected electronic structure of lanthanides and actinides

14:45–15:00 L. Petit, A. Svane, W.Temmerman, Z. Szotek
Electronic structure of americium compounds in the self-interaction corrected local-spin-density approximation

15:00–15:15 M. Pénicaud
Calculated equilibrium properties, electronic structures and structural stabilities of Th, Pa, U, Np and Pu

15:15–15:30 C. J. Pickard, B. Winkler, R. K. Chen, M.H. Lee, J.S. Lin, M. C. Payne, J. A. White, V. Milman, and D. Vanderbilt
Structural properties of lanthanide and actinide compounds within the planewave pseudopotential approach

15:30–16:00 Coffee

Saturday Afternoon Session, Parler room: EXC/QP

Chair: R. Del Sole

14:00–14:30 Lucia Reining and Valerio Olevano
Application of Green functions methods to the calculation of excited states

14:30–14:45 Michael Rohlfing and Johannes Pollmann
Surface excitons at the Si(111)-(2x1) surface

14:45–15:00 M. Kuzmin, C.D. Hogan, and C.H. Patterson
Quasi-particle band structures of wide-gap insulators

15:00–15:30 A. Rubio, I. Campillo, J. M. Pitarke, V. M. Silkin, E. V. Chulkov, P. M. Echenique
Lifetime of hot electrons in metals

15:30–16:00 Coffee

Saturday Afternoon Session, Ratgeb: SUPERC

Chair: E. Maksimov

14:00–14:30 Eva Pavarini, O. Jepsen, and O. K. Andersen
Hyperfine fields in cuprate superconductors

14:30–14:45 Claudia Ambrosch-Draxl, Pavel Korzahvyi, and Börje Johansson
Ab initio study of the oxygen orderig in $YBa_2Cu_3O_{7-x}$

14:45–15:00 C. Franchini, S. Massidda, A. Continenza, A. Gauzzi
Structural and electronic properties of $Hg_{1-y}Mo_yBa_2CuO_{4+\delta}$

15:00–15:15 Barry M. Klein
Instabilities in A15 compounds: A first-principles study

15:15–15:30 P. Süle and C. Ambrosch-Draxl
Hole doping in the $HgBa_2CuO_{4+\delta}$ *high* T_c *superconductor*

15:30–16:00 Coffee

Saturday Late Afternoon Session, Baldung room: F-EL & MAGNET

Chair: O. Eriksson

16:00–16:30 M.S.S. Brooks
Relativistic effects in f-electron systems

16:30–16:45 P. M. Oppeneer, T. Kraft, M. S. S. Brooks
Electronic structure of plutonium monochalcogenides

16:45–17:00 L. M. Sandratskii
Incommensurate magnetic structures in relativistic systems

17:00–17:30 Lars Nordström
Magnetism of the rare earth from first principles calculations

17:30–17:45 L. Steinbeck, M. Richter, and H. Eschrig
Itinerant-electron magnetocrystalline anisotropy energy of rare-earth transition-metal intermetallics from density functional calculations

17:45–18:00 Stefaan Cottenier and Heinz Haas
Hyperfine fields and local relaxations for impurities in bcc Fe: an FLAPW study

Saturday Late Afternoon Session, Parler room: MATER
Chair: B. Winkler

16:00–16:15 A. V. Postnikov, P. Entel, P. Ordejón
Structure and electronic properties of non-metallic surfaces and nanoparticles

16:15–16:30 M. Šob, L.G. Wang, V. Vitek
Theoretical tensile strength in metals and intermetallics

16:30–17:00 O. Jepsen and O.K. Andersen
Early slackness in high pressure phases

17:00–17:15 V. Crisan, H. Ebert, P. Entel, H. Akai
Stability and ordering in AlZn alloy system

17:15–17:30 R.I. Eglitis, E.A. Kotomin, and G. Borstel
Computer modelling of ABO_3 perovskites

17:30–17:45 W. Münch, K.-D. Kreuer, J. Maier, G. Seifert
Investigation of the proton diffusion mechanism in liquid imidazole using ab initio and quantum molecular dynamics simulations

17:45–18:00 K. Parlinski
Ab initio calculations of lattice dynamics and phase transitions

Saturday Late Afternoon Session, Ratgeb room: QMC
Chair: E. Koch

16:00–16:30 R.J. Needs, A.R. Porter, M.D. Towler, Y. Lee, W.K. Leung, G. Rajagopal, P.R.C. Kent, R.Q. Hood, W.M.C. Foulkes, S. Itoh, and S. Ihara
Accurate QMC calculations for ground and excited states

16:30–17:00 Claudia Filippi

Energy derivatives in quantum Monte Carlo: forces and optimization

17:00–17:30 Michel Caffarel

Zero-Variance principle for classical and quantum Monte Carlo algorithms

17:30–18:00 F. Becca, L. Capriotti, and S. Sorella

Stability of d-wave superconductivity in the t-J model

Saturday Early Evening Session, Parler room: SUMMARY

Chair: O.K. Andersen

18:05–18:35 V. Heine

Summary of the Conference

18:35–18:45 P.J. Durham

Closing of the Conference

2.2.7 List of contributed talks

Contributed talks

Bandstructure methods

H. Eschrig and Klaus Koepernik

Density functional theory of low temperature phase diagrams: Magnetism in the $[Fe(Mn)]_{(1-x)}Al_x$

E. Sjöstedt and Lars Nordström

A cautious linearization of the full potential APW method

A. Mavromaras, A. Ponceau, I. Lado Tourio, and F. Tsobnang

Optimized basis sets in a full potential LMTO method

M. Hytha, Jiří Vackář, and Antonin Šimůnek

Core-level shifts within pseudopotential framework

A. Šimůnek and Jiří Vackář

Semicore states in all electron pseudopotentials: ground state properties of NaCl

G. Theurich and N. A. Hill

General local spin density approximation for plane wave pseudopotential calculations

Correlated systems

M. Fleck, E. Pavarini and O. K. Andersen

Electronic structure of the striped phase in $La_{2-x-y}Nd_ySr_xCuO_4$

V. Drchal, J. Kudrnovský, and V. Janiš

Dynamical electron correlations in transition metals and their alloys

K. Terakura, Z. Fang, K. Miura, and J. Kanamori

Ferromagnetism and antiferromagnetism in double perovskites: La_2FeCrO_6, Sr_2FeMoO_6 and Sr_2FeWO_6

T. Fujiwara, Michael Korotin, and Vladimir Anisimov

Long period orbital order with hole stripes in $La_{7/8}Sr_{1/8}MnO_3$

P. Blaha, K. Schwarz, and P. Novak

Charge distribution and EFGs in cuprates using LDA+U within the LAPW method

R. Tyer, W.M. Temmerman, Z. Szotek, H. Winter, and G.A. Gehring

Application of the self-interaction correction to $LaMnO_3$ and $CaMnO_3$

F. Manghi, Stefano Monastra, and Catia Arcangeli

On-site correlation in the photoemission of transition metals

C. Patterson and M. Nicastro

Exchange coupling in the manganites and cuprates

E. Koch and Stefan Goedecker

Decay properties of the density matrix and Wannier functions for interacting systems

H. Rosner, S.-L. Drechsler, K. Koepernik, R. Hayn, and H. Eschrig

The electronic candidate for $CuSiO_3$ - a possible candidate for a new inorganic spin-Peierls compound?

Density Functional Theory

P. Garcia-Gonzales, Paula Sánchez-Friera, and R. W. Godby

Self-consistent calculations of the total energies of electron systems using many-body theory

S. Kurth, J. P. Perdew, A. Zupan, P. Blaha

Accurate density functional with correct formal properties: A step beyond the generalized gradient correction

C. Ullrich and Giovanni Vignale

Linewidth of collective intersubband transitions in quantum wells

R. Nesbet

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Surface relaxation and electronic structure of SnO_2 *(110) surface*

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P113. I. Galanakis, M. Alouani, H. Dreyssé, P. M. Oppeneer, P. Ravindran, L. Nordström, P. James, and O. Eriksson

Anomalous orbital magnetism: VAu_4

P114. Alexei Grechnev, Rajeev Ahuja, and Olle Eriksson

Magnetooptical Kerr effect in Fe/Au superlattices: theory

P115. Jürgen Henk and Börje Johansson

Quantum-size effects in photoemission from ultra-thin films: theory and application to Cu-films on fcc-Co(001)

P116. L. Hozoi, A.H. de Vries, C. de Graaf, P.S. Bagus, and R. Broer

Theoretical study of XPS spectra in late transition metal oxides

P117. Tilman Huhne and Hubert Ebert

Magneto-optical properties of multilayer- and surface layer systems

P118. P. Krüger, S. Tellmann, and J. Pollmann

Near-edge fine-structure of semiconductors: results from ab-initio studies

P119. Mariana Weissmann and Ana Maria Llois

Observation by STM of 3d transition metal atoms and clusters adsorbed on the Au(111) surface: Signatures derived from one-electron calculations

P120. J. A. Maytorena, B. S. Mendoza, W. L. Mochán

Visible-infrared sum and difference frequency generation at adsorbate-covered Au

P121. J. Minár, V. Popescu, H. Ebert, L. Sandratskii, A. Mavromaras

Treatment of non-collinear spin-structures in photo emission and X-ray absorption

P122. R. Monnier, S. Massidda, and E. Stoll

Electronic structure of alkaline earth hexaborides

P123. V. Popescu, H. Ebert, and A. Rogalev

Magnetic circular X-ray dichroism investigations on US and UGa_2 compounds

P124. S.L. Molodtsov, W. Schneider, J.J. Hinarejos, C. Laubschat, S.V. Halilov, V.D.P. Servedio, and Manuel Richter

Cooper minima in solids

Superconductivity

P125. H. Auer, C. Ambrosch-Draxl and P. Süle

Doping and pressure dependence of the Raman active A_{1g} modes of $HgBa_2CuO_{4+\delta}$

P126. Lars Fast, Miguel Marques, E. K. U Gross, and M. Lüders

First principle calculation of superconducting transition temperatures using DFT

P127. Josep M. Oliva, Pablo Ordejón, Enric Canadell, and Ruben Weht

Electronic Structure of the Superconducting Layered Ternary Nitrides $CaTaN_2$ and $CaNbN_2$

P128. I. Opahle, H. Rosner, and H. Eschrig

Electronic structure of LaT_2B_2C

P129. P. Puschnig and C. Ambrosch-Draxl

Electronic properties and Raman spectra of rare-earth carbide halides investigated from first principles

Surfaces

P130. DM Bird and MC Graham

Electron-hole pair production in H/Cu(111) scattering

P131. K.-P. Bohnen and R. Heid

Stress in heteroepitaxial growth: Ag/Pt (111)

P132. Juarez L. F. da Silva, M. Scheffler, and Catherine Stampfl

Adsorption of Xe atoms on metal surfaces: surprising results and understanding – a DFT study

P133. Thomas Demuth, Lubomir Benco, Jürgen Hafner, and Herve Toulhoat

Adsorption of organic molecules in zeolites

P134. Alexander Dvořák, Jürgen Fritsch, Stefan Tausendpfund, and Ulrich Schröder

Adsorption of Bi *on* InAs*(110)*

P135. A. Eichler and J. Hafner

Adsorbate induced vacancy formation and substrate relaxation on Cr(100)

P136. Jürgen Fritsch

Structure and dynamics of Cr_2O_3*(0001)*

P137. Tomohiro Hayashi, Yoshitada Morikawa, and Hisakazu Nozoye

The adsorption of dimethyldisulfide on Au(111): theoretical and experimental work

P138. Karoliina Honkala and Kari Laasonen

O_2 *adsorption and precursor states on Pd(111) surface*

P139. Robert Keyling, Wolf-Dieter Schöne, and Walter Ekardt

Lifetime of image and surface states of Al and Cu surfaces

P140. A. Kiejna and B. I. Lundqvist

First principles study of surface and subsurface O structures at Al(111)

P141. D. Ködderitzsch, W. Hergert, Z.Szotek, and W.M. Temmerman

Ab initio study of transition-metal oxide surfaces

P142. C. Cheng, K. Kunc, and M. H. Lee

Structural and electrostatic properties of the $SrTiO_3$ *(001) surfaces*

P143. Weixue Li, Catherine Stampfl, and Matthias Scheffler

Theory of oxygen adsorption on Ag(111): A DFT-GGA investigation

P144. Markus Lischka and Axel Groß

Ab initio calculations of hydrogen adsorption on palladium (210)

P145. A. Marmier, A. Alavi and M. Finnis

Free energy of α*-*Al_2O_3 *surfaces*

P146. F. Mittendorfer and J. Hafner

Desulphurization of thiophene/Ni(100)

P147. J. Oviedo and M. J. Gillan

Reduction and oxidation processes at the SnO_2 *(110) surface*

P148. N.I. Papanicolaou, V. Papathanakos, and G.A. Evangelakis

Investigation of exchange diffusion mechanisms on Cu(111) and Ag(111) surfaces by molecular dynamics simulations

P149. Päivi Pirilä, Karoliina Honkala, and Kari Laasonen

Co-adsorption of CO and NO on Pd(111) surface

P150. X. Qian, W. Hubner, and P.M. Marcus

Surface stress and the effects of relaxation

P151. K. Reuter, M.V. Ganduglia-Pirovano, M. Scheffler, and C. Stampfl

Initial stages of the Ru(0001) oxidation:
from subsurface oxygen to surface oxide formation

P152. A. V. Ruban

Local equilibria in Fe/Ru(0001)

P153. Stefan Tausendpfund, Jürgen Fritsch, Alexander Dvořák, Ulrich Schröder

Chemical reactions of ammonia on nitride semiconductor surfaces

P154. E. Wachowicz and A. Kiejna

Multilayer relaxations at the (0001) surface of Be and Mg

3 News from the TMR1 Network

"Interface Magnetism"

3.1 Workshop Announcements

3.1.1 Workshop on GMR and TMR

TMR-Network Magnetoelectronics

Dresden

November 30th - December 03rd, 2000

Purpose: Presentation and discussion of results and concepts to elucidate the microscopic origin of GMR, TMR and related phenomena.

Arrival: Thursday, November 30th, 2000

Departure: Sunday, December 03rd, 2000

We plan to have longer contributions (40 minutes) and short contributions (20 minutes) + discussions starting Friday morning, Saturday and Sunday morning.

Requirements:

Please confirm your participation by sending me an e-mail indicating the accompanying guests and any request concerning the accomodation until

August 31st, 2000.

Please fill out the following form and e-mail it back to:

mertig@theory.phy.tu-dresden.de

Name:

Postal Address:

Telefon/Fax:

e-mail:

Share room with:

Title of your contribution, if any:

Please send me a short abstract in latex form for each contribution, suitable to be presented in the Ψ_k-Newsletter, until

September 30th, 2000.

Ingrid Mertig

Technische Universitt Dresden	e-mail:	mertig@theory.phy.tu-dresden.de
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D-1062 Dresden, Germany		

3.1.2 XRMS-2000 Workshop

International Workshop on X-ray Magnetic Spectroscopies 2000 (XRMS-2000)

Organized by:

K. Starke, Physik, FU Berlin, Germany

H. Ebert, Dept. Chemistry, Phys. Chemistry, University Muenchen, Germany

Supported by:

TMR-Network: "Ab-initio Calculations of Magnetic Properties of Surfaces, Interfaces and Multilayers"

RTN-Network: "Computational Magnetoelectronics"

SCOPE:

The international workshop on X-ray magnetic spectroscopies will bring together theoretical and experimental scientists who work in the field of X-ray spectroscopies applied to research in magnetism. The one-day meeting provides an opportunity to discuss current advances in the field, as well as to visit the German synchrotron-radiation facility BESSY 2 in Berlin.

