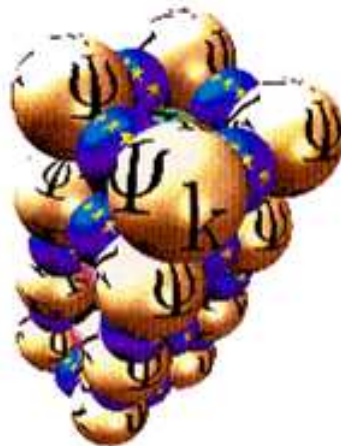

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 72

December 2005



Editor: Z. (Dzidka) Szotek
E-mail: psik-coord@dl.ac.uk

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1 Editorial

First, note that the front page of the newsletter has been changed and now includes also the Psi-k logo and the names of the sponsors. The UK's CCP9 (Collaborative Computational Programme on "Computational Studies of the Electronic Structure of Solids") has sponsored the newsletter since its very beginning. Throughout the years the CCP9 has been joined by a variety of EU and ESF networks in sponsoring the newsletter, but at present it is just the ESF Psi-k Programme, which will run until 2007. See Volker Heine's concluding remarks in the ESF section on the future of Psi-k beyond 2007. In the same section we have some remarks on the Psi-k 2005 Conference and its scientific highlights by Risto Nieminen, the Conference chairman.

As usual, the newsletter is started with an editorial followed by a short obituary of Paolo Carra, Theory Group, ESRF Grenoble. The RTN network on "f-electrons" has its annual report published in this newsletter, with a short summary of scientific highlights. The general workshop/school/conference and available position announcements can be found in their usual sections, followed by abstracts of newly submitted or recent papers. The newsletter is finished with the scientific highlight of the month on "ONETEP: linear-scaling density-functional theory with plane waves" by Peter D. Haynes (Cavendish Laboratory, Cambridge, UK), Chris-Kriton Skylaris (Oxford University, UK), Arash A. Mostofi (MIT, USA) and Mike C. Payne (Cavendish Laboratory, Cambridge, UK).

The *Psi-k* has a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:

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

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

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

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

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

2 General News

2.1 Obituary Paolo Carra

Head of the ESRF Theory Group, Grenoble, France

Paolo Carra passed away on 18th of October 2005. He had a cardiac arrest while sleeping.

Paolo Carra was a very bright theoretical physicist in condensed matter physics. He joined the ESRF in 1990, and since then he worked on problems requiring the deepest understanding of the interaction of condensed matter with the electromagnetic field, and in particular with x-rays. His work, carried out by himself, with his team, in collaboration with other re-known theoreticians, among them Theo Thole, and with experimentalists, gave milestone results. This work is internationally recognized as being one among the most important theoretical achievements in x-ray physics during the last 10 or 20 years. The derivation of new optical sum rules, applicable to the x-ray region, has had, and continues to have, a major impact on the understanding of subtle magnetic, electronic and structural properties of the most advanced and complex materials. Its relevance goes well beyond the simple theoretical understanding of a subtle physical phenomenon – this is demonstrated on how x-ray spectroscopy and scattering analytical techniques, since Paolo and co-workers discoveries, can serve the material science community to understand and design new advanced materials. This work was internationally recognized by the assignment to Paolo Carra of the Hewlett-Packard Europhysics Award in year 2000 for “the pioneering work in the development of the field of x-ray magnetic dichroism”. This prize was shared with G. van der Laan and G. Schutz.

Paolo Carra was appointed as Head of the ESRF Theory Group in 2000. He leaves his wife, Antonella, and two sons, Lorenzo and Enrico, 19 and 8 years old, respectively.

The ESRF Directors

3 News from the RTN on "f-electrons"

"Ab-initio Computation of Electronic Properties of f-electron Materials"

3.1 Third Annual Report

RTN Network Title : Ab-initio Computation of Electronic Properties of f-electron Materials.
Network Short Title : Psi-k f-electron
Contract No. : HPRN-CT-2002-00295
Commencement date of contract : 01-09-2002
Duration of Contract : 48 months
Reporting Period : 3rd: 01-09-2004 - 31-08-2005

Name of co-ordinator : Associate Prof. Axel Svane
Address : Department of Physics and Astronomy,
Ny Munkegade,
DK-8000 Aarhus C, Denmark
Telephone : +45 8942 3678
Telefax : +45 8612 0740
E-mail : svane@phys.au.dk

Network home page : <http://www.phys.au.dk/~svane/rtn.htm>

Part A: Research Results

A.1.: Scientific Highlights

Methodological Developments

A new method of numerical simulations for correlated electron systems based on the continuum-time QMC approach has been implemented and used to investigate the interplay of the on-site Kondo effect and inter-site exchange interactions. This interplay is of crucial importance for physics of anomalous f-electron systems like Kondo lattices (Nijmegen group).

The DMFT scheme has been implemented into the KKR computer code to facilitate a coherent potential description of disordered correlated systems (Nijmegen).

A new solver for the LDA+DMFT calculations with arbitrarily strong spin-orbit coupling has been implemented by the Nijmegen postdoc.

The Uppsala group has developed a many-body projector orbitals method for electronic structure theory of strongly correlated electrons, with the purpose of computing crystal-field excitations in f-materials in a DFT framework.

Work on ab-initio derivation of many-body Hamiltonians, in particular the computation of the Hubbard U parameter and the development of the DMFT(GW) methodology has been carried out by the Paris-Rutgers-Nijmegen collaboration.

Photoemission spectra of f-electron solids.