VENUE:

Berlin, Germany, Synchrotron-Radiation Facility BESSY 2, Berlin-Adlershof
(see http://www.bessy.de)

DATE:

Saturday, 9th December 2000 (after the BESSY user meeting; see
http://www.bessy.de/INFO/nt.htm)

SCIENTIFIC PROGRAMME:

There will be several invited and contributed talks and a poster session.

PRELIMINARY LIST OF SPEAKERS:

G. van der Laan (*Daresbury*)	L. Braicovich (*Milano*)
J. Tobin (*LLNL*)	J. Kortright (*LBNL*)
T. Eimueller (*Wuerzburg*)	H. Wende (*FU Berlin*)
E. Dudzik (*HMI Berlin*)	I. Idzerda (*NRL*) (*)
C. Vettier (*ESRF*) (*)	P. Strange (*Keele*) (*)
C. Natoli (*INFN*) (*)	W. Kuch (*Halle*) (*)
J. P. Hill (*BNL*) (*)	

(*) to be confirmed

REGISTRATION:

Until 6th of October via FAX or EMAIL to:

K. Starke fax: +49-30-838-53336
starke@omega.physik.fu-berlin.de

or

H. Ebert fax: +49-89-2180-7584
he@gaia.cup.uni-muenchen.de

Please specify: - oral contribution (if possible)
- poster contribution

Submit the title and a half page abstract (Latex preferred) not later than 6th of October, because a booklet of abstracts will be distributed.

FURTHER INFORMATION:

A web page will be available after middle of August via:

http://www.dl.ac.uk/TCSC/HCM/PSIK/workshops.html

This will also supply information on hotels.

Looking forward to meet you in Berlin,

Kai Starke & Hubert Ebert

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 expect (subject to completion of contract negotiations) to have openings 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 should be 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@mpi-halle.de)
- **Ferromagnet/ Superconductor Interface**. For more detail please contact Balazs Gyorffy (b.gyorffy@bristol.ac.uk)
- **Magnetic Nanostructures**. For more detail please contact Laszlo Szunyogh (szunyogh@dirac.phy.bme.hu)
- **Magnetooptics**. 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.

The Network activily 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 ESF Programme

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

5.1 Reports on Workshops/Conferences

5.1.1 Report on CECAM-ESF Workshop

ELECTRONIC AND OPTICAL PROPERTIES OF SEMICONDUCTING GLASSES

13−16 June, 2000

Lyon, France

The workshop was held at CECAM in Lyon (France), from June 13 to June 16, 2000. It was organized by David Drabold (Ohio University), Normand Musseau (Ohio University), Gerard Barkema (University of Utrecht) and Pablo Ordejón (CSIC-Barcelona), and sponsored by CECAM and the ESF Programme on "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" (Psi-k). It was organized in the CECAM style, with 23 invited speakers (plus the organizers). The workshop was intended to be a forum for discussion, and therefore plenty of time after each talk and at focused discussion sessions was available.

The prime goal of the meeting was to bring together active theorists and experimentalists working in the area of amorphous and glassy materials. We wanted to explore the current state of the art in methods of simulation (eg, molecular dynamics, Wooten-Weaire-Winder methods, activation-relaxation technique, etc), strengths and weaknesses of various descriptions of interatomic interactions (ranging from Keating springs to post-LDA). We wanted to determine how to better interact with experimental research in the field – what

experimentalists would most like us to compute. We focused both on the technical issues of these techniques, and on how can they be used to explain and predict the experimental behavior of glasses. More precisely, we wanted to see the following points addressed:

- How important are the details of structure to electronic properties? In which cases can we get away with modeling structure and electronic properties at different levels of accuracy (*eg.*, model potentials for structure and *ab initio* methods for electrons)?

- How can we get the appropriate structure using the most advanced *ab-initio* interactions? To obtain a network in agreement with electronic and optical properties, what level of modeling regime (eg. WWW bond-switching, MD, ART...) and Hamiltonian (empirical interatomic potentials to *ab initio* [LDA, LSDA, GGA...]) is necessary? How does this depend upon the l?

- Can atomistic level calculations provide useful input to phenomenological theories of transport and defect equilibria (the defect pool model)?

- Can conventional *ab initio* methods reliably model light-induced structural rearrangements? How accurate must the excited states be?

- Does the adiabatic (Born-Oppenheimer) approximation lead to significant errors in dynamics for photo-excited or doped systems?

- What are the characteristics of a structural model that is able to reproduce band tail states (which are critical to transport and optical processes)?

- What is the mechanism of doping in an amorphous material? Why is a very large concentration ($\sim 1 - 10\%$) of impurities required?

- Experimentally, the method of preparation influences greatly the electronic and optical properties of these glasses - is there any way to replicate such variations numerically?

- Dynamical properties appear to be one of the most promising approaches to characterize these materials; how far can we push the study of the dynamics of electrons?

- Glasses are known to show dynamics on a wide range of time scales. Can we extend the simulation time scales significantly?

All of these issues were discussed over the four days of the meeting. Some issues were resolved and of course others were not. In addition, we believe that the understanding

between experimentalists and theorists was much improved – *e.g.*, what can or cannot be measured (or computed) and why. We think that this type of understanding is essential to developing the field, especially one in which the interaction between experimentalists and theorists is so essential.

The meeting ran from approximately 9AM until 6PM on June 13,14,15 and half a day on June 16. The abstracts of talks are included below. Most talks were half an hour long with an additional 10 minutes scheduled for discussion. There were also four one hour review talks given as described below. The tone of the meeting was cordial and we maintained a frank and open discussion about the current understanding of the field, strengths and weaknesses of various theoretical schemes for modeling, and what was needed to improve the interaction between experimental and theoretical research in the field. Two 1.5 hour "roundtables" involving all participants were held to further clarify points raised in the lectures.

A "round table" discussion was led by Mike Thorpe: *In search of the perfect amorphous structure*. After a good deal of discussion and many helpful comments from the several experimentalists present, it was clear that many open questions remain, and the role of simulation is crucial. One example is the question of whether odd-membered rings in the archetypal amorphous semiconductor *a*-Si can be directly experimentally measured. It is not clear that this is possible!. A good deal of discussion focused on recent neutron diffraction experiments which suggest a surprisingly low average coordination for *a*-Si.

Martin Stutzmann led a roundtable discussion on *Electronic and optical properties*. The discussion focused on electron-phonon coupling, metastability and the need for theory to compute appropriate matrix elements in an attempt to interact more directly with experiments like Raman scattering in amorphous materials. It emphasized the need from the experimentalist for even approximate calculations of a range of quantities that had not been considered by computational researchers.

This workshop was a real success. The considerable amount of time allotted for discussion both after each talk and at the round tables promoted a healthy exchange of ideas. In particular, it was noted that a number of fundamental problems were still pending. Many suggestions and promises regarding how to solve these in the coming years were made and we look forward to progress along these directions and new fruitful collaborations initiated by this workshop.

ORGANIZERS

David A. Drabold, Department of Physics and Astronomy, Ohio University (USA)

Normand Mousseau, Department of Physics and Astronomy, Ohio University (USA)

Gerard Barkema, University of Utrecht, (The Netherlands)

Pablo Ordejón, Institut de Ciència de Materials de Barcelona, CSIC (Spain)

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S.N. Taraskin, University of Cambridge, UK

Mike Thorpe, Michigan State University, USA

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The influence of Coulomb interactions on the energy levels and transport properties in disordered systems

Guy J. Adriaenssens
Universiteit Leuven, Belgium
Vladimir I. Arkhipov
Philipps-Universität Marburg, Germany
Evguenia V. Emelianova
Universiteit Leuven, Belgium

In the description of transport in disordered semiconductors, the distribution in energy of the localized states that serve as either traps or hopping sites to the charge carriers is generally represented by a fixed density-of-states function. However, such fixed distribution of necessity does not include the varying Coulomb interactions between mobile excited charge carriers and the original (and now oppositely charged) lattice sites they occupied before excitation. Accounting for such Coulomb interactions on the basis of an Onsager pair dissociation probability allows the formulation of a model for low-temperature variable-range hopping conductivity which encompasses the various exponential temperature dependencies from $T^{-1/4}$ to $T^{-1/2}$ as a function of variations in temperature and density of localized states.

Another example of the role of Coulomb interactions is provided by the way in which an ionized dopant atom will locally modify the general density-of-states distribution of its surroundings. Simple arguments show how this results in a strong reduction of the efficiency with which the Fermi level of the semiconductor can be moved about, even when the dopants do ionize.

Nature of impurity states in amorphous silicon

G. Allan, C. Delerue and M. Lannoo
Universite de Lille, France

Low doping efficiency is observed in *a*-Si:H. This necessittates high impurity concentrations which are much larger than the ones generally used for bulk crystalline semiconductors. The low doping efficiency is attributed to the belief that almost all the impurities are incorporated into inert three-fold coordinated sites whereas the remaining four-fold coordinated impurities essentially follow the common rules, i.e. they give shallow levels near the band edges and they bring an extra carrier to the system.
For comparison to the undoped material the electronic structure of *a*-Si:H is calculated in the tight-binding approximation. Hydrogenic substitutional impurities are randomly introduced in a model *a*-Si:H we have built from the 4096 atoms *a*-Si model of B. R. Djordjevic, M. F. Thorpe, and F. Wooten [Phys. Rev. B **52** 5685 (1995)]. We show that most of the hydrogenic impurities in four-fold coordinated sites give localized states in the bandgap which result from the interplay of Coulomb potential of the impurity and the potential fluctuations induced by the disorder. This leads to a large broadening of the Urbach edge.

Internal rotations in solids

E. Artacho, María V. Fernández-Serra
Universidad Autónoma de Madrid, Spain
Kanwal G. Singh
Wellesley College, USA
Guillermo Gomez-Santos
Universidad Autónoma de Madrid, Spain

"Floppy modes" in the context of glasses and amorphous solids, and "rigid unit modes" in the context of complex crystalline solids like minerals, are low-frequency motions of atoms that can, in principle, include some motions of rotational character, i.e., modes for which the associated generalized (internal) coordinate can be assimilated to an angle. This possibility is clear when thinking of lattices or networks of low average coordination like silica, silicates, and some other glass-forming materials. The simplest way of viewing

these rotations is thinking about an oxygen atom turning around the axis that joins its two neighbors.

These motions are, however, systematically treated as "modes", what means that their dynamics and collective behavior are assumed to be well described by the phonon paradigm, and the general laws it implies at low energy. However, extending that paradigm to rotational motions is misleading at the least. The quantization of the kinetic energy in any rotational dynamics brings about substantial differences in behavior. This will be illustrated with the study of a simple model of network with rotational degrees of freedom. The phase diagram associated to the model will be presented, which shows a phase of rotonic excitations unlike phonons (gapped excitations) and a quantum phase transition to a phononic-like phase at higher rotor-rotor interactions. Numbers will be presented for silica.

Computer generation of well-relaxed amorphous structures

G.T. Barkema
University of Utrecht, The Netherlands
N. Mousseau
Ohio University, Athens (OH), USA

This talk gives an overview of a range of computer algorithms used for generating amorphous structures as well as their advantages and drawbacks. These methods can be divided into two classes.

(1) Bond-tranpositions techniques, such as that introduced by Wooten, Winer and Weaire. The goal here is to produce a final configuration as close as possible to the ideal continuous random network or experimental results; the route to getting there is irrelevant and all tricks are allowed. Because of its focus on the results, these techniques have systematically produced the best configurations over the years.

(2) Dynamical approaches, such as molecular dynamics and the activation-relaxation technique, are also preoccupied with describing the route to amorphization correctly. Because of this, these techniques are much more sensitive to the details of the interaction potential. Molecular dynamics is a well established method but suffers from strong limitations regarding the time scales available. The activation-relaxation technique, while still being in development, has already produced a wide-range of high-quality amorphous samples.

Both methods will be discussed and compared.

Tight-binding calculations on ART- and WWW-prepared configurations of a-Si

P. Biswas

University of Utrecht, The Netherlands

Two empirical approaches have been used to generate atomic configurations of a-Si: the activation-relaxation technique (ART) and an improved version of the well-known Wooten-Winer-Weaire (WWW) approach. In our work, we have started from these configurations and investigated the electronic density of states, using modified Goodwin-Skinner-Petifor semi-empirical parameters; we particulary looked at the states in and around the band gap and will discuss the nature of these states.

Light-induced metastability and mobile H excitation in hydrogenated amorphous silicon

Howard M. Branz

National Renewable Energy Laboratory Golden (CO), USA

The light-induced Staebler-Wronski metastability in hydrogenated amorphous silicon (a-Si:H) likely involves excitation of bonded H (Si-H) to bond-centered H by carrier recombination. This leaves a threefold-coordinated dangling-bond defect at the site of excitation. In some H models, this is the final step of metastability. Other models hypothesize long-range diffusion of this mobile H (the analogue of bond-centered H in c-Si), to accomodate the constraint on dangling-bond/H separation which is imposed by electron spin resonance.

Experiments and theory related to the mobile H hypothesis will be described. Recent metastability experiments probing both the temporal [Stradins et al, J. Non-Cryst Solids, in press] and spatial [Tzanetakis and Branz, unpublished] domains suggest that mobile H may be an intermediate precursor between electron-hole recombination and defect creation in amorphous silicon. First-principles calculations [Zhang and Branz, PRL, vol 84, 967, 2000] reveal a pathway for excitation of bond-centered H from Si-H by recombination of a trapped biexciton. This mechanism also accounts for efficient non-radiative carrier

recombination without multiphonon emission.

Vibrations in Network Glasses: Neutron Inelastic Scattering in the Ge-As-Se and As-Se-Br Systems*

R. L. Cappelletti
NIST, USA
Birgit Schwickert
UC Berkeley, USA

Determinations of the generalized vibrational density of states (VDOS) made on samples of Ge-As-Se and As-Se-Br glass alloys by neutron inelastic scattering at the NIST Center for Neutron Research are presented. These covalent glass forming systems of Periodic Table row neighbors were chosen to probe only connectivity in network glasses containing 4-3-2 and 3-2-1 coordinated atoms respectively since they have very similar masses and not very different neutron scattering lengths. The Ge-As-Se system exhibits nearly identical VDOS up to a characteristic frequency for glasses having the same average coordination number $\langle r \rangle$. This vibrational isocoordinate rule is one of many isocoordinate rules for a variety of properties found in several network glass systems. A recent computational study of vibrations in 4-3-2 networks by Mousseau et al. shows very similar behavior. In the As-Se-Br system the network connectivity is modified by presumably one-fold coordinated Br atoms. Theory proposes that the average number of mechanical constraints per atom, $\langle c \rangle$, depends both on $\langle r \rangle$ and the Br content, so that constant $\langle r \rangle$ and constant $\langle c \rangle$ lines in the ternary phase diagram do not coincide. No! simple correlation was observed between the measured VDOS and either $\langle r \rangle$ or theoretical $\langle c \rangle$. A contrasting feature in competition with mechanical constraints is the tendency towards chemical association which favors certain bonding arrangements and the emergence of distinctive clusters in the network depending on composition. We provide evidence for the ability of the Ge-As-Se system to express these features in the form of As_4Se_4 cage molecules partially opened out and bonded into the network.

*This work was supported by NSF under Grant No. DMR 9604921.
Measurements were performed at the NIST Center for Neutron Research.

Molecular dynamics simulation of the growth of nanostructured amorphous carbon films by cluster beam deposition

L. Colombo, D. Donadio, P. Milani, and G. Benedek
Istituto Nazionale per la Fisica della Materia, Italy

Supersonic cluster beam deposition (SCBD) has recently emerged as a powerful technique for the growth of nanostructured carbon thin films. When the incident energy of clusters accelerated in a supersonic expansion is small enough to prevent massive fragmentation, films are obtained in a large, albeit controllable variety of morphologies. Such films are shown to retain a memory of the precursor clusters and to display a disordered graphite–like character with a prevalent three-fold coordination. Furthermore, they display a porous structure, consisting of closed graphitic particles and curved graphene foils embedded in an amorphous matrix. This makes these systems appealing for possible applications, e.g., in gas sensing and gettering. Moreover, carbon cluster assembling has been suggested as a possible route to the formation of negatively curved graphitic carbon (random schwarzites).

A key feature of SCBD is the relationship between the structure and size (of a few up to several hundreds atoms) of the clusters in the beam and the resulting structural and functional properties of the film. Due to the large variety (as regards size, isomerization and reactivity) of clusters, the effects of cluster–cluster interaction on the substrate and the extent of rebonding during the film growth are hard to predict and control. Thus the cluster assembling during the beam deposition and the structure of the resulting films at the nano– and meso–scale is still a matter of discussion.

Despite the above unclear scenario, a number of facts and key parameters governing the SCBD film growth have been identified: (i) experimental results based on ion-drift measurements have shown that small carbon clusters (roughly below 40 atoms) have chain or ring structures, whereas larger clusters tend to form fullerenic cages; (ii) the actual mass distribution and deposition energy deeply affect the final atomic–scale structure, notably the density and the porosity of the sample; (iii) the vibrational temperature of the impinging clusters, the geometrical parameters of the beam–substrate interaction (e.g., incidence angle), as well as the energy distribution within the beam can vary in a wide range.

In this work we present and discuss a computer study, tailored on SCBD experiments

and based on classical molecular dynamics (MD) simulations, aimed at improving our basic understanding of the SCBD growth phenomena. Our MD simulations, besides providing a full atomic–scale characterization of these new materials, enable us to establish a rational link between the physical properties of the grown films and the beam features. In particular, MD simulations of the SCBD process with small (< 10 atoms) low–energy clusters yield the first clear evidence that random schwarzites are formed.

Work supported by INFM under the Advanced Research Project CLASS.

Electronic structure of amorphous insulators and atomistic theory of photo-structural processes

D. A. Drabold

Ohio University, USA

In this talk I discuss recent work on the electronic structure of amorphous insulators with a special emphasis on a-Si. I briefly discuss the nature of the electron states, particularly in the vicinity of the gap from very large scale calculations performed on truly realistic models of a-Si (due to Djordjevic, Thorpe, Wooten and Mousseau and Barkema). Then the effects of thermal disorder are considered, first in the harmonic approximation, with the explicit computation of electron-phonon couplings or "ab initio" deformation potentials, and also by thermal molecular dynamics simulation. It is found that *localized* electron states are very sensitive to thermal disorder. The couplings are largest for conduction tail electrons and *acoustic* phonons. This situation is contrasted with a-Se in which both the acoustic and optical modes play a major role in coupling to the conduction tail states.

I will spend the remainder of the talk describing recent work on modeling photo-structural response of a-Se. A simple model for the light-solid interaction is used (as in studies of the a-Si Staebler-Wronski effect with Fedders and Fu), in conjunction with a realistic model of a-Se. Promise and problems with the method will be pointed out for discussion.

Photo-induced metastability in chalcogenide glasses

Stephen Elliott

University of Cambridge, UK

Chalcogenide glasses exhibit a wide variety of photoinduced phenomena, including photodarkening/bleaching, dilation/contraction etc.. Perhaps of most interest are anisotropic effects induced by polarized light, e.g. dichroism, birefringence. Obtaining a microscopic explanation of these changes represents a big challenge for theory. In this talk, I will describe some recent work in which polarized light can cause mechanical displacement of a cantilever with a chalcogenide layer on top, and evidence for two mechanisms of dichroism in arsenic-rich films.

Amorphous Si:H Supercells and Real Amorphous Si:H

P. Fedders

Washington University, USA

It is presumably well known that good a-Si:H supercells should possess radial distribution function close to those found in experiments, concentrations of H similar to that found in good lab grown material, and should possess only zero or one electronic defect state in the gap if they are to be similar to real lab grown material. At least for band tail states, it has been shown that their structure depends crucially on the presence of hydorgen. However, there are many other properties that a-Si:H supercells should possess if they are to be realistic models of the actual material. The average supercell properties (gap, bond angle and bond length distributions, etc) should be time independent for as long a time as possible although individual bond lengths and angles may change slightly. Real material contains both clustered and isolated H atoms and they may well act in different ways. Since experiments show that dangling bonds are not located near H atoms, this should also be reflected in supercells. This is not so simple since the removal (either on a computer or thermally in the actual material) of an H atom in an H-clustered region will leave a dangling bond with near H neighbors. This must either be energetically very unfavorable or must quickly change to a configuration where one does not have a dangling bond near the H atoms. Further, experiments show a very localized spin density for dangling bonds although not necessaritly a well localized charge density. We will discuss these properties

in detail with respect to supercells that we have created over the years.

Modification of carbon systems for potential applications in electronic devices

Thomas Frauenheim, G. Jungnickel, Th. Koehler, M. Amkreutz and G. Seifert
University of Paderborn, Germany

Semiconductor devices based upon carbon would be very attractive by taking advantage of the short and stiff carbon-carbon bonds. Exceptional high thermal conductivity and stability combined with large band gap and a high saturation velocity for electrons as in diamond would make it a superior material for superfast, high-power, high-temperature applications working under harsh environment.

Application of diamond itself, unfortunately, still suffers from difficulties to prepare an n-type doped high quality crystalline material. Low solubilities and strong relaxation processes of potential dopants causing deep levels to appear greatly reduce the applicability of diamond.

However, the multitude of carbon allotropes provides alternative ways of finding dopable sufficient large band gap systems. The electronic modification and doping behaviour in carbon has, therefore, been studied for various carbon modifications such as amorphous systems, hypothetical carbon allotropes and novel sidewall functionalized carbon nanotubes using approximate density-functional-based simulation techniques.

The theoretical investigations with the focus on boron, nitrogen and phosphorous doping at substitutional lattice sites revealed that in regular lattices a rather special local environment is needed to prevent the impurities from relaxing off center and removing the potential shallow doping levels. On the contrary in amorphous materials the dopant states interact with band tails and are frequently found to become deactivated. While incorporation of fluorine into amorphous carbon doesn't yield an improvement of the doping capability, sidewall fluorination of nanotubes provides a potential basis for tailoring nanoscale electronic components in molecular electronics.

Radiation induced changes in bonding in glass

J. Jain

Lehigh University, Bethlehem (PA), USA

It is now well established that electromagnetic radiation can alter the structure of glass permanently or temporarily during the exposure. For example, electronic defects or color centers such as E-centers in oxide glasses analogous to those in crystals, are often created by ionizing radiation. These changes have been characterized extensively, however, much less is known about the structural changes induced by light of bandgap energy. In this regard, the structure of semiconducting chalcogenide glasses is particularly sensitive to irradiation, which is the basis of several interesting novel scalar and vector optical phenomena such as the opto-mechanical effect. We are characterizing the origin of these changes in the bonding characteristics of prototypic amorphous As-Se by high-resolution x-ray photoelectron spectroscopy. The results show that irradiation by He-Ne laser light (l = 633 nm) produces permanent changes in the valence band, which can be traced to the compositional changes within the probed region. In addition, there are reversible changes, which indicate transfer of lone-pair states of Se to a new kind of bonding states deeper in the band; the latter are only weakly populated in the absence of light.

In comparison to chalcogenide glasses, oxide glasses such as alkali silicates are far more resistant to visible light. Nonetheless, we observe significant changes in their valence band under x-irradiation, which are then correlated with the changes in composition and structure. For example, a prolonged exposure to monochromatic Al-Ka_{α} x-rays alters the concentration of alkali ions in the probed region. Although the number of network forming atoms (Si and O) remains unaffected, the fraction of charge compensating non-bridging oxygen varies concurrently. The implications of these observations is discussed also for ion transport in the same glasses.

Bulk and Surface Structure of Amorphous Silicon

Efthimios Kaxiras
Harvard University, USA
Martin Bazant
MIT, USA

Based on many experimental and theoretical studies, it is widely accepted that a-Si has the basic structure of a Continuous Random Network (CRN) of tetrahedrally bonded atoms, but the question of departures from the CRN has been the subject of considerable debate in recent years and remains controversial. Experimental results appear to favor under-coordinated, three-fold bonded atoms as the dominant defects (so-called "dangling bonds"). On the other hand, theoretical simulations, using a wide variety of *ab initio*, semi-empirical and empirical methods, consistently produce both under-coordinated as well as over-coordinated (five-fold bonded) defects, with a significant preference for the latter. The typical five-fold bonded defect (the so-called "floating bond") was originally proposed and studied theoretically by Pantelides, who argued that the experimental evidence for dangling bonds could be just as easily support the existence of (theoretically favored) floating bonds.

The type of bonding arrangements at the surface of a-Si is even less clear than in the case of bulk defects, since surface-specific measurements are not readily available. Of course, a surface created by terminating the CRN at a plane would have only under-coordinated atoms, but the possibility of surface reconstruction has not yet been thoroughly explored. Indeed, it has been reported that *ab initio* relaxation of a bulk-terminated CRN model produces a surface with roughly equal numbers of three-fold and five-fold bonded atoms. Deviations from the tetrahedral bonding pattern, either in the bulk or at the surface, are crucial in determining the electronic properties of the material because they introduce states in the gap. We will discuss our recent work on bulk and surface structures of amorphous silicon, using a combination of empirical and *ab initio* approaches to generate and relax the atomic models.

Structure of amorphous tetrahedral semiconductors: *Acta est fabula?**

Laurent J. Lewis

Université de Montréal, Canada

In spite of years of experimental and theoretical effort, the structural and dynamical properties (in particular relaxation) of amorphous tetrahedral semiconductors are not completely understood. The elaboration of precise, fully-relaxed models of these materials have long suffered from computational limitations in both size and time, though recent advances in the description of total energies (e.g., tight-binding molecular dynamics[1]) as well as relaxation schemes (e.g., ART[2]) have allowed rapid progress to be achieved within the last few years. Concurrently, proper, reliable, and extremely precise experimental data have become available, putting models under severe tests. For instance, the high-resolution x-ray measurements of Laaziri et al[3] reveal that fully-annealed, ion-implanted a-Si is on average slightly undercoordinated, to about 3.88, compared to about 3.79 in the as-prepared material. The annealing process, further, is found to take place at *constant density*, suggesting that relaxation proceeds via the annihilation of point defects. For the III-V compounds, careful EXAFS measurements[4] of material produced by ion implantation indicate that a-GaAs is undercoordinated to about 3.85, with a density slightly less than that of the corresponding crystalline phase; in contrast, a-InP is denser and slighly overcoordinated, to about 4.16, and possesses wrong bonds in a proportion of about 14%.

In this talk, I will review our recent work in modelling a-Si and the III-V's using state-of-the-ART numerical methodology. While computer models evidently have reached a level of precision quite comparable to that afforded by experiment, several questions remain unanswered. The coordination number of the prototypical material a-Si, for instance, is still subject to discussion and interpretation; the precise value of this number is important for assessing the presence of defects and thus the processes that lead to relaxation. Likewise, the error bars on the parameters that describe the local structure in III-V compounds are large, and models are thus important in interpreting or complementing the experimental data.

*Work done in collaboration with many people, including Normand Mousseau, Hyangsuk Seong, Alessandro De Vita, Roberto Car and Cristiano Luis Dias.

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Monte Carlo Simulation of Heteroepitaxial Growth of Semiconductor Compounds with Large Mismatch

R. Malek

Ohio University (USA)

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We have performed atomic scale simulation of the heteroepitaxial growth of semiconductor systems with large mismatch by associating Monte Carlo (MC) technique with an energetic model derived from the Valence Force Field (VFF) approximation. The energy model allows us to determine stress and strain in the deposited film by minimizing the total energy, and to calculate the stress dependent probabilities. The MC technique is needed to describe the kinetic of growth, and thus to handle the random nature of the atomic motions based on Arrhenius law and Poisson process. We have shown that the growing film presents 3D islands or cavities with (111) facets. In the first case, the interlayer migrations avoid coalescence of clusters to form a planar film and favor the formation of large and high islands. In the second case, the cavities are filled by the growth on (111) facets and lead to the formation of point defects, like a bulk vacancies, and their association to form extended defe! cts, like a vacancy lines and vacancy clusters. The creation of these defects is related to atoms in handing positions which are the results of reactions between atoms in interstitial positions. The strain relaxation is shown to be performed in few atomic layers and not uniform inside a given island. The maximum strain relaxation is located in the border of these islands where the strain energies are small and the atomic displacements are large.

Intermediate range order in disordered Ge_xSe_{1-x} systems: interplay between structural and electronic properties

C. Massobrio

CNRS, Strasbourg, France

Interest in disordered Ge_xSe_{1-x} systems is motivated by the peculiar structural changes exhibited over the whole compositional range, which reflect variations in the nature of bonding. On the Se rich side (x=0.2, $GeSe_4$ and x=0.33, $GeSe_2$), intermediate range order (IRO) which establishes on length scales significantly more extended than nearest-neighbor distances gives rise to the presence of a first sharp diffraction peak (FSDP) in the total neutron structure factor. First principle molecular dynamics studies have shown that liquid $GeSe_4$ is a chemically ordered system[1], i.e. the number of heteropolar bonds is maximized. On the other hand, in liquid $GeSe_2$ the chemical order is broken due the presence of miscoordinated atoms and homopolar bonds which coexist with $GeSe_4$ tetrahedra[2]. The existence of homopolar Ge−Ge bonds for this composition has been recently firmly established for amorphous $GeSe_2$ by using the method of isotopic substitution in neutron diffraction[3].

To highlight the intimate relationship between bonding and intermediate range order in disordered network-forming systems, liquid $GeSe_2$ has been investigated by adopting two distinct functionals for exchange and correlation within density functional theory. It was found that a generalized gradient approximation (GGA) is required to reproduce a FSDP in the total structure factor, while, when the local density approximation (LDA) is used, the FSDP is absent[4]. To link these findings to specific bonding features we have first considered one single configuration of liquid $GeSe_2$, for which we have obtained the electronic structures pertaining to both energy functionals and we have calculated the corresponding electronic densities of states (EDOS). Comparison of the charge density plots shows that the occurrence of the IRO can be associated with the more ionic bonding found within GGA which promotes the formation of $GeSe_4$ tetrahedra[4]. Analysis of the two EDOS on the basis of this single atomic configuration reveals that this enhanced ionicity arises from states lying well below ($\sim$ 1eV) the Fermi energy. Moreover, the more ionic character found within GGA it is not necessarily correlated with the shape of the EDOS at the top of the valence band, which gives a more pronounced pseudogap in the LDA case.

The behavior of the EDOS at the Fermi level and the description obtained in terms of charge densities, as expressed on the basis of a single atomic configuration analysis, can be fully reconciled by calculating EDOS *time averages* of the electronic density of states (EDOS) on atomic configurations obtained within LDA and GGA first principles molecular dynamics. The importance of fully accounting for the atomic relaxations is reflected by the behavior of the upper valence states, which now consistently yield a deeper pseudogap in the GGA case.

This work has been performed in collaboration with Alfredo Pasquarello (Lausanne) and Roberto Car (Princeton).

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Review of first-principles electronic structure calculations

Pablo Ordejón

CSIC, Barcelona, Spain

With the incredible rate of improvement in computers, and the developement of more efficient computational techniques, the application of first-principles electronic structure methods to the study of disordered systems is becoming increasingly important in recent years. This is due to the fact that the system sizes that can currently be handled are large enough to represent with sufficient accuracy the structure of disordered systems. I will review the advances in the electronic structure calculations techniques which are allowing these studies, and will give some examples of recent work in our group on several disordered systems.