The spectral functions of several actinide systems have been calculated within the dynamical mean-field theory. The spectra of PuSe and Am have been obtained using a simplified model of the conduction electron combined with an exact diagonalization of the ensuing impurity problem (Aarhus). The comparison to experimental photoemission spectra is quantitatively accurate, and allows for a detailed identification of the origin of the most distinct features of the spectra in terms of the quantum state of the f-shell. In another study by the Nijmegen post-doc the spectra of USe, UTe, PuSe and PuTe have been calculated solving the impurity problem in the T-matrix FLEX approach, emphasizing improvement over the static LDA+U results. In a joint paper, the Aarhus, Nijmegen and Uppsala groups have calculated the photoemission of rare-earth systems TmCh (Ch=S,Se and Te) [3] and a paper on the the elemental metals is in preparation. In these cases the photoemission is dominated by the atomic-like multiplets of the photoexcited f-shell, and these features are quantitatively accurately reproduced with the Hubbard-I type approximation for the f spectral function.

The $\alpha - \gamma$ transition in cerium

The $\alpha - \gamma$ isostructural transition in cerium has been studied by the Daresbury and Aarhus

collaboration [11] and by the Paris group [12], by two different models. The first approach involves self-interaction corrected density-functional calculations in a disordered alloy of α -like and γ -like cerium atoms, the disorder being described by the coherent potential approximation. The second approach involves the dynamical mean-field treatment of the cerium solid with extensive quantum Monte Carlo calculations of the ensuing Kondo impurity problem. Common to both approaches is the conclusion that it is the entropy of the γ -phase that drives the transition.

The Mott transition in f-systems, with emphasis on the CeTh alloy, has been studied in a DMFT treatment of the Hubbard model including hybridization and finite temperature, and a first order transition between Kondo screened phase and local moment behavior is found [1] (Paris-Rutgers collaboration). Additionally, it is demonstrated that both an upper and a lower critical temperature exist, a fact corroborated by experimental evidence.

The equation of state of the Ce₄₃Th₅₇ alloy has also been studied using DFT and CPA for disorder by the Nijmegen post-doc.

Rare-earth oxides and rare-earth doped high T_c superconductors.

Electronic structure calculations were performed for the rare-earth high T_c superconductors CeBa₂Cu₃O₇, PrBa₂Cu₃O₇, NdBa₂Cu₃O₇, GdBa₂Cu₃O₇, and TbBa₂Cu₃O₇. Special emphasis was put to the valency of the rare-earth ion, which is computed with the self-interaction corrected local-spin-density energy functional. These studies indicated that the non-superconductivity in PrBa₂Cu₃O₇ is due to the tetravalency of Pr which leads to a magnetic and divalent Cu for which superconductivity cannot occur. The situation for the rare-earths in the superconductors is quite parallel to that of the rare-earth oxides, for which the tetravalent dioxides are only found for Ce, Pr and Tb [2,4].

Magnetism and Fermi surface properties

Magnetic x-ray scattering of praseodymium has been calculated (Daresbury with external team members) [5]. The cerium 115 compounds CeMIn₅ (M=Co, Rh, and Ir) have been studied using the LDA implemented in the FPLO method with both itinerant and localized description of the f-electrons. Fermi surface details (de Haas-van Alphen frequencies) show best agreement with experiments for itinerant f-treatment in the M=Co and M=Ir compounds, but localized f-treatment in the M=Rh case [6,7].

A.2.: Joint Publications

Network post-docs are underlined.

1. L. de'Medici, A. Georges, G. Kotliar and S. Biermann, *Mott transition and Kondo Screening in f-electron Metals*, Phys. Rev. Lett. **95**, 66402 (2005). ENS-ULM and RUTGERS partners.
2. L. Petit, A. Svane, Z. Szotek and W.M. Temmerman, *First principles Study of rare earth*

- oxides*, Phys. Rev. B, to appear (2005). UAA and CCLRC partners.
3. S. Lebègue, G. Santi, A. Svane, O. Bengone, M. I. Katsnelson, A. I. Lichtenstein, and O. Eriksson, *A Theory for calculating the photoelectron spectra of strongly correlated materials*, Phys. Rev. B, to appear (2005). UAA, KUN and UPPSALA partners.
 4. L. Petit, A. Svane, Z. Szotek and W.M. Temmerman, *Electronic Structure of rare earth oxides*, Topics in Applied Physics, Springer Verlag, to appear (2005). UAA and CCLRC partners.
 5. E. Arola, M. Horne, P. Strange, H. Winter, Z. Szotek and W.M. Temmerman, *Self-interaction corrected relativistic theory of magnetic scattering of x-rays: Application to praseodymium*, Phys. Rev. **B70**, 235127 (2004) (cond-mat/0404543). CCLRC with external team members in Keele and Karlsruhe.
 6. S. Elgazzar, I. Opahle, R. Hayn, and P.M. Oppeneer, *Electronic Structure and de Haas-van Alphen quantities of $CeMIn_5$ ($M=Co, Rh, \text{ and } Ir$) compounds*, J. of Magn. and Magn. Mater. **290-291**, 388 (2005). DRESDEN and UPPSALA partners.
 7. S. Elgazzar, I. Opahle, R. Hayn, P.M. Oppeneer, *Calculated de Haas-van Alphen quantities of $CeMIn_5$ ($M=Co, Rh, \text{ and } Ir$) compounds*, Phys. Rev. B **69**, 214510 (2004). DRESDEN and UPPSALA partners.
 8. J. Laverock, S. B. Dugdale, Zs. Major, M. A. Alam, N. Ru, I. R. Fischer, G. Santi and E. Bruno, *Fermi surface nesting and charge-density wave formation in rare-earth tritellurides*, Phys. Rev. B **71**, 85114 (2005). UAA with CCLRC external team member Bristol.
 9. S. Y. Savrasov, A. Toropova, M. I. Katsnelson, A. I. Lichtenstein, V. Antropov, and G. Kotliar, *Electronic structure and magnetic properties of solids*, Z. Kristallogr. **220**, 473 (2005). RUTGERS and KUN collaboration.
 10. S. Biermann, A. Poteryaev, A. I. Lichtenstein, and A. Georges, *Dynamical Singlets and Correlation-Assisted Peierls Transition in VO_2* , Phys. Rev. Lett. **94**, 026404 (2005). ENS-ULM and KUN partners.
 11. M. Lüders, A. Ernst, M. Däne, Z. Szotek, A. Svane, D. Ködderitzsch, W. Hergert, B. Györfy and W. M. Temmerman, *Self-interaction correction in multiple scattering theory*, Phys. Rev. B **71**, 205109 (2005). UAA and CCLRC partners with external team member Bristol.
 12. B. Amadon, S. Biermann, A. Georges, and F. Aryasetiawan, *The alpha-gamma transition of Cerium is entropy-driven*, preprint cond-mat/0504732. ENS-ULM and KUN partners.