A novel approach to electron localization in noncrystalline materials

L. Colombo
Università di Cagliari, Italy
M. Peressi and R. Resta
Università di Trieste, Italy

The insulating state of matter is characterized by the excitation spectrum, but also by qualitative features of the electronic ground state. The insulating ground wavefunction in fact: (i) displays vanishing dc conductivity; (ii) sustains macroscopic polarization whenever the electronic Hamiltonian is noncentrosymmetric; and (iii) is localized. The idea that the insulating state of matter is a consequence of electron localization was first proposed in 1964 by W. Kohn[1].

We present a novel definition of electron localization[2–4], rather different from Kohn's, and deeply rooted in the modern theory of polarization, based on a Berry phase[5]. In fact the present approach links the two features (ii) and (iii) above, by means of essentially the same formalism. In the special case of an uncorrelated crystalline solid, the localization of the many–body insulating wavefunction is measured by the spread of the Wannier orbitals; this spread diverges in the metallic limit.

We discuss here the case of a noncrystalline solid in any independent–electron approximation (Hartree–Fock, Kohn–Sham). Our approach measures the localization of the many–body wavefunction as a whole, instead of focussing on features of the individual eigenstates of the one–electron Hamiltonian; such measure is a function of the Fermi–level position. Actual calculations are in progress for a model of a–Si, whose structure is generated according to WWW[6], and where a tight–binding approximation is adopted for the independent–electron Hamiltonian. Preliminary results will hopefully be presented.

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Successes, failures and opportunities for thoery in amorphous carbon

J. Robertson

Cambridge University, UK

The talk will review the successes and failures of theory in the field of amorphous diamond-like carbon. In particular, in electronic structure, deposition processes, spectroscopies such as Raman and in electron field emission.

Electronics in tortured topologies: Nanoporous titania and silicon

N. Kopidakis, P. Rao, E. A. Schiff, Q. Yuan

Syracuse University, USA

L. Tsybeskov, P. Fauchet

University of Rochester, USA

A. J. Frank, N.-G. Park and J. van de Lagemaat

National Renewable Energy Laboratory, USA

Sponge-like, "bicontinuous" materials with nanometer scale feature sizes can have exciting electronic properties. Porous silicon emits light with an efficiency enormously greater than the single crystal silicon from which it is made, as discovered by Canham about nine years ago. Porous titanium dioxide is the basis of an extraordinary solar cell invented by Graetzel and O'Regan at about the same time.

In this presentation we report transient measurements of photocarrier drift and diffusion in these topologically disordered materials. Porous silicon is created by electrochemical etching of crystal silicon, and its structure is arguably fractal. The photocarrier drift measurements are "dispersive" and consistent with a random walk on a fractal, and they yield a random-walk dimensionality consistent with a percolation network. This

behavior is very surprising, since we expect that quantum confinement effects associated with the nanoporosity would have led to a rugged energy landscape for transport and a qualitatively different behavior. We speculate upon the relative importance of disorder and nanoporosity for porous silicon's electronic structure.

Porous titania is created by sintering of colloidal nanocrystals to form a porous structure. In common with porous silicon, electron diffusion on the porous structure does not appear to be dominated by an energy landscape. On the other hand, the diffusion is very strongly nonlinear: the electron "typical" diffusion coefficient rises proportional to the total density of electrons. We are exploring Coulomb blockade models for this behavior.

Amorphous Silicon Suboxides: From Semiconductor to Insulator

M. Stutzmann, R. Janssen, A. Janotta

Technische Universität München, Germany

Hydrogenated amorphous silicon suboxides, a-SiO_x:H, span the so far relatively unknown region between the most studied amorphous semiconductor, a-Si:H, and the technologically important insulating glass a-SiO_2. Therefore, in principle a lot can be learned about how the basic structural and electronic properties of disordered networks containing Si, O, and H depend on the relative concentrations of the constitutent atoms as well as on doping with electronically active impurities (e.g. B and P). The purpose of this presentation is to summarize the main results of a recent, systematic study of PECVD-deposited Si suboxides (bonding statistics, vibrational properties, optical bandgaps and bandtails, luminescence, deep defects, doping efficiency, stability, transport, and device properties)and to discuss these results from an experimental point of view in terms of present phenomenological models. Of particular interest are questions such as

- The influence of oxygen on preferential hydrogen bonding.
- The effect of small oxygen concentrations on the Urbach tail width and the deep defect density.
- A comparison of local oxygen vibrational modes in crystalline versus amorphous silicon.

- The relative effects of hydrogen versus oxygen content on the effective optical bandgap of silicon rich alloys.
- The dependence of the doping efficiency of boron or phosphorus on the oxygen concentration.
- Bipolar a-SiO_x:H pin diodes and the defect pool model

A central aim of this phenomenological discussion is the identification of basic questions requiring further input from reliable microscopic models of such amorphous alloy systems.

Some problems around the optical gap in chalcogenide glasses

Keiji Tanaka
Hokkaido University, Japan

The optical absorption edge of chalcogenide glasses has been studied extensively after Kolomiets and Tauc, while the nature is not yet elucidated.Forinstance,interpretations of Tauc gap and Urbach edge are still ambiguous. We cannot yet explain the origin of the weak-absorption tail(extending below the Urbach edge), which limits the application of chalcogenide glasses to optical fibers. In addition, although the mobility-edge and charged-defects concepts proposed by Mott and others have been employed frequently, we have no direct evidence demonstrating the existences. Clear-cut descriptions of these features are indispensable for the understanding of a variety of photoinduced phenomena. I will talk about these problems on the basis of recent spectral data of optical absorption, photoconduction[1,2], and photoluminescence in As_2S_3 and related materials. For instance, the mobility edge in As_2S_3 is assigned at 2.7 eV. Origins of the Urbach edge and the weak-absorption tail are discussed.

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Atomic vibrations in disordered structures

S.N. Taraskin and S.R. Elliott
University of Cambridge, UK

The nature and properties of vibrational excitations in disordered materials are discussed. Our approach includes analytical (e.g., coherent potential approximation) and numerical (e.g., normal mode analysis, fast evolution method) techniques. The problems of interest are (i) dispersion law in disordered materials, (ii) density of vibrational states (low-frequency regime and the boson peak), (iii) wave propagation (the Ioffe-Regel crossover), (iv) multifractal properties of localized states. Systems under analysis include vectoral multi-dimensional toy models, icosahedral glass, structural models of realistic glasses (e.g. vitreous silica and germania) constructed by means of classical molecular dynamics.

Self- Organization in Network Glasses

Michael F. Thorpe and M. V. Chubynsky
Michigan State University, USA

The continuous random network model is widely used as a realistic description of the structure of covalent glasses and amorphous solids. We point out that in real glasses and amorphous materials, there are non-random structural elements that go beyond just simple chemical ordering. We propose that the network can self-organize at its formation or fictive temperature, and examine some of the possible consequences of such self-organization. We find that the absence of small rings can cause the mechanical threshold to change from a second order to a first order transition. We show that if stressed regions are inhibited in the network, then there are two phase transitions and an intermediate phase that is rigid but stress-free. This intermediate phase is bounded by a second order transition on one side and a first order transition on the other. Recent experiments in chalcogenide glasses give evidence for this intermediate phase.

Hydrogen diffusion and metastability in hydrogenated amorphous silicon

Chris G. Van de Walle

Xerox PARC, USA

Hydrogen passivates defects in amorphous silicon, but is also generally accepted to be involved in defect *generation*. We have addressed the interactions of hydrogen with amorphous silicon by focusing on the local environment around the hydrogen atom, carrying out first-principles calculations for hydrogen in a crystalline lattice with and without defects. The computational results have all been obtained using density-functional theory, *ab initio* pseudopotentials, and a supercell geometry.

We have carefully investigated the dissociation path for the breaking of a Si-H bond. The vibrational characteristics of this process provide an immediate explanation for the large isotope effect (H vs. D) observed for Si-H bond breaking on surfaces and at interfaces; whether the enhanced stability of Si-D bonds can also benefit amorphous silicon has not been established yet.

By linking the microscopic phenomena to the macroscopic diffusion process we can compare the predicted Fermi-level dependence with the observed one. This leads to some interesting conclusions about the nature of hydrogen trapping sites.

Finally, I will discuss an exchange process between trapped and interstitial hydrogen that plays a significant role in diffusion processes. A metastable SiH_2 complex plays an important role in this exchange; I will speculate on the potential role of this complex, and of the H_2 molecule, in metastable defect formation.

I gratefully acknowledge collaborations with B. Tuttle, C. Herring, W. Jackson, N. Johnson, N. Nickel, and R. Street.

5.2 Reports on Collaborative Visits

Report on a Collaborative Visit of Dr Sergey Ostanin (University of Glasgow, UK) to Professor Hubert Ebert (LMU, Munich, Germany)

June 7-12, 2000

I was visiting Prof. Ebert's group at Department of Chemistry of L.-M. University in Munich from 7 June to 12 June 2000. Our collaborative work initiated before, at my previous visit, has been completed.

One of the main objects discussed with Prof. H. Ebert and Dr. V. Popescu were the x-ray magnetic circular-dichroism (XMCD) spectra calculated for ordered and disordered Co-Rh and Fe-Pd alloys. These theoretical data, obtained by the fully relativistic SP-KKR-CPA method, were examined against the available experimental XMCD findings. We analysed an origin of the XMCD changes due to both disordering and structure-distortion effects. The latter one is very important because some recent XMCD measurements have been done using the thin-film site-ordered specimens distorted tetragonally along the out-of-plane film direction.

The SPR-KKR-CPA calculations were able to confirm the magnetisation induced in the $4d$ transition metals by their alloy partners. Because XMCD is dominating in the white line region, the XMCD sum-rules in their integral form can supply reliable estimations of the component-resolved spin and orbital magnetic moments in Co-Rh and Fe-Pd.

In the near future we are planning to submit a paper on the XMCD in Co-Rh and Fe-Pd alloys including the original experimental XMCD data.

I am very grateful to the network for support.

Dr. Sergey Ostanin
Department of Physics and Astronomy, University of Glasgow
Glasgow, UK

June 14, 2000

Report on a Collaborative Visit of Mads Brandbyge (Technical Univ. of Denmark) to Pablo Ordejon (Autonoma Univ. Barcelona)

2 June – 24 June 2000

I visited Prof. Pablo Ordejon and his group at the Institut de Ciencia de Materials de Barcelona from 2. June to 24. June, 2000. The aim of my visit was to initiate a collaboration on ab initio calculations of electrical transport on the atomic scale - e.g. through atom sized metal point contacts or molecular contacts. Especially, we want to be able to calculate the non-linear conductance of atomic/molecular scale systems self-consistently within density functional theory.

The specific goal of the visit was to combine the SIESTA code – a LCAO O(N) density functional package

(D. Sanchez-Portal, P. Ordejon, E. Artacho and J. Sole, Int. J. Quantum Chem. 65, 453 (1997)), with the non-equilibrium Greens function transport scheme, as implemented in a semi-empirical self-consistent tight-binding version (M. Brandbyge, N. Kobayashi, and M. Tsukada, Phys. Rev. B 60, 17064 (1999)).

During my stay I have implemented the first version of the connected code. Its main ingredient is the SIESTA–transport-code interface which communicate the hamiltonian and overlap parameters to the transport code, and return the non-equilibrium densitymatrix to the LCAO-DFT code. The transport code calculate the densitymatrix corresponding to the contact/scattering region coupled to bulk electrodes (with difference in Fermi energy for finite voltage bias).

Simple tests for one-dimensional chains of gold atoms where performed, but more extensive tests of the code for the case of three-dimensional structures with a finite voltage bias remains to be done.

Mads Brandbyge

Report on the collaborative visit of Ulrich Freking (Münster) to Wroclaw within the STRUC-Psi_k ESF Programme

17th June - 1st July 2000

Within the STRUC-Psi_k ESF Programme, I spent two weeks (17.06.2000 - 01.07.2000) at the University of Wroclaw in the group of Professor Maria Steslicka to continue a joint scientific project on 'Electronic properties of superlattices (SL's) from pseudopotential calculations'. My stay in Wroclaw focused on a theoretical investigation of AlGaAs-based biperiodic superlattices in which every second GaAs slab ('quantum-well' layer) and/or every second GaAs slab ('quantum-barrier' layer) is of a different width. Biperiodic SL's exhibit superior characteristics as compared to usual SL's with simple two-layer well-barrier period, and therefore they are found to be promising for novel applications in optoelectronics. The starting point of our studies were computer codes using pseudopotentials within a plane-wave basis set which I have written at the University of Münster during my studies for a PhD.

During my stay in Poland, together with members of the group of Prof. Steslicka we were able to reach the two following main aims:

First, together with Dr. Robert Kucharczyk I discussed several results obtained for biperiodic SL's by using a modern empirical pseudopotential of Mäder and Zunger [K. Mäder and A. Zunger, Phys. Rev. B**50**, 17393 (1994)]. We carried out calculations of the electronic level structure and space-charge distributions for [100]-oriented bioperiodic $(\mathrm{GaAs})_k(\mathrm{AlAs})_l(\mathrm{GaAs})_m(\mathrm{AlAs})_m$ SL's with variable layer thicknesses. The SL potential resulting from the two different GaAs and/or AlAs slabs within the SL period yields miniband splittings and specificial spatial redistributions of states. Our results obtained for the GaAs $\Gamma - v$alley-derived minibands reproduce the characteristics predicted by simple-model approaches. While corresponding features of the AlAs X-valley-derived minibands are neglected in most model studies, our pseudopotential approach allowed us to discuss them for biperiodic SL's for the first time. Our results will be presented at the ECOSS conference in Madrid in September 2000 and they will be published in the Proceedings of the conference in 'Surface Science'.

Second, I installed a more sophisticated, self-consistent version of my program code,

using norm-conserving pseudopotentials of Kleinman and Bylander [L. Kleinman and D.M. Bylander, Phys. Rev. B**48**, 1425 (1982)]. We were able to obtain first results for [100]-oriented superlattices on a two processor workstation of the University of Wroclaw. A PhD student in the group of Professor Steslicka, to whom I explained the underlying density functional theory and the use of my codes, has continued these studies after my return to Münster. The interpretation of the results will be done in close collaboration.

In summary, my stay in the group of Prof. Maria Steslicka in Wroclaw enabled us to continue more realistic electronic structure calculations of semiconductor superlattices. Neither the calculations themselves nor the interpretation of the respective results would have been possible without this collaboration.

Ulrich Freking

Mnster, July 13th, 2000

5.3 Workshop Announcements

5.3.1 Workshop on Materials Modelling

MML2000 International Workshop on Materials Modelling

Oxford, UK, 18-20 September 2000
http://users.ox.ac.uk/ mml2000/

Committee: Prof David Pettifor, Prof Adrian Sutton,
Dr Robert Rudd and Dr Steven Kenny

MML2000 will highlight applications of materials modelling to systems with multiple length scales. A large range of state-of-the-art modelling will be covered, and we aim for the talks to be given at a level accessible to non-experts and young scientists. This year's workshop will complement MML99 which focussed on methodologies, and again this year we expect participants whose interests range from quantum chemistry to continuum modelling, with attendees coming from both academia and industry.

The style of the workshop will be informal. There will be four keynote talks the first day, followed by six one-hour talks on each of the two following days. The Oxford venue is the same as last year: the lecture theatre of the Computing Laboratory in the Wolfson Building for the lectures and St. Edmund Hall for accommodations and meals (including the banquet). Each of these is outstanding in its own right, and together they promise to help make MML2000 a great success.

We have invited an outstanding group of speakers. The preliminary programme is available at the MML2000 web site:

http://users.ox.ac.uk/ mml2000/programme.html

The confirmed speakers include Pettifor (Oxford), Windle (Cambridge), Gilmer (Lucent),

Farrugia (Corus), Kremer (Mainz), Theodorou (Patras), Paul (Mainz), Willis (Cambridge), Rudd (Livermore), Jenson (MIT), Evans (Swansea), Grant (Oxford) and Phillips (Brown).