Single-institution post-doc Publications

13. L. V. Pourovskii, M. I. Katsnelson, and A. I. Lichtenstein, *Correlation effects in electronic structure of actinide monochalcogenides*, Phys. Rev. B **72**, 115106 (2005).

14. L. V. Pourovskii, A. V. Ruban, L. Vitos, H. Ebert, B. Johansson, and I. A. Abrikosov, *Fully relativistic spin-polarized exact muffin-tin-orbital method*, Phys. Rev. B **71**, 094415 (2005).
15. A. Landa, P. Soderlind, A. Ruban, L. Vitos, and L. V. Pourovskii, *First-principle phase diagram of the Ce-Th system*, Phys. Rev. B **70**, 224210 (2005).
16. R. Laskowski, N. E. Christensen, G. Santi and C. Ambrosch-Draxl, *Ab-initio calculations of bound excitons in GaN*, Phys. Rev. B **72**, 035204 (2005).
17. G. K. H. Madsen and G. Santi, *Anharmonic lattice dynamics of type-I clathrates from first-principles calculations*, submitted to Phys. Rev. Lett. (2005).
18. O. Eriksson, J. M. Wills, M. Coliaretì-Tosti, S. Lebegue, and A. Grechnev, *Many-body projector orbitals for electronic structure theory of strongly correlated electrons*, Int. J. Quant. Chem. **105**, 160 (2005).
19. F. Lechermann, S. Biermann, A. Georges, *Interorbital charge transfers and Fermi-surface deformations in strongly correlated metals: models, BaVS₃ and Na_xCoO₂*, cond-mat/0505241 (Prog. Theor. Phys. Supp., in press (2005)).

Part B: Comparison with the Joint Programme of Work

B.1.: Research Objectives

The research objectives of the Network remain unchanged with respect to the work programme of the contract: theoretical investigations of the physical properties of materials containing atoms with incompletely filled *f*-shells. These objectives are still relevant and achievable.

B.2.: Research Method

The research methodology of the Network remains unchanged with respect to the work programme of the contract: *ab-initio* quantum mechanics based upon Density Functional Theory and enhanced with the Dynamical Mean Field Theory capability.

B.3.: Workplan

The Network Workplan is largely unchanged with respect to the contract. The major breakdown in 6 tasks is still valid. We propose that the subtask 3.7 'magneto-caloric materials' be replaced by 'Novel superconducting f-solids'. As the research interests of the partners, and indeed of the community as such, have evolved in the last few years, the exciting discoveries of unconventional and rather high temperature superconductivity in the PuCoGa₅ and CeMnIn₅ and related compounds have gained high priority, while the magneto-caloric materials have proven to be of more conventional character. This development was unforeseen at the time of contract completion.

• Schedule and Milestones

The Work Program comprises the following sub-projects: Milestones for first results of each of the subtasks are given in bold. Comments on the last years progress are given.

1. Dynamical Mean Field Theory in the Linear Muffin-Tin-Orbital method (Task leader: ENS-ULM, collaborating with UAA, CCLRC, RUTGERS, KUN and UU)

1.1 Impurity solvers.

1.1.A IPT (**12 months**) Done. Other impurity solvers, like spin-polarized plus spin-orbit T-matrix plus FLEX (SPTF) have been developed.

1.1.B Extended NCA and other new impurity solvers. (**24 months**) Done. Extended NCA is now largely abandoned at the expense of better tools. Solution of impurity cluster problem is implemented and first papers published. Exact diagonalization of relativistic atom interacting with dispersionless bath.

1.1.C QMC (**18 months**) Done. Continuous time, full-interaction vertex, multiorbital QMC scheme for fermions has been developed. First applications (5-orbital model) done. Test application to trimer on surface published. This QMC-scheme will be used for calculation of Ce on Ag(111) surface (task 3.3). QMC with NMTO implementation of Hamiltonian has been tested (generalized QMC scheme for non-diagonal, low-symmetry matrix form of the local temperature-dependent Green-function within NMTO-TB) Application for transition-metal perovskite and for cerium published.

1.2 Green's Functions.

1.2.A $T = 0$, full self-energy (**24 months**) A significant development of the DMFT methodology is towards the integration with the GW-approximation, which combines the DMFT treatment of strongly correlated degrees of freedom with approximate (random-phase-approximation) treatment of screening of the nearly-free electron degrees of freedom. This rather ambitious development most likely will outdate the IPT and extended NCA impurity solvers in terms of accuracy. On the other hand the technical problems in connection with generating a full GW-DMFT self-energy are large, and developments continue. A realistic milestone for first applications is extended to 48 months. First papers on formalism published.