We hope MML2000 will attract a diverse group of participants from the UK, Europe and beyond. Some bursaries will be available for students from the conference organisers, and more substantial financial assistance will be available from SIMU for its members (not just students) who participate.

Please have a look at our web site, http://users.ox.ac.uk/ mml2000

Online registration is available at the web site. Please register as soon as possible if interested.

MML2000 Organising Committee
Department of Materials
University of Oxford
Oxford OX1 3PH, England

fax: +44 1865 273789
mml2000@materials.oxford.ac.uk
`http://users.ox.ac.uk/~mml2000/`

6 General Workshop/Conference Reports

6.1 Symposium on Spin-Electronics

Halle, Germany, July 3-6, 2000

The "Symposium on Spin-Electronics" (`http://www.mpi-halle.de/~sse2000`)

was held in Halle (Germany) on July 3-6, 2000. This was the first international symposium specifically devoted to spin-electronics. It has been organized by the Max-Planck Institute of Microstructure Physics.

Spin-electronics (also dubbed "spintronics" or "magneto-electronics") is a new field of science and technology aiming at merging electronics and magnetism in order to realize new electronic devices in which the spin of the electron plays an active role. Of particular interest is the realization of non-volatile magnetic random-access memories (M-RAM) that could offer a number of advantages as compared to conventional C-MOS RAMs: non-volatility, better scalability, lower energy consumption and heat dissipation. On the long term perspective, spin-electronics also appears as a promising candidate for the realization of solid-state quantum computers. Besides its strong technological potential, spin-electronics is also an extremely attractive area from the point of view of fundamental science.

The purpose of the "Symposium of Spin-Electronics" was to bring together scientists active in the field of spin-electronics and spin-dynmics in order to the latest experimental and theoretical developments, as well as technological applications. The subtopics covered various apspects of spin-dependent transport, electronics, and optics:

- materials for spin-electronics (hybrid FM/SC systems, oxides, etc.)
- GMR, tunneling MR, and other spin-dependent transport effects
- femtosecond spin-dynamics (pump-probe experiments, etc.)
- gigahertz spin-dynamics in semiconductors

- applications and devices (GMR heads and sensors, MRAMs, etc.)
- new directions (spin transistors, etc.).

The response to the Symposium has been extremely positive and the participation was very important for a newly created Symposium: more than 300 persons (including approximately 20 persons from the USA and 40 from Japan) attended the Symposium and presented more than 260 contributions (12 invited papers, 67 contributed oral papers, and 184 posters). Besides scientific discussions, the participants of the Symposium also had the opportunity of discovering the city of Halle, by attending a symphonic concert at the Georg-Friedrich-Haendel Concert Hall and by enjoying the beautiful landscape from the Biergarten "Bergschänke". The visit of the Max-Planck Institute of Microstructure Physics, after the end of the Symposium, attracted more than hundred visitors. The evaluation carried out at the end of the meeting regarding the scope, scientific program, and organization has given very positive results, and the participants almost unanimously voted in favor of a further "Symposium on Spin-Electronics."

The RTN on "Computational Magneto-electronics" has been very actively involved in the conception of the Symposium (five members of the Network were among the members of the Inernational Advisory Committee or of the Program Committee of the Symposium), and 27 members of the Network attended the Symposium and presented 33 contributions. From the point of view of the Network, the Symposium offered an unique opportunity of exchanging view with experimentalists and scientists of the semi-conductor community.

P. Bruno
Co-chair of the Symposium

7 General Workshop/Conference Announcements

7.1 Winter School in Cargese

EUROPEAN WINTER SCHOOL

STATE OF THE ART SIMULATIONS
IN ELECTRONIC STRUCTURE AND TOTAL ENERGY
FOR SURFACE SCIENCE

Institut d'Etudes Scientifiques de Cargèse
Cargèse (Corse) FRANCE

February 19^{th} - March 3^{rd} 2001

Scientific Committee:
M.C. Desjonquères (Saclay), M. Finnis (Belfast), C. Noguera (Orsay), M. Scheffler (Berlin), P. Soukiassian (Saclay), D. Spanjaard (Orsay), E. Tosatti (Trieste), E. Wimmer (Le Mans)

Local Committee:
M.C. Asensio (Orsay, Madrid), C. Barreteau (Saclay), M.C. Desjonquères (Saclay), T. Deutsch (Grenoble), F. Finocchi (Orsay), D. Spanjaard (Orsay), G. Tréglia (Marseille)

PRELIMINARY PROGRAMME

1. Electronic structure: Methods

a) General introduction to density functional theory (1H30), pseudopotentials and plane waves (1H30), linear response and molecular dynamics (1H30): D. VANDERBILT (Rutgers University, USA)

b) FLAPW and FPLMTO Methods (3H): E. WIMMER (Le Mans, France)

c) Tight-binding methods (1H30): C. BARRETEAU (Saclay, France)

2. Electronic structure: Applications and Experiments

a) Kinetic Monte-Carlo method: from microscopic to macroscopic properties (3H): P. KRATZER (Berlin, Germany)

b) Quantum wells (1H30): E. GARCIA-MICHEL (Madrid, Spain)

c) Theory of Photoemission (1H30): M. LINDROOS (Tampere, Finland)

d) Photoemission experiments (1H30): M.C. ASENSIO (Orsay, France and Madrid, Spain)

e) Theory of Scanning Tunneling Microscopy (1H30): F. FLORES (Madrid, Spain)

f) Scanning Tunneling Microscopy experiments (1H30): S. ROUSSET (Paris, France)

3. Empirical potentials and applications

a) General introduction (3H): G. ACKLAND (Edimbourg, Scotland)

b) Kinetic Tight-Binding Ising Model and its applications to alloying at surfaces (1H30): G. TREGLIA (Marseille, France)

c) Order/Disorder at surfaces (3H) E. TOSATTI (Trieste, Italy)

4. Surface Magnetism

a) General introduction to surface magnetism and role of the electronic correlations (3H): G. SAWATZKY (Gröningen, Netherlands)

b) Theory of surface magnetism: Coupling between magnetism and atomic structure - Multilayers (3H): S. BLÜGEL (Jülich, Germany)

c) Magnetism of metals, magnetic dichroïsm (3H): F. GAUTIER (Strasbourg, France)

5. Excitations at surfaces

a) General introduction (1H30): P. THIRY (Namur, Belgium)

b) Optical response of surfaces (1H30): G. ONIDA (Roma, Italy)

c) Surface vibrations (1H30): P. DUMAS (Orsay, France)

d) Electronic excitations (1H30): V. STAEMMLER (Bochum, Germany)

6. Physisorption and Chemisorption

a) General introduction (3H): J.K. NORSKOV (Lyngby, Denmark)

b) Physisorption (1H30): C. RAMSEYER (Besançon, France)

c) Ab-initio methods in chemisorption (1H30): H. TOULHOAT (Rueil-Malmaison, France)

d) Chemisorption experiments (3H): D.A. KING (Cambridge, UK)

The programme will be organized in 9 working days during which there will be 4 lectures (1H30 each, including 15' for discussions)

7.2 ADFT2001 Vienna, Austria

International Conference on Applied Density Functional Theory

January 14-17, 2001 in Vienna, Austria

Honorary Chairman: Walter Kohn

The Workshop's web site:

http://www.physics.at/dft2001

This four day symposium will focus on the application of Density Functional Theory to problems in physics, chemistry and materials science.

The list of confirmed invited speakers includes:

- Ole Andersen (Stuttgart): *Beyond linear methods*
- Peter Bloechl (Zuerich): *Insights on the Dielectric Breakdown in Transistors from Density* Functional Calculations
- Roberto Car (Princeton)
- Boerje Johansson (Uppsala)
- Walter Kohn (Santa Barbara): *Van Der Waals Attraction and Time-Dependent DFT: An Extended Regime.*
- Dimitrios Papaconstantopoulos (Washington): *The NRL Tight-Binding Method*
- David Singh (Washington): *A band structure view of some metallic correlated oxides.*
- Erich Wimmer (Paris): *The Impact of Density Functional Theory on Industrial Research*

WORKSHOP ANNOUNCEMENT

We are pleased to announce the first

7.3 International Workshop in Barcelona

on

"Modelling of the Growth and Interface Properties of Thin Films and Multilayers through Molecular Dynamics"

9-10 November 2000 - Barcelona, Spain

organised by the Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC) and promoted by the European Thematic Network MULTIMETOX.

This Workshop is intended to bring together computer simulation methods in crystal growth and interfaces properties, and thin and ultra thin experimental preparation techniques. The lectures are oriented to PhD students, although postdocts and researchers are not excluded. Participants are welcome to present results of their own field of research, either molecular dynamics calculations on physico-chemical mechanisms of growth and interfaces, or deposition and characterisation of surfaces, interfaces and nanometer-scale structures.

Tentative list of Invited Lecturers:

Dr. J. Gale, Imperial College of Science, Technology and Medecine, London, UK "Molecular Dynamics Simulations"

Dr. A.R. Gonzalez-Elipe, Instituto de Ciencia de Materiales de Sevilla, Spain "Evolution of Crystal Structure during Thin Films Growth"

Dr. P. Kratzner, Fritz-Haber-Institute, MPG, Berlin, Germany "Surface Diffusion and Crystal Growth in GaAs"

Dr. E. Hernandez, Instituto de Ciencia de Materiales de Barcelona, Spain "Molecular Dynamics Simulations of Growth of Fullerenes and Nanotubes"

Dr. M.S. Islam, University of Surrey, Guilford, U.K. "Ionic Transport in Perovskites: a Computer Modelling Tour"

Dr. I. Turek, Institute of Physics of Materials, Brno, Czech Republic "Ab-Initio Theory of Magnetoresistance in Layered Magnetic Systems"

More information about the workshop can be found in the workshop website:

http://www.icmab.es/multimetox/md2000.html

We look forward to see you in Barcelona.

The Organising Committee:

Pablo Ordejon
Josep Santiso
Gemma Garcia
Alber Figueras

8 General Job Announcements

Post-doctoral Position

CONQUEST Order-N Project
University College London, UK

A post-doctoral position is available immediately to work in the group of Professor Mike Gillan on the CONQUEST Order-N Project. The aim of this well-established project is to develop a fully functional code to do static and dynamic first-principles calculations on systems of thousands of atoms using density-functional theory. An essential part of this aim is that the code runs efficiently on massively parallel machines. Development of the CONQUEST code (Concurrent O(N) QUantum Electronic Simulation Technique) began in 1995, and its practical O(N) (linear-scaling) behaviour on parallel machines was demonstrated over two years ago on systems of over 5,000 atoms. Three researchers are currently working on CONQUEST at University College London: Mike Gillan, David Bowler and Tsuyoshi Miyazaki, and the person appointed to the position will work closely with Gillan and Bowler.

The project has access to major parallel computer resources. A new facility was recently established at UCL. Known as HiPerSPACE (Hi-PERformance Service for Physics, Astronomy, Chemistry and Earth Sciences), this consists of two Origin 2000 machines, giving a total of 72 R12000 processors with 48 Gigabytes of memory. In addition, the CONQUEST project has allocations of time on the Manchester CSAR service, whose main machine is a 816-processor Cray T3E with 148 Gbyte of memory. The CONQUEST O(N) project is being carried out in the framework of the U.K. Car-Parrinello consortium, a collaboration of computational condensed-matter groups at UCL, Cambridge, Oxford, Edinburgh, Belfast, Bath and Daresbury Laboratory.

The project: the successful applicant will work on improving the efficiency and reliability of the CONQUEST code, and will use the code to do innovative first-principles calcu-

lations on complex nano-structures on semiconductor surfaces. A major target for the immediate future is to incorporate a more efficient representation of the localised orbitals using atomic-like orbitals.

Duration: grant funding is available now to support a post-doctoral position for 12 months. Actions are underway to secure additional funding for a further 2- or 3-year period.

Salary is on the Research Council RA1A scale, currently 15,735 - 23,651 (plus 2,134 London allowance) UK pounds per year, pay award pending.

Location: the work will be carried out in the CMMP section (Condensed Matter and Materials Physics) of the Physics and Astronomy Department at University College London. This is in central London near Regents Park.

Qualifications: candidates must have (or expect to obtain soon) a Ph.D. in theoretical or computational condensed-matter physics, chemistry, materials science or a related discipline. A strong and documented track-record in writing practical large-scale computer code is essential. Experience with parallel computers is highly desirable.

Applying for the position: enquiries and applications, the latter including curriculum vitae and the names of at least two (preferably three) referees, should be sent to Dr. David Bowler. E-mail address: david.bowler@ucl.ac.uk Postal address: Physics and Astronomy Department, University College London, Gower Street, London WC1E 6BT.

Further information can be found on the following web sites:

University College London: www.ucl.ac.uk
Physics and Astronomy Department: www.phys.ucl.ac.uk
CMMP group: www.cmmp.ucl.ac.uk

CONQUEST: www.cmmp.ucl.ac.uk/ conquest

Positions in Electronic-Structure Theory

University of Saarland, Saarbrücken, Germany

At the Department of Physical Chemistry, University of Saarland, Saarbrücken, Germany, we are currently building up a new theory group and have some openings for Ph. D. students or post-doc fellows.

Our research activities concentrate on the development and application of computational methods for the studies of electronic and structural properties of specific systems, most notably polymers, chain compounds, clusters, and colloids, but also solids and molecules will be treated, and later also photonic crystals will be a subject of our research. Many of the activities will be in close contact with experimental groups in the chemistry and physics departments of the University of Saarland.

Those who are interested in joining these activities and helping building up the new group are asked to contact me at the address below.

The University of Saarland encourages in particular women to apply for those positions.

Michael Springborg
Physical Chemistry
University of Saarland, Bau 9.2
66123 Saarbrücken
Germany

Tel: +49-681-302-3856
Secr: +49-681-302-3855
Fax: +49-681-302-3857
email: m.springborg@mx.uni-saarland.de

1 POST-DOCTORAL AND 2 Ph.D. POSITIONS

University of Twente, The Netherlands

1 postdoc and 2 Ph.D. positions are available in the research group of Prof. Paul J. Kelly in the Physics Department at the University of Twente in the Netherlands.
Information about the group can be found at http://www.tn.utwente.nl/cms/

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

The aim of the theoretical work is to bridge the gap between realistic ab-initio descriptions of the electronic structure in layered magnetic materials (P.J. Kelly: University of Twente and Philips Research Laboratories Eindhoven) and phenomenological transport models of GMR (G.E.W. Bauer: Delft University of Technology) . Candidates should have experience of first-principles electronic structure calculations. Knowledge of transport theory would be very welcome but is not a prerequisite. The research position will be based in Enschede (Twente) and the post-doc will maintain intensive contact with other members of the node in Delft and Eindhoven.
* Only nationals of Member States or Associated States of the EU (but not the Netherlands) are eligible for the position allocated to the Dutch node.

In addition we have 1 position available to do a Ph.D on spin transport in layered magnetic materials on the basis of realistic electronic structure calculations.

A second position is available for a Ph.D on transport through single molecules, also on the basis of realistic electronic structure calculations.

Applications should be sent to
Prof. P.J. Kelly,
Faculty of Applied Physics,

University of Twente,
P.O. Box 217,
7500 AE Enschede,
The Netherlands

email: p.j.kelly@tn.utwente.nl
Tel.: +31-53-4893166
Fax: +31-53-4892910

Postdoctoral Position

Quantum Simulations Group, Condensed Matter Division, Physics Directorate Lawrence Livermore National Laboratory

Applications are invited for a postdoctoral position in the area of structural, electronic, and optical properties of nanostructure materials. The Quantum Simulations Group at LLNL currently consists of: Troy Barbee, Lorin Benedict, Giulia Galli, Jeffrey Grossman, Francois Gygi, Randy Hood, Roy Pollock, Eric Schwegler, and Andrew Williamson. We are developing a new initiative focused on nanostructure research and are seeking candidates with experience of electronic structure calculations. The salary range is $50,000-60,000 per year.

Applicants should send a curriculum vita and letters of reference to:

Jeff Grossman or Andrew Williamson
7000 East Ave.
P.O. Box 808
L-415
Livermore
CA 94551

email: williamson10@llnl.gov

POSTDOCTORAL POSITION

Department of Physics, University of Cambridge, UK

A postdoctoral position is available from 1st October 2000 to work on ab initio electronic structure calculations with the group of Dr Richard Needs. We use quantum Monte Carlo methods and density-functional methods to study problems in condensed matter physics. More information on the work of the group can be found at:

`http://www.tcm.phy.cam.ac.uk/~rn11/`

The successful candidate should have a PhD in Physics, Chemistry, Materials Science or a related subject. Preference will be given to candidates with a strong background in electronic structure calculations.

Details of how to apply can be found at:

http://www.tcm.phy.cam.ac.uk/advert.html

Richard Needs,
TCM Group, Cavendish Laboratory,
Madingley Road,
Cambridge CB3 0HE,
UK

e-mail: rn11@phy.cam.ac.uk

Postdoctoral Position in
Theory of Atomic and Molecular Manipulation
Department of Applied Physics
Chalmers/Göteborg University
Göteborg, Sweden

A postdoctoral position within the TMR network on "Atomic/Molecular Manipulation" is open in the group of Materials and Surface Theory. The successful applicant will work on the theoretical description and modeling of manipulation of individual atoms and molecules with the scanning tunneling microscope under supervision of Mats Persson and in collaboration with the theory and experimental groups of the network.

Candidates should have a PhD and a strong background in the theoretical and computational methods of condensed matter physics. The post is for 1+1 year and starting date will be as soon as possible. Further details about the position can be obtained from Mats Persson. (See, e.g. http://fy.chalmers.se/ap/msp/ and http://fy.chalmers.se/ap/TMR/ for some information about our group and the network, respectively).

Please note that this position is funded by the TMR program of the EU so only candidates from (non Swedish) European countries and associated members, that is, Iceland, Israel, Lichtenstein and Norway, can apply.

Applicants should send a CV, a list of publications and names of a few reference persons with phone numbers to:

Prof. Mats Persson,
Department of Applied Physics,
Chalmers/Göteborg University,
S-412 96 Göteborg, SWEDEN
e-mail: tfymp@fy.chalmers.se
phone: +46-31-7723666

POSTDOCTORAL POSITION

in Computational Physics

University of Natal at Pietermaritzburg, South Africa

Contact person: Dr. N. Chetty, chettyn@phsc.unp.ac.za

A postdoctoral position is available in the field of Computational Solid State Physics or Statistical Physics for two years renewable for a third year, to commence in August 2000. The candidate should have an expertise in Fortran 77/90, UNIX /LINUX systems, and an interest in parallel computing on a cluster of pentiums running PVM/MPI. An experience in the quantum mechanical modelling of solids or atomistic models in simulations will be considered an advantage. The candidate will also be required to teach a single module of 24 lectures per semester in the undergraduate Programme in Computational Physics. Remuneration will be commensurate with experience, and a PhD is the minimum qualification. Please send a CV and a list of three referees to the above address.

Ph. D. Studentships

Computational Materials Physics Group

University of Edinburgh, UK

Engineering and Physical Science Research Council (EPSRC) funded PhD places available for students with first or upper second class degrees (or equivalent) in a relevant subject. All projects involve the atomistic modelling of materials using state of the art computer simulations in the Computational Materials Physics Group at the University of Edinburgh, commencing 1st October 2000.

Successful applicants will learn the theory and practice of quantum mechanical calculations, employing and developing existing codes on systems of material interest. Three projects are available, applying quantum physics to electronics, robotics and geophysics.

Anchoring of Liquid Crystal molecules to surfaces

Liquid crystals are formed by long, thin molecules which align in a particular direction. This enables them to act as light polarisers which, because of their liquid nature, can be rapidly switched in direction. An unknown aspect of their behaviour is how they interact with surfaces (e.g. on display devices), whether they are bonded (chemisorption) or not (physisorption). This project will build on recent work with simpler molecules to formulate a theoretical understanding of the processes involved. This will guide electronic engineers towards a more systematic way of tailoring the properties of newly synthesised molecules.

Shape Memory Alloy

Shape memory alloys are a class of material which can be deformed at one temperature, and then resume their original shape when returned to their previous temperature. As such they can be used as motorless robots, or in medical applications where a support or tool is inserted and then expands to an appropriate shape. This behaviour depends crucially on the microstructural ability of the material to change crystal structure under

anisotropic strain. This project is to calculate the strain dependence of the phase stability of NiTi, the archtype shape memory alloy, to obtain an understanding which can guide improvements in the alloy composition and manufacture and to derive simple models of that behaviour at large scale.

Mantle mineralogy

The earth's mantle is composed of minerals comprising silicon, magnesium, aluminium and oxygen in various concentrations. The equilibrium form under the extreme conditions of pressure and temperature is uncertain, and intractible to experiment, yet crucial for understanding the mantle convection currents which drive plate tectonics. This project is to map out the stable compostions as a function of temperature and pressure, including both chemical decomposition and changes in crystal structure. This will produce a definitive phase diagram for the materials which compose most of the planet.

The Department of Physics and Astronomy was rated 5 in the last research assessment exercise and has the largest research income of any university department in Scotland. We also have unrivalled access to supercomputing facilities through the Edinburgh Parallel Computing Centre.

Potential applicants should contact either Dr S.P. Bates (S.P.Bates@ed.ac.uk) or Dr G.J.Ackland (G.J. Ackland@ed.ac.uk) for more information.

9 Abstracts

Real-Space Imaging of Two-Dimensional Antiferromagnetism on the Atomic Scale

S. Heinze,[1,2] M. Bode,[1] A. Kubetzka,[1] O. Pietzsch,[1] X. Nie,[2]
S. Blügel,[2] and R. Wiesendanger[1]
1: Institute of Applied Physics and Microstructure Research Center,
University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany
2: Institut für Festkörperforschung, Forschungszentrum Jülich,
D-52425 Jülich, Germany

Abstract

A two-dimensional antiferromagnetic structure within a pseudomorphic monolayer film of chemically identical manganese atoms on tungsten (110) was observed with atomic resolution by spin-polarized scanning tunneling microscopy at 16 Kelvin. A magnetic superstructure changes the translational symmetry of the surface lattice with respect to the chemical unit cell. It is shown, with the aid of first-principles calculations, that as a result of this, spin-polarized tunneling electrons give rise to an image corresponding to the magnetic superstructure and not to the chemical unit cell. These investigations demonstrate a powerful technique for the understanding of complicated magnetic configurations of nanomagnets and thin films engineered from ferromagnetic and antiferromagnetic materials for magnetoelectronics.

(Science **288**, 1805 (2000))

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

Influence of perpendicular magnetic anisotropy on closure domains studied with x-ray resonant magnetic scattering

E. Dudzik, S. S. Dhesi, H. A. Durr, S. P. Collins, M. D. Roper, G. van der Laan,
K. Chesnel, M. Belakhovsky, A. Marty, and Y. Samson
Daresbury Laboratory, Daresbury, Warrington, Wa4 4AD, UK

Abstract

FePd thin film samples with perpendicular magnetic anisotropy (PMA) have been studied with x-ray resonant magnetic scattering (XRMS), both at the Fe and at the Pd L_3 edges. In these samples the competition between PMA and shape anisotropy leads to the formation of highly-ordered striped domain patterns with a magnetization component perpendicular to the film plane. These striped domains give rise to magnetic satellite peaks in the diffraction pattern. Magnetic diffraction rod scans of these satellites were analysed to obtain information about the magnetic depth profile of the films. It was found that flux closure occurs in samples with a low to medium PMA, while a high PMA impedes the formation of closure domains. Data analysis gives a depth of the closure domains extending to 85 Å, with approximately half the magnetic moment aligned in-plane.

(Tentatively scheduled for 1 September 2000, Physical Review B, Volume 62, Number 9)
Preprints available from: g.vanderlaan@dl.ac.uk

A First-Principles Theory of Bloch Walls in Ferromagnets

J. Schwitalla[a], B. L. Györffy[a], and L. Szunyogh[b,c]

[a] *H.H. Wills Physics Laboratory, University of Bristol, UK*

[b] *Department of Theoretical Physics,*

Budapest University of Technology and Economics, Hungary

[c] *Center of Computational Materials Science,*

Technical University Vienna, Austria

Abstract

We present a first principles account of Bloch Walls on the basis of relativistic Spin-Density Functional Theory in the Local Density Approximation (LDA). We argue that calculations based on this description will provide useful and novel informations about the physics of this important element of micro-magnetics. To illustrate the points we wish to make we implement the proposed calculations for Fe and determine the Bloch Wall thickness ℓ_{BW}. Moreover we study features of the electronic structure which arise due to the presence of the Bloch Wall.

(Submitted to PRB, 4 July 2000)

Postscript preprints available from: `szunyogh@heisenberg.phy.bme.hu`

This paper includes acknowledgement to the TMR Network on "Ab initio calculations of magnetic properties of surfaces, interfaces and multilayers" (Contract: ERBFMRXCT96-0089).

Oscillatory Exchange Coupling across $Cu_{(1-x)}Ni_x$ spacers: A first principles calculation of the amplitudes and phases using asymptotic analysis

N. N. Lathiotakis and B. L. Györffy

H. H. Wills Physics Laboratory, University of Bristol,

Tyndall Ave, BS8 1TL Bristol, U.K.

E. Bruno and B. Ginatempo

Dipartimento di Fisica and Unità INFM,

Università di Messina, Salita Sperone 31,

98166 Messina, Italy

Abstract

We apply a recently developed first-principles asymptotic approach to the problem of the oscillatory exchange coupling (OEC) in the $Co/Cu_{(1-x)}Ni_x/Co$ trilayer system for all (100), (110) and (111) directions of growth. We compare results of the asymptotic analysis with full calculations. Our results are consistent with the available experimental data and give strong evidence for the existence of the exponential decay in the asymptotic form of the OEC for $x > 0.04$. Moreover, we discover a caliper vector of the alloy Fermi surface, $Q^{(3)}_{(100)}$, which did not exist in the case of pure Cu, but contribute to the OEC significantly for $x \geq 0.11$.

(to appear in: Physical Review B **62**, Number 13, 1 October 2000)

Latex-file available from: n.lathiotakis@bristol.ac.uk

Multilayer relaxations at the (0001) surface of Be and Mg

E. Wachowicz and A. Kiejna,
Institute of Experimental Physics, University of Wrocław,
plac M. Borna 9, 50-204 Wrocław, Poland

Abstract

Density functional theory and a plane-wave basis pseudopotential technique is applied to calculate relaxations of the first three interlayer spacings at the (0001) surface of thick Be and Mg slabs. For both metals the calculated outward relaxation of the topmost layer and small relaxations of the deeper layers are in a good agreement with experiment and previous calculations. The calculated multilayer relaxations are analyzed in terms of the electron charge density profile perpendicular to the surface which shows an oscillatory character with a period consistent with the long-range Friedel oscillations. Our results provide arguments for the generalization of the physical model relating the origin of multilayer relaxation to Friedel oscillations at the bulk truncated surface.

(Accepted by Solid State Commun.)
Copy available from: kiejna@ifd.uni.wroc.pl

Acknowledgement includes: STRUC-Ψ_k Programme of the European Science Foundation.

Ferromagnetic zigzag chains and properties of the "charge ordered" state in the 50% perovskite manganites

I. V. Solovyev

JRCAT-Angstrom Technology Partnership,

1-1-4 Higashi, Tsukuba, Ibaraki 305-0046, Japan

and

Institute of Metal Physics, Russian Academy of Sciences,

Ekaterinburg GSP-170, Russia

Abstract

The low-temperature properties of the so-called "charge ordered" state in the 50% doped perovskite manganites are described from the viewpoint of the magnetic spin ordering. In these systems, the zigzag antiferromagnetic ordering, combined with the double-exchange physics, effectively divides the whole sample into the one-dimensional ferromagnetic zigzag chains and results in the anisotropy of electronic properties. The electronic structure of one such chain is described by an effective 3×3 Hamiltonian in the basis of Mn($3de_g$) orbitals. We treat this problem analytically and consider the following properties: (i) the nearest-neighbor magnetic interactions; (ii) the distribution of the Mn($3de_g$) and Mn($4p$) states near the Fermi level, and their contribution to the optical conductivity and the resonant x-ray scattering near the Mn K-absorption edge. We argue that the anisotropy of magnetic interactions in the double-exchange limit, combined with the isotropic superexchange interactions, readily explains both the local and the global stability of the zigzag antiferromagnetic state. The two-fold degeneracy of e_g levels plays a very important role in the problem and explains the insulating behavior of the zigzag chain, as well as the appearance of the orbital ordering in the double-exchange model. Importantly, however, the charge ordering itself is expected to play only a minor role and is incompatible with the ferromagnetic coupling within the chain. We also discuss possible effects of the Jahn-Teller distortion and compare the tight-binding picture with results of band structure calculations in the local-spin-density approximation.

(Submitted to Phys. Rev. B)

Manuscripts available from: igor@jrcat.or.jp

Ab-initio Theory of Valency in Ytterbium Compounds

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Abstract

The electronic structure of 26 Yb compounds is calculated with the *ab-initio* self-interaction corrected local-spin-density approximation. In this approach f-electrons can be described as either localized or delocalized. Hence, a divalent Yb ion is represented with a completely localized f^{14} shell, while a trivalent Yb ion is represented with a localized f^{13} shell with the remaining 14^{th} f-electron giving rise to a very narrow f-resonance, which straddles the Fermi energy. The systems studied comprise the Yb monopnictides and monochalcogenides as well as a series of intermetallic compounds. Experimental equilibrium volumes are well reproduced. The results provide quantitative support to the experimental classification of Yb compounds in terms of effective valencies.

(Submitted to Phys. Rev. B)

Manuscripts available from: svane@ifa.au.dk

Electronic structure and magnetism in disordered bcc Fe alloys

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Abstract

We here study electronic structure and magnetic properties of bcc Co_xFe_{1-x}, Cr_xFe_{1-x} and Mn_xFe_{1-x} in their ferromagnetic phases using Augmented space recursion technique coupled with tight-binding linearized muffin tin orbital (TBLMTO) method. We make a systematic study of magnetic properties like magnetic moment and Curie temperature and try to draw some conclusions on their variation across the row of 3-d transition metal series in periodic table using arguments based on effects like charge transfer,exchange splitting and hybridization.

(Submitted to Journal of Phisics C: Condensed Matter)

Latex-file available from : subhra@boson.bose.res.in

Experimental and theoretical x-ray magnetic circular dichroism study of the magnetic properties of $Co_{50}Pt_{50}$ thin films

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Abstract

An experimental and theoretical investigation of the structural and micro-magnetic properties of the $Co_{50}Pt_{50}$ ordered alloy is presented. The Co-3*d* and Pt-5*d* orbital and spin magnetic moments and their anisotropies are determined by means of angle-dependent x-ray magnetic circular dichroism measurements. Our calculated spin magnetic moments of both Co and Pt are in good agreement with our experiment results, while the orbital magnetic moments are underestimated. The reduction of the 3*d* and 5*d* orbital magnetic moments, observed when the spin magnetic moment is forced out of the easy axis of magnetization, is reproduced by the theory. The calculated XMCD reproduces semi-quantitatively the experimental spectra and underestimates the so-called branching ratio. The computed magneto-crystalline anisotropy is of the same order of magnitude as the experimental one with the correct sign.