A second new development is that of Cluster-DMFT. Within this scheme non-local spin and orbital fluctuations can be investigated. Several applications in joint publications.

1.2.B Finite T (**36 months**) Done. Applied to CeTh alloy.

1.3 Combine 1.1 with 1.2 (**24 months**) Done. Applied to CeTh alloy.

1.4 Include phonons in 1.3. (**48 months**) Done. DMFT phonons of δ -Pu and Am. Applied to discussion of superconductivity in Am.

2. **Actinides:** (Task leader: UU, collaborating with UAA, CCLRC, RUTGERS, IFW-DRESDEN, KUN, and ENS-ULM)
- 2.1 **Phase Diagram of Pu** (sub-task leader: RUTGERS)
- 2.1.A δ -phase ($T = 0$: **18 months**, finite T : **48 months**) Several attacks on the Pu δ -phase have been made by network partners ($T = 0$). Spectral function for high-temperature have been compared with photoemission experiments. Start of calculations of δ -Pu with QMC in LDA+DMFT scheme.
- 2.1.B ϵ -phase ($T = 0$: **18 months**, finite T : **48 months**) Has been initiated.
- 2.1.C α -phase (**36 months**) Has not been completed.
- 2.1.D Pu compounds (**36 months**) The superconducting PuCoGa₅ compound has attracted quite extensive interest, and several Network contributions have been published. Also, the Pu valency and crystal field splitting in the PuO₂ compound has been investigated, and several joint publications published. Recent applications of DMFT to PuCh (Ch=Se and Te) published.
- 2.2 Am and compounds. (**24 months**, finite T : **48 months**) Disordered local moments theory of actinide metals has been investigated and a paper completed. Am metal including high pressure phases and phonons in DMFT treatment has been published. The trends of f-electron localization through the actinide chalcogenides and pnictides has been studied...
- 2.3 Np (**24 months**) and compounds. ...including NpPn and NpCh...
- 2.4 U (**24 months**) and compounds. ...as well as UPn and UCh! The U valency in UX₃ compounds has been investigated, revealing a shift in the series X=Rh, Pd, Pt, Au. Magnetism of UO₂ has been the subject of a study. U adlayers on W surfaces have been studied (also part of task 4). Photoemission of USe and UTe based on DMFT(FLEX) has been completed.
3. **Rare-earth systems:** (Task leader: KUN, collaborating with UAA, CCLRC, RUTGERS, IFW-DRESDEN, ENS-ULM, UU and MD)
- 3.1 Ce (**24 months**, finite T : **48 months**) Improved and simplified SIC methodology has been developed and tested on the $\alpha \rightarrow \gamma$ phase transition of Ce, including finite T . The high temperature optical conductivity of Ce in both the α and the γ phase has been calculated within DMFT. DMFT(QMC) calculation of energy and entropy has been completed and published.
- 3.2 Optical properties of pigments such as Ce₂S₃ (**36 months**) (sub-task leader: MD) Geometry optimizations for CeS, Ce₂S₃ and Ce₃S₄ compounds have been completed. Initial results for optical excitations have been obtained with the LDA+U method.
- 3.3 Ce on Ag(111) (**24 months**) DMFT methodology development completed. Test for trimer Kondo atoms on surface published.
- 3.4 SmS and TmSe (**36 months**) (sub-task leader: UAA) SmX and TmX compounds are done and published.

- 3.5 rare-earths in high- T_c superconductors (**18 months**) (sub-task leader: CCLRC) Several RE-Ba₂Cu₃O_{6+x} compounds have been studied. Systematic picture emerges, and joint publication in preparation.
- 3.6 luminescence (**48 months**) Still testing approaches.
- 3.7 magneto-caloric materials (**36 months**) → Novel superconducting f-solids (sub-task leader: UU) Nothing has been completed on magneto-caloric materials. We suggest to replace this subgoal of the network research with 'Novel superconducting f-solids'. The research interests of the Network partners have shifted more towards the newly discovered superconducting compounds like PuCoGa₅ etc, and CeMIn₅ (M=Co, Rh, and Ir). Several Network publications have emerged, and important theoretical insights continue to be developed within the network. Several contributions at the 2. annual workshop in Paris discussed PuCoGa₅.
4. **Surface magnetism:** (Task leader: IFW-DRESDEN, collaborating with CCLRC, UU and MD)
- 4.1 Gd(0001) and related systems (**18 months**) In a study of the Sm(0001) surface the Sm atoms have been shown to exhibit divalency, as opposed to the trivalency of bulk Sm. Magnetic anisotropy has been investigated by LSD and LDA+U methods in bulk (hcp) Gd. The methodology to calculate accurate total energies and surface dipoles has been completed by the Dresden post-doc.
- 4.2 non-collinear moments (**30 months**) Non-collinear moments of (bulk) LaCrSb₃ and UO₂ were studied.
5. **Workshops:** (Task leaders: UAA and CCLRC, involves all partners)
- 5.1 5 Annual progress workshop (**0-1, 12, 24, 36 and 48 months**) The first annual meeting was organised in November 2003 in Aarhus with 35 attendees. Second annual meeting was organized in december 2004 in Paris with 40 attendees. The Midterm Review meeting followed this workshop. A winterschool on the physics of the lighter actinides was organised in Riksgränsen, Sweden in May 2004 (37 attendees). Third annual workshop was replaced by the PSIK2005 conference in september 2005, while a fourth annual workshop is scheduled for Lyon around June 2006. A one-day mini-conference was organised in Hamburg in May 2005 in connection with the Hands-on-DMFT course.
- 5.2 DFT and DMFT tutorial workshop (**18 months**) DMFT tutorial workshop was organized in Daresbury in June 2003.
- 5.3 Industry workshop (**36 months**) (sub-task leader: MD) Scheduled for 2006.
- 5.4 Hands-on course (**48 months**) FPLO hands-on-courses were organized in Dresden in March 2003, in UC Davis, USA in June 2004 (not network financed), and again in Dresden in March/April 2005. A KKR hands-on-course was organised in München in June 2005 with 28 attendees and 20 lecturers. A Hands-on-DMFT course took place in Hamburg in May 2005 with 47 attendees.

6. **Newsletter and Home page:** (Task leader: CCLRC, involves all partners) 6 Newsletters have been published in second network year (October, December 2004, February, April, June, August 2005). The maintenance of the network homepage has been outsourced to partner UU.

• **Research Efforts of the Participants**

The research efforts of the Participants are summarized as follows:

Involvement								
task	UAA	CCLRC	RUTGERS	DRESDEN	KUN	ENS-ULM	UU	MD
1.1.A			x			X	x	
1.1.B	x		x		x	X		
1.1.C			x		x	X	x	
1.2.A	x	X	x		x	X	x	
1.2.B	x	X	x		x	X	x	
1.3	x	X	x		x	X		
1.4			X		x	x		
2.1.A	x	x	X		x		X	
2.1.B		x	x				X	
2.1.C			x				X	
2.1.D	x	x			x		X	
2.2	x	x	x	x	x	x	X	
2.3	x	x	x	x			X	
2.4	x	x	x	x	x		X	
3.1	x	x	x	x	X	x	x	
3.2	x						x	X
3.3					X			
3.4	X	x		x	x		x	
3.5	x	X						
3.6					X		x	
3.7	x			x			X	
4.1		x		X			x	x
4.2	x			X	x		x	x
5.1-4	X	X	x	x	x	x	x	x
6.1	x	X	x	x	x	x	x	x

Table 1: Involvement of the individual Research Teams. Task leaders are given in bold.

B.4.: Organisation and Management

B.4.1. Management.

The Network's scientific programme is broken down into sub-tasks each of which is managed by a board of two or more node leaders, coordinated through the Network Coordinator and the Network Secretary. The major part of network management happens through frequent email contact. Whenever appropriate, short-term secondments and mini-meetings between two or more network partners, including post-docs, are used to plan the near future scientific research programme of the sub-tasks. Major organisational planning is usually done in connection with Network meetings. One Network Board meeting was held in the reporting year, in connection with the second annual/Midterm review meeting. A second Board meeting was held in connection with the PSIK2005 conference in September 2005.

Network announcements, including abstracts of submitted papers, vacant positions, and network meetings, are announced in the bimonthly Psi-k newsletter, which currently is distributed to more than 1500 email addresses worldwide. The dissemination of scientific results is taking place through publication in research journals as well as presentations at conferences. Newsletters are available at:

<http://psi-k.dl.ac.uk/index.html?newsletters>

The Network home page is:

<http://phys.au.dk/~svane/rtn.htm>

B.4.2. Main network meetings.

- *Electronic Structure of Correlated Materials*, 2nd annual Workshop, Paris, France, Dec. 8-10, 2004. 40 attendees. One external expert was financed (after Commission approval): F. Aryasetiawan, Research Institute for Computational Sciences, AIST, Tsukuba University, Japan, giving a seminar on *Ab-initio schemes for correlated electrons and the Hubbard U*. Aryasetiawan stayed with ENS-ULM for a few days after the meeting for collaborative consultations.
- Network Board Meeting, Paris, France, Dec. 9, 2004. 8 attendees.
- Network Midterm Review Meeting, Paris, France, Dec.10, 2004. 19 attendees.
- FPLO hands-on course, Dresden, Germany, March 30-April 3, 2004. 40 attendees.
- DMFT hands-on course and mini-conference, Hamburg, Germany, May 17-20, 2005. 50 attendees.
- KKR hands-on-course, Munich, Germany, June 9-11, 2004. 48 attendees.

B.4.3. Networking.

from to	UAA	CCLRC	RUTGERS	IFW	KUN	ENS	UU	MD
UAA CCLRC	3	5		4			6	
RUTGS IFW				2a	2d	2b	2c	
KUN ENS	1a	1b	1c,7,10	1d	1e		1f	1g,8,9
UU MD								

Table 2: Secondments and visits. Numbers refer to list below.

1. At the Paris Workshop and Midterm Review Meeting, Dec. 8-10, 2004 participated:
 - a) A. Svane, G. Santi, from UAA.
 - b) W. M. Temmerman, Z. Szotek, M. Lüders, from CCLRC and P. Strange from CCLRC external team member Keele.
 - c) G. Kotliar and S. Ping from RUTGERS.
 - d) I. Opahle, F. Tasnadi and M. Richter from IFW-Dresden.
 - e) M. Katsnelson and L. Pourovskii from KUN.
 - f) O. Eriksson, S. Lebegue, A. Grechnev, P. Souvatzis, T. Bjørkman and P. Oppeneer, from UU and T. Gouder, and R. Eloirdi from UU external team member ITU Karlsruhe.
 - g) E. Wimmer and R. Windiks from MD.
2. At the DMFT hands-on course and mini-conference in Hamburg, May 17-20, 2004 participated:
 - a) F. Tasnadi from IFW-Dresden.
 - b) S. Biermann, A. Poteryaev, F. Lechermann, and J. M. Tomczak from ENS-ULM.
 - c) T. Bjørkman and B. Sanyal, from UU
 - d) M. Katsnelsson and L. Pourovskii from KUN.
3. A. Svane from UAA visited CCLRC June 1-3, 2005, to give a seminar and collaborative discussion.
4. M. Richter from IFW-Dresden visited CCLRC October 14-16, 2004, to give a seminar and collaborative discussion.
5. W. M. Temmerman from CCLRC visited external team member Karlsruhe, Jan. 24-27, 2005, for collaborative consultations.