(Physical Review B **62**, 1157 (2000))

Reprints available from: Iosif.Galanakis@ipcms.u-strasbg.fr

Interface magnetism in ultra-thin Fe/W(110) films from first-principles

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Abstract

An *ab-initio* study of the magnetic properties of Fe ultra-thin films on top of a W(110) substrate shows that for one Fe layer the magnetization axis is in-plane. For an additional layer of Fe, the magneto-surface and magneto-elastic anisotropies favor a magnetization axis perpendicular to the substrate, but the total energy including the shape anisotropy is minimal for the spin axis in-plane. In the case of the tri-layer film all anisotropies favor an in-plane magnetization axis. The spin magnetic moment of the first Fe atomic layer is close to the bulk value while that of the second and third Fe atomic layers are considerably increased. The W atoms at the interface are weakly antiferromagnetically coupled to Fe. The orbital magnetic moment anisotropy of all the atoms is shown to be directly related to the calculated x-ray magnetic circular dichroism anisotropy.

(Physical Review B, to be published August 2000)

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On perpendicular magnetic anisotropy of binary alloys: A total energy calculation

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Abstract

Using the state-of-the-art relativistic full-potential version of the linear-muffin-tin orbital method we have performed *ab-initio* calculations to study the magnetic properties of eight transition-metal binary alloys (FePt, CoPt, FePd, FeAu, $MnPt_3$, $CoPt_3$, VAu_4 and $MnAu_4$). Both the local spin-density approximation (LSDA) and the generalized gradient approximation (GGA) to the exchange-correlation potential are used in the computation. The resulting spin and orbital magnetic moments of both approximations are similar and agree nicely with experiment, however different values are found for the magneto-crystalline anisotropy energy (MCA), especially for $MnPt_3$, $CoPt_3$ and $MnAu_4$. For all the other alloys the difference between the MCA values calculated within LSDA and GGA is less than 1 meV. The volume shape anisotropy (VSA) is found to be important for the FePd and $MnPt_3$ thick films, while it is negligible for the other binary alloys.

(Physical Review B, to be published September 2000)

Manuscripts available from: Iosif.Galanakis@ipcms.u-strasbg.fr

The CO/Pt(111) puzzle

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Abstract

Notwithstanding half a dozen theoretical publications, well-converged density-functional calculations, whether based on a local-density or generalized-gradient exchange-correlation potential, whether all-electron or employing pseudopotentials, underestimate CO's preference for low-coordination binding sites on Pt(111) and vicinals to it. For example, they imply that CO should prefer hollow- to atop-site adsorption on Pt(111), in apparent contradiction to a host of low temperature experimental studies.

(Submitted to: J. Phys. Chem.)

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The GaAs(001) surface under conditions of low As pressure: Evidence for a novel surface geometry

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Abstract

Using density-functional theory we identify a new low-energy structure for GaAs(001) in an As-poor environment. The discovered geometry is qualitatively different from the usual surface-dimer based reconstructions of III-V semiconductor (001) surfaces. The stability of the new structure, which has a $c(8 \times 2)$ periodicity, is explained in terms of bond saturation and favorable electrostatic interactions between surface atoms. Simulated scanning tunneling microscopy images are in good agreement with experimental data, and a low-energy electron diffraction analysis supports the theoretical prediction.

(Submitted to: Phys. Rev. Lett.)

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Atomic structure of the stoichiometric GaAs(114) surface

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Abstract

The stoichiometric GaAs(114) surface has been prepared using molecular beam epitaxy (MBE) followed by annealing in ultra-high vacuum. Based on in-situ scanning tunneling microscopy (STM) measurements and first-principles structure calculations, we determine the surface reconstruction which we call $\alpha 2(2 \times 1)$. Contrary to what is expected for a high-index surface, it is surprisingly elementary. The (2×1) unit cell contains two As dimers and two rebonded Ga atoms. The surface energy is calculated as 53 meV/Å^2 which falls well within the range of low-index GaAs surface energies.

(Submitted to: Phys. Rev. Lett.)

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Decay properties of the one-particle Green function in real space and imaginary time

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Abstract

The decay properties of the one-particle Green function in real space and imaginary time are systematically studied for solids. I present an analytic solution for the homogeneous electron gas at finite and at zero temperature as well as asymptotic formulas for real metals and insulators that allow an analytic treatment in electronic-structure calculations based on a space-time representation. The generic dependence of the decay constants on known system parameters is used to compare the scaling of reciprocal-space algorithms for the GW approximation and the space-time method.

(Submitted to: Phys. Rev. B)

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Mechanism of island dissolution during capping layer growth interruption

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Abstract

Combining real-time experiments and density functional calculations, we demonstrate how the wetting phenomenon can be exploited to improve the size homogeneity of an ensemble of quantum dots by introducing a growth interruption during the capping layer growth. We use in-situ reflectance anisotropy spectroscopy, atomic force microscopy and transmission electron microscopy to investigate redistribution of material during the growth interruption. Density functional calculations identify the tendency of InAs to form a wetting layer on GaAs as the main driving force for this redistribution.

(Submitted to: Phys. Rev. Lett.)

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The electronic and optical properties of Si/SiO_2 superlattices: role of confined and defect states

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Abstract

The Si layer thickness dependence of the optical properties of Si/SiO_2 superlattices has been, for the first time, theoretically investigated. In our first principle calculation we consider both fully passivated interfaces and the presence of oxygen vacancy at the interface. Our results show the key role played both by the quantum confined states and interface states in the experimentally observed visible luminescence in Si/SiO_2 confined systems.

(Accepted by Surface Science)

Manuscripts available from: degoli@aries.unimo.it

Gallium and Indium under High Pressure

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Abstract

Ga and In crystallize in unusual open ground-state crystal structures. Recent experiments have discovered that Ga under high pressure transforms into a close-packed structure, while this has so far not been observed for In. Results from first principles calculations explain in a simple way this difference in behavior. We predict a so far undiscovered transition of In to a close-packed structure at extreme pressures and show that the structure determining mechanism originates from the degree of s-p mixing of the valence orbitals. Group-III elements are shown to strongly disobey the standard corresponding-states rule.

(Physical Review Letters)

Preprints available from: sergeis@fy.chalmers.se or via

http://fy.chalmers.se/ sergeis/research.html

Parallelization of the FLAPW Method

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Abstract

The FLAPW (full-potential linearized-augmented plane-wave) method is one of the most accurate first-principles methods for determining structural, electronic and magnetic properties of crystals and surfaces. Until the present work, the FLAPW method has been limited to systems of less than about a hundred atoms due to the lack of an efficient parallel implementation to exploit the power and memory of parallel computers. In this work, we present an efficient parallelization of the method by division among the processors of the plane-wave components for each state. The code is also optimized for RISC (reduced instruction set computer) architectures, such as those found on most parallel computers, making full use of BLAS (basic linear algebra subprograms) wherever possible. Scaling results are presented for systems of up to 686 silicon atoms and 343 palladium atoms per unit cell, running on up to 512 processors on a CRAY T3E parallel supercomputer.

(To appear in Computer Physics Communications (submitted Jan. 2000))

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Theoretical description of the Fano-effect in the angle integrated valence band photoemission of paramagnetic solids

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Abstract

A theoretical description of the Fano-effect in the angle integrated valence band photoemission of paramagnetic solids is presented that is based on the one-step-model of photoemission and relativistic multiple scattering theory. Applications to fcc-Cu led to a very satisfying agreement with recent experimental data that show the Fano-effect, i.e. a finite spin-polarisation for the spectra is found for excitation with circularly polarised radiation. As can be demonstrated by model calculations this finding is caused by the presence of the spin orbit coupling. To allow for a more detailed discussion of the spectra a simplified description of the Fano-effect is presented that treats spin orbit coupling as a perturbation.

(Submitted to *Phys. Rev.*

Manuscript available as ps-file on request from:

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A relativistic theoretical description for spin-resolved CVV-Auger electron spectroscopy with application to Pd and Fe

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Abstract

A theoretical description of spin-resolved CVV (core-valence-valence) Auger electron spectroscopy is presented. The approach is derived on the basis of a fully relativistic description of the electronic structure of magnetic materials. As a consequence, spontaneous exchange splitting as well as spin-orbit coupling – two possible and important sources for a spin-polarization of Auger electrons – are accounted for on the same level. This is demonstrated by application to paramagnetic fcc-Pd and ferromagnetic bcc-Fe. In both cases spin-resolved CVV Auger electron spectra are presented and discussed emphasizing the role of the spin-orbit coupling. Comparison is made with available experimental data as far as possible.

(Submitted to *Phys. Rev.*
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Field induced magnetic circular dichroism in paramagnetic solids

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Abstract

The magnetic circular dichroism in X-ray absorption (MCXD) is now a standard tool to probe the spin and orbital moments in spontaneously magnetized materials by exploiting the so-called sum rules. On the other hand, it is known that the magneto-optical Faraday effect, for example, can be observed for magnetic materials as well as for non-magnetic materials if the later ones are exposed to a magnetic field. Accordingly, magnetic circular dichroism in X-ray absorption should be induced in non-magnetic materials by an external magnetic field. A theoretical description of such an experiment is presented, that is based on a combination of a fully relativistic linear response formalism and a corresponding treatment of magnetic circular dichroism. It is demonstrated that application of the magnetic sum rules now gives access to the spin and orbital element projected susceptibility of the system under investigation. In particular one finds that it is only the VanVleck-like contribution to the orbital susceptibility that is probed.

to be published in *Lecture Notes in Physics*
Proceedings of the Workshop *"New trends in synchrotron radiation and magnetism"*,
Mittelwihr (Haut-Rhin, France), April 13 -14 2000.
Manuscript available as ps-file on request from:
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10 Book Announcement

ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF SOLIDS

"The use of the LMTO method"

Hugues Dreyssé (Ed.)

in *Lectures Notes in Physics - Springer*

Based on the Workshop held in Mont Sainte Odile, October 1998

and organized by the TMR network "Interface Magnetism"

Contents

11 SCIENTIFIC HIGHLIGHT OF THE MONTH

First-principles modelling of magnetic tunnel junctions

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Introduction

Magnetic tunnel junctions (MTJ) are promising candidates for applications in spintronic devices such as magnetic random access memories, read heads and sensors [1]. The MTJs consist of two ferromagnetic layers separated by an insulating barrier layer. The physical quantity measured for signal detection is the tunnelling magnetoresistance (TMR), i.e. the relative difference in the resistance between parallel and antiparallel magnetizations of the electrodes. It was found that the TMR could be as high as 30% at room temperature in tunnel junctions based on ferromagnetic 3d-metal electrodes when alumina is used as the barrier layer (for a recent review, see [2]).

The magnitude of the TMR is determined by the spin polarization (SP) of the tunnelling current, which can be measured in experiments on superconductors [3]. It was generally accepted that the SP of the tunnelling current is an intrinsic property of the ferromagnets and is determined by the SP of the electronic density of states (DOS) at the Fermi energy [4]. Experimental results show, however, that the SP of the tunnelling current is strongly dependent on the structural quality of the tunnel junctions. Improvements in the quality of the alumina barrier and the metal/alumina interfaces result in an enhancement of the measured values of the SP. Experiments also show that the SP is dependent on the choice of the tunnelling barrier. Negative values of the SP were obtained at low applied voltage

when tunnelling occurs from Co across a $SrTiO_3$ barrier [5], whereas it is positive across an alumina insulating layer [3]. We see, therefore, that the SP is *not* an intrinsic property of the ferromagnet alone but depends on the structural and electronic properties of the entire junction including the insulator and the ferromagnet/insulator interface. Thus, the realistic description of the magnetic tunnel junctions becomes increasingly important for a quantitative description of the SDT and for an accurate prediction of the TMR. This is a very complicated problem especially due to the *amorphous* structure of the alumina barrier layer and the lack of direct atomistic information about the structure and bonding at the ferromagnet/alumina interface. This is quite different from the situation with other metal/alumina interfaces so far studied in which the metal is grown on top of *crystalline* Al_2O_3 (see, for example, [6], [7, 8]).

As a first step in understanding the properties of $Co/Al_2O_3/Co$ tunnel junctions we want to address two principal issues: 1) the atomic structure of the MTJ, and 2) the electronic structure of the MTJ. We have considered both Al- and O-terminated interfaces in coherent geometries which provide the *smallest* possible lattice mismatch between bulk fcc cobalt and crystalline α-alumina and have performed full geometry optimization of the structure by self-consistent spin-polarized calculations within density functional theory and the generalized gradient approximation using the total energy plane-wave pseudopotential code CASTEP [9]. The spin-polarized electronic structure of the Co/Al_2O_3 interfaces was studied by means of the scalar-relativistic linear muffin-tin orbital (LMTO) method [10]. Electronic properties of the $Co/Al_2O_3/Co$ MTJ are discussed with the focus to understand mechanisms responsible for spin-dependent tunneling.

Atomic structure

We have constructed a realistic model for the atomic structure of the cobalt/alumina/cobalt tunnel junction within a supercell approach by incorporating most of the important features of the real Co/Al_2O_3 thin-film system. The MTJs are produced by depositing a few tens of monolayers of aluminium film on top of the crystalline ferromagnet layer followed by thermal- or plasma- assisted oxidation to create the alumina tunnelling barrier (see e.g. [11]). The TEM images show that the alumina layer is grown on top of the (111) plane of fcc cobalt which exhibits large, predominantly [111] oriented grains [12]. Therefore, it is reasonable to assume that the cobalt film (deposited at the beginning of the manufacturing cycle) serves as a base with the bulk lattice parameter fixed in the

plane parallel to the interface. The alumina is then formed by adjusting its structure to that of cobalt during the course of oxidation.

The amorphous state of alumina can not be directly modeled at present by first-principles methods due to the large number of atoms needed in the simulation cell. Therefore, we consider crystalline α-Al_2O_3 with the [0001] orientation on top of fcc (111) Co, as a first step in modelling a realistic Co/Al_2O_3/Co MTJ. We have carefully studied all the possibilities of relative crystallographic alignments of cobalt and alumina and identified the crystal structure with the minimal lattice mismatch. The lateral dimensions of our supercell correspond to a 2x2 surface unit cell of the (111) plane of fcc cobalt with the theoretical lattice parameter $a = 5.057$ Å. The experimental lattice parameter a of corundum is 4.759 Å which results in a 6% lattice mismatch. Two limiting cases of oxygen-rich and aluminium-rich interfaces were modeled in order to get a feeling of the influence of oxidation on the SDT device characteristics. For both the O- and Al-terminated interfaces we use a seven-layer-thick cobalt slab with four cobalt atoms per layer (28 cobalt atoms in total) and a seven-layer-thick alumina slab, the composition of the latter being dependent on the termination.

Spin-polarized plane-wave pseudopotential calculations of the MTJ in supercell geometry were made within the generalized gradient approximation with the code CASTEP [9]. In order to determine the relaxed structure of the MTJ, it was critical to perform an optimization of all the internal coordinates of the atoms as well as the height of the unit cell. The constraints of fixed lateral cell dimensions and frozen three middle layers of cobalt were imposed in order to simulate the experimental conditions of the growth on the cobalt base. For a given cell size the atomic internal degrees of freedom were relaxed to give the minimum energy structure. The cell size was then varied and the relaxed structure was deduced from the minimum of the resultant binding energy curve. The relaxed structures are shown in Fig. 1.

We see from Fig. 1 that at the O-terminated interface the three oxygen atoms in the O{1} layer participate in bonding with the four cobalt atoms in the Co{3} layer. Since the O-terminated interface possesses P-3 symmetry all three oxygen atoms are equivalent so we label them O. Looking at the cobalt side, the four cobalt atoms are divided into the three equivalent atoms Co2 and the single atom Co1 which is centered on the axis of symmetry. This Co1 atom forms three equivalent bonds with surrounding O atoms with a bond length R(Co1-O)= 2.12 Å, whereas each of the other three Co2 atoms forms

a bond with a single oxygen with a bond length R(Co2-O)= 1.97 Å. This difference in bond number between the Co sites causes the O-terminated interface to ripple by 10%. From the Al_2O_3 side of the interface, every oxygen atom has two inequivalent bonds R(Co1-O) and R(Co2-O) with the Co1 and Co2 atoms plus two inequivalent bonds with the aluminium atoms Al1 and Al2 in the layer Al{1} (R(Al1-O)= 1.84 Å and R(Al2-O)= 1.95 Å). In both interface terminations Al1 labels the aluminium atom within the first alumina layer Al{1} that is closest to cobalt, whereas Al2 labels the aluminium atom within the same Al{1} layer, but shifted along the z-direction towards the alumina side. The average Co-O bond length of 2.04 Å is within 5% of that in bulk CoO [13].

Fig. 1. The relaxed structure of the (a) O-terminated and (b) Al-terminated MTJs. The left-hand panel is a side view of the supercell, the right-hand panel is a layer-by-layer projection of the structure onto the (0001) plane using the Co{3} layer as reference. The layers are labeled by the chemical symbol of the element comprising the layer and are numbered from the bottom to the top.

At the Al-terminated interface two aluminium atoms in the Al{1} layer interact with the four cobalt atoms in the Co{3} layer as shown in Fig. 1. Atom Al1 occupies the fcc hollow site in the next layer, and the Al2 atom is at the hcp hollow site (these positions are identified as hcp or fcc with respect to in-plane coordinate stacking). The Co1 atom does not have any bonds with the interfacial Al{1} layer, and each of the three equivalent Co2 atoms is bonded to one Al1 atom with a bond length 2.40 Å and to one Al2 atom with a bond length 2.58 Å . From the alumina side of the interface one Al1 atom is bonded

to three Co2 atoms and the Al2 atom also has three Co2 nearest neighbours. The P123 symmetry of the cell includes a 3-fold rotation in addition to reflection. All the three Al-Co bonds originating from a particular Al atom are identical, the Co2-Al2 bond lengths being the longest. Interestingly, the average value of the Co-Al bond lengths, namely 2.49 Å, is equal to the average Al-Co bond lengths in CoAl intermetallic compound [14].

Electronic structure

The resulting spin- and layer-dependent DOS for the O-terminated interface are shown in the left hand panel of Fig. 2. The top two panels (a) and (b) display the LDOS of the O{2} and Al{2} layers in the middle of the oxide. We found that these LDOS are very similar to those obtained for the bulk α-Al_2O_3 [15], [16]. In the bulk α-Al_2O_3 the valence and the conduction bands are separated by a band gap which is, according to our results, equal to 6.2 eV at the Γ-point. Although this value is less than the experimental band gap of 8.8 eV [17] as a result of using the local density approximation (LDA), it is in good agreement with an all-electron full-potential LDA calculation [18]. In the presence of the interface with the Co metal the LDOS within the band gap of alumina (layers O{2} and Al{2}) is not exactly zero showing the presence of electronic states of the Co metal that propagate into the insulator barrier, decaying exponentially with the distance in the oxide layer. These metal-induced states are spin-polarized and are responsible for the spin-dependent tunnelling [3]. The Fermi level lies within the band gap of Al_2O_3 at about 3.5 eV above the top of the valence band.

The DOS of the inner Co{0} layer (panel (f)) is similar to the bulk DOS of fcc Co [19]. Although the major features of the DOS of the interfacial Co{3} layer bear close resemblance to that of the bulk Co{0} layer, we observe some differences as a result of the reduced symmetry of the interface as compared to the bulk and the covalent bonding between this Co{3} layer and the adjacent oxygen O{1} layer of Al_2O_3. In particular, the d band of the interfacial Co{3} layer is smeared out compared to the bulk (compare (e) and (f)), and the electronic states extend down to -10 eV as a result of the bonding with oxygen. This bonding does not, however, quench the interface magnetism, the magnetic moment of the interfacial Co{3} layer being 1.68 μ_B. This is different from what was found for the Co/HfO_2(001) interface [20], where the majority d band of the interfacial Co layer was not completely occupied and consequently the magnetic moment of this layer was strongly reduced compared to the bulk.

The DOS of the oxygen O{1} layer at the interface is very different from that in the 'bulk' of alumina O{2} layer (compare (d) and (a)) due to the covalent bonding between the $2p$ orbitals of oxygen and the $3d$ orbitals of cobalt. The pronounced four peaks in the energy interval between -3 eV and -8 eV for both the majority- and minority-spin electrons are associated with the formation of the bonding states. In addition to the bonding levels below the d bands, the oxygen DOS displays a broad band of antibonding states that extends up to about 2 eV above the Fermi energy. The exchange splitting of the d bands of Co and the bonding between the d orbitals of Co and the p orbitals of O induce a splitting of these antibonding states. Contrary to the bonding states, this splitting is large, mirroring the exchange splitting of the surface Co d states. The antibonding states are almost fully occupied for the majority spins and are partly occupied for the minority spins. This leads to an induced magnetic moment of 0.07 μ_B on the oxygen sites. The LDOS at the Fermi energy is larger for the minority-spin electrons as compared to the minority-spin electrons, i.e. the spin polarization in the density of states at the Fermi energy is negative. The DOS of the Al{1} layer adjacent to the interfacial O{1} layer does not differ significantly from the DOS of the Al{2} layer in the bulk of alumina (compare panels (c) and (a)). Although a trace of the antibonding Co-O states is still visible at the energies within the band gap, the bonding between the Al and O dominates in the LDOS formation within this layer.

The electronic and magnetic properties of the Al-terminated interface differ from those of the O-terminated one. The main difference comes from the fact metallic character of the metal/oxide interaction (see below) results in the sizeable LDOS of the interfacial Al{1} layer at the Fermi energy which is typical for metals (see the right hand panel (d) in Fig. 2). The DOS of the oxygen and aluminium layers within the interior alumina are qualitatively similar to those obtained for the O-terminated interface (compare panels (a) and (b) in Fig. 2). There is, however, a difference in the position of the Fermi energy: in the case of the Al-terminated interface it is shifted towards the bottom of the conduction band. As can be seen from panel (d), the SP of the LDOS at the Fermi level on the interfacial Al{1} layer is slightly negative.

Fig. 2. Layer-projected spin-dependent densities of states of the O-terminated $Co/Al_2O_3/Co$ MTJ (left hand panel) and Al-terminated $Co/Al_2O_3/Co$ MTJ (right hand panel) as a function of electron energy. The majority- and minority-spin densities of states are shown by arrows pointed up and down respectively. The Fermi level is denoted by the vertical line.

Character of bonding at the interfaces in $Co/Al_2O_3/Co$ MTJ

The electronic structure results indicate strong covalent bonding at the interface between Co{3} layer and the adjacent oxygen O{1} layer of Al_2O_3 in O-terminated MTJ. Fig. 3a shows charge-density contours of the Co/Al_2O_3 system in the (100) Miller plane of the supercell. The O atom at the interface shares the charge with the two interfacial Co1 and Co2 atoms. This partial localization of the electron density in the region between the atoms is an additional evidence of the covalent character of the Co-O bonding. The strongest covalent bonding is between the Co2 and O atoms which have the smallest bond length of 1.97 Å. The Co1 atom at the interface has much weaker bonding with O. There

is little electron charge propagating from the O atom to the nearest Al1 atom and the region between them is characterized by a very low charge density. This fact and the sizeable charge transfer between the Al and O demonstrate the dominance of the ionic character in the Al-O bond, which is known from previous studies of bulk alumina [17].

Fig.3. Charge density contours (in atomic units) of the (a) O-terminated and (b) Al-terminated $Co/Al_2O_3/Co$ MTJ.

The Al-terminated interface is characterized by metallic character of bonding as it was evidenced from resulting electronic structure. The interfacial Al{1} layer can be considered as a termination of a metal substrate comprising the Co metal layer and the Al monolayer and the LDOS of the interfacial Al{1} layer is sizeable at the Fermi energy which is typical for metals. Fig. 3b shows the charge-density map of the Al-terminated Co/Al_2O_3 system in the (110) Miller plane of the supercell. As is seen from the Fig. 3b, the value of the charge density at the interface is comparable with that in the interstitial region of bulk Co, which indicates the metallic character of the bonding between Co and Al at the interface.

As is known from previous studies, bonding at the metal-ceramic interfaces is accompanied by substantial charge transfer between metal and ceramic atoms [7],[21]. We calculated the Mulliken charges on all the atoms in the MTJ and plotted their distribution in the direction perpendicular to the interface in Fig. 4 for the O-terminated (a) and Al-terminated (b) MTJs. Usually, the oxide side acquires electrons and metallic atoms become positively charged. This is obviously the case for the O-terminated interface, where the oxygen O{1} layer tries to restore its favorable valence state by attracting electrons from the cobalt side. The four atoms of the Co{3} layer transfer

+0.15 electrons per atom to the O{1} layer, where each of the three O atoms carries -0.86 charge. There is also an additional transfer of electrons from the Al{1} layer where each of the two Al atoms donates extra 0.2 electrons per atom to the oxygens in the O{1} layer in addition to the usual charge transfer to oxygens in the bulk alumina.

Fig.4. Layer-resolved charge distribution (average charge per atom) across the O-terminated and Al-terminated $Co/Al_2O_3/Co$ MTJs. The interface boundary is marked by dotted vertical line.

The picture of the charge distribution across the Al-terminated interface (see Fig. 4b) is different from that in the O-terminated interface. Like in the bulk alumina, the interfacial Al{1} layer has an appreciable positive charge +2.42 (+1.21 per atom) due to sizeable charge transfer to the adjacent O{1} layer. This positive charge is screened very quickly within the Co layer as a result of the metallic character of interaction between the Co{3} and Al{1} layers. This screening is reminiscent of the Friedel oscillations since we also observe the charge alternation from plus to minus and the interfacial Co{3} layer acquires a considerable negative charge of about -0.2 per atom. The transfer of electrons to the Co{3} from the Al{1} layer has further consequences in terms of interfacial magnetism and interfacial energetics. As a result of the charge transfer to the Co{3} layer we observe the

reduction of the average magnetic moment within the Co{3} layer down to approximately 1.15 μ_B per atom. As can be seen from panel (e) of Fig. 2, the Fermi level lies above the majority d bands and the reduction in the magnetic moment is mainly due to the minority d band filling (compare with the bulk DOS shown in panel (f)).

The reduction of the surface magnetism results in lowering the interfacial work of separation which is defined as $W_{sep} = (E_{\mathrm{Co}} + E_{\mathrm{Al_2O_3}} - E_{int})/2A$. Here E_{int} is the total energy of the supercell containing the MTJ, E_{Co} and $E_{\mathrm{Al_2O_3}}$ are the energies of the same supercell containing a single slab of pure Co and Al_2O_3, A is the area of the interface [21]. We found that within the spin-polarized total energy framework the work of separation for the O-terminated interface is equal to 6.35 J/m^2 and for the Al-terminated interface is equal to 3.64 J/m^2. In order to reveal the influence of magnetism on interfacial energetics, we have performed spin-restricted calculations for both terminations. It turned out that in the case of the O-terminated interface the difference between spin-polarized and spin-unpolarized values for the work of separation is less than 0.1 J/m^2. This result is not unexpected: the O-terminated MTJ and the single slab of pure Co have similar magnetic moments, therfore, the magnetic contributions to the total energy are subtracted in the work of separation since the alumina part of interface is nonmagnetic. However, in the case of the Al-terminated interface the quenching of the surface magnetism due to the charge screening effects costs +0.7 eV per interface and reduces the work of separation by 0.5 J/m^2 as compared to the spin-restricted value.

Spin-dependent tunnelling

Although we have not evaluated yet the conductance of the $Co/Al_2O_3/Co$ junction, some conclusions about the mechanism of spin-dependent tunnelling can be made based on the LDOS considerations. The quantity which is relevant to the tunnelling is the LDOS at the Fermi energy across the insulating barrier. This quantity characterizes the decay of the evanescent metal-induced electronic states within the band gap of alumina and could, therefore, be used for elucidating the factors responsible for the spin polarization of the tunnelling current. We have performed an additional electronic structure calculation in which the thickness of the α-alumina insulating barrier in the O-terminated Co/Al_2O_3 structure was increased by 12 extra monolayers of alumina (i.e by the size of the conventional unit cell of bulk alumina).

Fig. 6a illustrates the behaviour of the LDOS at the Fermi energy for the majority and minority spin electrons as a function of the distance from the interface Co layer. Evidently, the LDOS decreases exponentially with the distance. Although the minority DOS is larger at distances near the interface, it decays more rapidly as compared to the majority LDOS. Eventually the majority LDOS starts to dominate over the minority LDOS resulting in the positive SP. This can be seen from Fig. 6b, which shows the SP of the DOS at the Fermi level as a function of the distance from the interface Co layer. The SP is defined by $(D_\uparrow - D_\downarrow)/(D_\uparrow + D_\downarrow)$, where $D_\uparrow$ and $D_\downarrow$ are the LDOS for the majority and minority spins respectively. It is clear from Fig. 6b, that the layer-averaged SP increases gradually without showing a tendency for saturation.

Fig. 6. The local density of states at the Fermi energy for the majority- (circles) and minority- (squares) spin electrons (a) and the spin polarization of the DOS (b) as a function of the distance from the interface Co layer.

In order to obtain quantitative information about the behaviour of the LDOS within the barrier, we fitted the two curves presented in Fig. 6a by the exponential function $A\exp(-2\kappa z)$, where A is the constant, z is the distance from the interface, and κ is the decay constant. We found that $\kappa_\uparrow = 0.48$ Å^{-1} and $\kappa_\downarrow = 0.54$ Å^{-1} for the majority and

minority spins respectively. This corresponds to the decay lengths $l_\uparrow = 1.04$ Å and $l_\downarrow = 0.93$ Å. The decay constants determine the height of the effective potential barrier $U = \hbar^2\kappa^2/(2m^\star)$. Assuming that the effective electron mass $m^\star$ is equal to the free-electron electron mass, we obtain $U_\uparrow = 0.88$ eV and $U_\downarrow = 1.11$ eV. It is not surprising that these values of the barrier height are lower than the values of $2 \div 2.5$ eV extracted from experimental data (see, e.g. [2]), because LDA underestimates the band gap in insulators.

Since $U_\uparrow < U_\downarrow$ the tunnelling current should become 100% positive spin-polarized in the limit of large insulator thickness. This reflects the fact that the d-states of cobalt decay faster in the insulator barrier that the s-p states. Such a behaviour was predicted by theory for epitaxially-grown iron/semiconductor tunnel junctions [22]. In our case this conclusion might be precocious since the analysis is based on the LDOS at the Fermi energy. It is well-known that electronic states which correspond to different transverse momenta decay in the barrier with different decay lengths. In the case of alumina which has a minimum direct band gap at the Γ-point, the electronic states with zero transverse momentum have the lowest effective barrier height and consequently the longest decay length. In addition to this, as was shown in Ref. [22], the bands which are characterized by different symmetry, i.e. associated with different angular character within the barrier, can have unequal decay lengths. We conclude, therefore, that in order to fully understand the factors controlling the SP, further calculations are necessary, which include the explicit evaluation of the conductance and its analysis in terms of contributions from the states with different transverse momenta and orbital characters.

Acknowledgments

I.I.O. thanks DARPA for the financial support under Contract No.N00014-97-1-G015. E.Yu.T. thanks Hewlett Packard Laboratories, Palo Alto for the financial support through a collaborative research program. The calculations were performed in the Materials Modelling Laboratory at the Department of Materials and in the Oxford Supercomputer Centre, University of Oxford.

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