6. S. Lebegue from UU visited UAA for collaborative discussions, November 2004.
7. G. Kotliar from RUTGERS visited partner ENS-ULM, June 2005.
8. R. Windiks from MD visited ENS-ULM for collaborations January 2005.
9. R. Windiks from MD visited ENS-ULM for collaborative consultations May 2005.
10. G. Kotliar from RUTGERS is on a sabbatical at partner ENS-ULM, Sept 2005 - June 2006.

The following overseas travel was financed by the network contract after Commission approval:

1. W. M. Temmerman from CCLRC presented an invited talk at the APS March Meeting, in March 2005.
2. M. Taut from IFW-Dresden presented a poster at the 16th International Conference on Electronic Properties of Two-Dimensional Systems, Albuquerque, New Mexico, USA in July 2005.

Follow-up on Midterm review Meeting

After the Midterm Review Meeting two specific measures were recommended: increased collaboration with EXCITING network (2002-00317), and a young researcher's dedicated meeting.

Researchers from the present network have presented the network activities at a meeting of the EXCITING network (A. Svane and G. Santi, at the workshop EXCAAR in Aarhus (April 2004, previous reporting period). In Aarhus the present network's post-doc and the EXCITING post-doc (R. Laskowski) shared office, and several joint projects were started and lead to published papers (see post-doc reference list above).

Researchers from the partners IFW-DRESDEN, CCLRC and KUN of the present network participated in the EXCITING workshop in Berlin in March 2005 on 'Orbital Functionals', where they presented talks on their f-electron research and interacted scientifically with members of several EXCITING nodes.

The organisation of a young researcher's meeting was likewise initiated from the Aarhus post-docs: the coordinators of the two networks agreed to allot money for a joint 'f-electron' and EXCITING meeting, organised solely by the young researchers. However, after an initial enthusiasm among the young researchers, the initiative seems to have stranded.

B.5.: Training

B.5.1. The vacant Network positions have been publicised through the Psi-k Newsletter, the Psi-k mailing list and the CORDIS webpage.

B.5.2. A total of 71 post-doc and 2 pre-doc months of training has been delivered in the third year, for a total of 154.5 post-doc + 2 pre-doc months of training in the first three years. For the fourth year employments negotiated and confirmed by both parties (status A, B or C)

amount to 67 post-doc +6 pre-doc months, *i.e.* we aim at a total of 223.5 post-doc + 8 pre-doc months delivered at the end of contract. This is well in excess of the contract deliverable of 222 post-doc months. Currently, negotiations for still 6 months of post-doc training and 8 months of pre-doc training is on-going, specifically an extension of the Dresden post-doc till the network expiration date, and the hiring of a Romanian pre-doc at partner UU, respectively. As things have developed, the number of post-doc months delivered by the individual partners have changed in comparison with the contract forecast, and as a consequence some adjustments of the total budget have been agreed upon (see section **B.4.3**). At partners MD and ENS-ULM there will be two post-docs employed through the last network year. At node UAA the post-doc has left for his home country, and it has not been possible to find a candidate for short-term employment. At partner CCLRC the post-doc has been promoted into a permanent position. The post-doc formerly employed at partner KUN has moved into a network position at partner MD, while a new postdoc is employed at KUN. Tables 4 and 5 summarize the overall post-doc status. At the end of the third year 6 young researchers are employed while two more have started around Sep. 2005, at MD and ENS-ULM.

Young researcher person-months financed by the contract						
Participant	Contract deliverable			Financed sofar		
	Pre-doc (a)	Post-doc (b)	Total (a+b)	Pre-doc (c)	Post-doc (d)	Total (c+d)
1. UAA	0	36	36	0	25.5	25.5
2. CCLRC	0	30	30	2	23	25
3. RUTGERS	0	0	0	0	0	0
4. IFW-DRESDEN	0	30	30	0	24	24
5. KUN	0	30	30	0	24	24
6. ENS-ULM	0	30	30	0	21	21
7. UU	0	30	30	0	22	22
8. MD	0	36	36	0	15	15
Totals	0	222	222	2	154.5	156.5
First Year	0			0	16.5	16.5
Second Year	0			0	67	67
Third Year	0			2	71	73

Table 3: Network employment of young researchers.

Name	Place of work	Prev. with	emplymt. period other partner
Leena Torpo	MD, LeMans F	-	01-02-2003 to 30-06-2003
Martin Lüders	CCLRC, Daresbury UK	CCLRC	01-02-2003 to 31-12-2004
Gilles Santi	UAA, Aarhus DK	CCLRC	15-05-2003 to 30-06-2005
Leonid Pourovskii	KUN, Nijmegen NL	-	01-08-2003 to 31-07-2005
Leonid Pourovskii	MD, LeMans F	KUN	01-09-2005 to 31-08-2006
Ferenc Tasnadi	IFW-DRESDEN D	Dresden	01-09-2003 to 28-02-2006
Sebastien Lebegue	UU, Uppsala S	-	01-11-2003 to 31-10-2005
Frank Lechermann	ENS-ULM, Paris F	-	01-12-2003 to 31-08-2006
Daniel Rohe	ENS-ULM, Paris F	-	01-10-2005 to 31-08-2006
Markus Däne	CCLRC, Daresbury UK		8 mths. 2005/2006
Alexei Griechnev	KUN, Nijmegen NL	UU	01-07-2005 to 31-08-2006
Rene Windiks	MD, LeMans F	-	01-11-2004 to 31-08-2006

Table 4: Working place of Young Researchers and (projected) employment period. All are post-docs, except M. Däne, who has not yet completed his PhD.

4 News from the ESF Programme

”Towards Atomistic Materials Design”

4.1 Scientific Report on Psi-k2005 Conference

4.1.1 Psi-k 2005: Some Remarks by the Conference Chairman

In the two months after the Psi-k 2005 Conference in Schwäbisch Gmünd there has been some time to reflect more on scientific contents of the meeting and the message it delivered about the state of our field.

The first observation concerns the diversity of scientific questions now addressed by electronic-structure calculations. Heterogeneous catalysis and other surface reactions have long been in the repertoire of our community and continue to flourish. The same is true for metallic alloys and other structural materials, but we now see major efforts also in first-principles calculations for interface structures, for biological matter and biological processes, and for geophysics and earth sciences.

Quantum transport is another area where there has been major growth in the exploitation of electronic-structure methods. Density-functional theory can provide a realistic Hamiltonian to be plugged into the powerful methods developed in the mesoscopic-transport community. Devices based on nanoscale structures, ranging from single molecules attached to external leads to nanowires and ultrathin insulator layers, are now subject to quantitative modelling. Quantum transport in atomic-scale structures opens up also theoretical challenges, as it is not exactly clear what is the range of validity for the Landauer-type methods. Many-electron correlations, inelastic effects, and explicit time dependence are interesting topics now under intensive study.

The diversity also includes extensive work on quantum dots, rings and other nanostructures, where quantum confinement effects influence the physical properties, such as optical and other excitation spectra. Again, DFT methods can provide the benchmarks for small systems, which can be scaled up for investigations of the structural and electronic properties of large (million-atom) assemblies using simplified model Hamiltonians. There are also many other areas of nanoscience, where computational methods provide decisive input and insight, including nanomechanical phenomena and growth by self-assembly.

Nanoscale and complex magnetism is an exciting area where computational methods have shown their power. Magnetic ordering in thin films and superlattices has enormous technological potential, and new magnetic materials (such as multiferroics) are intensively explored. Spin switching, spin-transfer torque and the Rashba effect are examples of current topics in magnetoelectronics, another technologically interesting and rapidly expanding area. Intensive work continues in the search for useful materials for spintronics, such as dilute magnetic semiconductors. Their

properties are sensitive to the presence of defects and impurities, which need to be understood in great detail.

Let me round up the diversity argument by noting the progress made in first-principles approaches to superconducting materials. For many superconducting materials, the devil is in the details of the complex system, as both electronic properties and electron-phonon interactions depend critically on the atomic-scale composition and structure.

The second observation are the strong advances made in quantitative understanding of many-electron effects. It has long been known that these are important for strongly correlated materials, and that the mean-field description of standard DFT cannot treat them properly. On the other hand, the model Hamiltonians popular in many-body theories often fail to describe the real physical system of interest, or contain parameters that need to be adjusted. It has now become possible to intertwine many-electron theories and faithful atomic-scale description into a first-principles approach. A remarkable symposium on ab initio quantum many-body calculations ran through the whole Psi-k 2005 Conference. It brought together the practitioners of several approaches to the problems, such as dynamical mean-field theory, many-body perturbation theory, quantum Monte Carlo methods, and time-dependent current-density functional theory. For those who had the chance to follow these sessions during the conference, this provided a unique overview of the impressive development in both fundamental theories and applications to specific systems. The incorporation of these methods into everyday electronic-structure codes is now happening fast. It seems that in near future "beyond-LDA" or "beyond-GGA" methods will be almost routine, as it is becoming possible to overcome the technical and computational limitations. This is a truly remarkable development and opens many new possibilities for predictive work. The computational demands are strong, however, and for accurate descriptions of, say, van der Waals interactions in extensive systems, additional shortcuts should be explored.

This leads me to my third observation, concerning the vigorous development of new computationally efficient methods. Linear-scaling DFT codes have made impressive progress, which is also evident in quantum Monte Carlo methods. Molecular-dynamics and hybrid methods combining quantum mechanics with classical force fields are applied to demanding problems, for example in soft-matter and solvent systems. Time-dependent DFT methods and transport codes proliferate and are being commercialized. The workhorse DFT codes keep on adding features and functionalities and are also coupled to databases with structural and physicochemical information.

The much improved availability and documentation of electronic-structure and related computer codes have facilitated their widespread use also beyond academia. This is reflected in my final observation: the large number of industrially relevant, "dirty" real-world problems now being at least in part solved by the methods developed in and known to the Psi-k community. There is little doubt that "our" methods are now making a strong impact in applied research and technical development and have become an important tool for industrial research. We should all feel proud and encouraged by this.

Risto Nieminen
Psi-k 2005 Chairman

4.1.2 Summary of Concluding Remarks by Volker Heine at Psi-k2005 Conference

I want to talk mainly about the future of our Psi-k community because our present mode of funding is coming to a dead halt and will not be renewable from the end of 2007.

However, first to the science at this Conference. Of course there has been far too much and of too enormous a variety for anyone to summarise, but let me make a few brief comments. People are saying that the conference has been a great success, and there has been a real buzz about the place. In particular people have been keen to attend sessions on new developments which may have relevance for their field in the future. This is important because I had previously heard some suggestions that there may not be a need any more for Psi-k as an organisation, albeit a loose one. Clearly it is still useful for people to meet every few years as computationalists on electronic structure, not immersed in some larger group in their own special field of application. Thus I expect that your Psi-k Committee tomorrow will lay plans for another conference in 2010, though there is no sign of where the money will come from.

At the first general Psi-k conference in 1996, I drew a picture with Density Functional Theory at the centre and arms reaching out into all sorts of fields of research. Actually that was a bit optimistic: most of our calculations were not yet contributing very much to front-line research. But that has now changed. To DFT at the centre we must now add Computational Many-Body Theory, and the arms are certainly now contributing knowledge and understanding at the research frontier. For example at Cambridge University there are permanent staff members doing our type of work in five University Departments ranging from Physics and Chemistry through Earth Sciences and Materials Science to Engineering. And at this conference there have been several reports of applications in industry, particularly surface catalysis and drug discovery. We have clearly arrived as a significant scientific force.

But what of the future? The European Science Foundation (ESF) has been very helpful to our Psi-k community with two rounds of 5-year funding for the activities supporting our community taken as a whole. That will cease in 2007 with no chance of renewal on that kind of basis. Our problem is that there is no niche for us in the thinking of funding organisation as a human or dispersed infrastructure underpinning our research community as a whole, although the ESF referee reports were outstanding. When we applied (together with the Molecular Dynamic Simulation community) to the European Union for an Integrated Infrastructure Initiative grant, the opening sentence of the referee report said "This is not what is meant by computational science infrastructure". Clearly they were only interested in hardware and Grid types of things. At the ESF the national funding agencies that supply its funds do not like on-going infrastructural activities no matter how good the peer reviews: they only want sexy applications. On the latter front there have of course been many successes with EU Networks and national funding for particular projects.

Let me summarise how I see the Psi-k activities as infrastructure underpinning a lot of outstanding local work, and I am purposely going to start with the intangibles which are sometimes the most important in the long run. Our community taken as a whole has made Europe the

leading area in the world for our type of research. I am not interested in competing or being better than someone else, but I do care about excellence. I have heard it said that second rate research is almost worthless as far as extending the frontier of knowledge. Moreover it is clear to me that this excellence owes a lot to the high degree of cooperation across Europe that has been built up.

Put into human terms, many many young people from across the whole of the continent have been helped to participate in first class research, and either made a career there or moved on building on that experience. That to me is what Europe is all about, to achieve what we want to do by working together when one country is simply too small a unit by itself. For example I remember the intense discussions when the Car and Parrinello Phys. Rev. Letter first hit us, to understand its several ingredients and how to exploit them fully.

But it is not just a matter of sharing expertise. In some countries and some institutes our kind of calculations are not seen as 'proper' theoretical physics, or even as 'real' science at all. I was spared some of that prejudice in Cambridge because Hartree, a professor in the mathematics faculty, no less, had been pioneering Hartree Fock calculations on atoms for more than a decade, had written the first textbook on numerical methods, and had been instrumental in the building of the first electronic computer for scientific purposes on this side of the Atlantic.

Quite aside from prejudice, not every university can have a first class group in every new subject, and so good spreading of information and a ready welcome from elsewhere have been important. Just look at the lists of collaborators on most of the papers at this conference and the mix of national origins that they display. It is incredible. That in turn is sharing codes and spreading expertise around to establish more start-up groups. It has been a basic tenet of our Psi-k organisation to try to meet the needs of everyone in the whole community as far as practicable, and there are different ways of being isolated. I am thinking of one young person hired as a fresh PhD, pioneering our kind of ab initio simulation in a new field. She was not isolated in a general sense because hers was an institute with a worldwide reputation, but as the only person in electronic structure calculation there she clearly needed good contacts with other simulators to keep abreast of technical developments.

It is now easy to see how the various Psi-k activities fit in. The 10 to 20 workshops per year bring people together, in some cases for the first time ever in a subject, as for example in mineralogy. From these contacts EU Networks and other activities are spawned. The email address list of now 1500 names has become the leading medium in the world in our field for advertising jobs and activities such as conferences and workshops. The Psi-k Newsletter backs these up with reports for those who could not attend, and has a scientific highlight every two-monthly issue.

We have pioneered hands-on training in the use of codes, including the background theory needed to use them intelligently. I always find it remarkable that our type of simulation can be done at all, and it is clear that every kind of approximation, short cut and trick is needed for that. And if a person does not understand them enough to use them intelligently it leads to 'garbage in, garbage out' as the saying goes. For example the basic ideas have not changed in 25 years in pseudopotential calculations with plane waves and Hellmann Feynman forces, but look at the difference in sophistication now and the time it has taken to develop the method to that point.

Other activities include our 15 Working Groups, set up with no more bureaucracy than writing

one or two pages to outline what they hope to do. There has been a series of workshops with people in industry, particularly on catalysis. In the early days occasional short term or training visits were funded when these could not be supported from other sources. Several ESF EuResCo topical conferences were initiated, including the first one on the application of computer simulation in biology, until that whole programme collapsed. There have been various activities not funded by the ESF grant all making their contribution, such as the workshops associated with Trieste. Cooperation has been built up with other organisations, particularly CECAM over joint workshops and training.

The purpose of listing these activities is for you to ask yourselves whether they are worth continuing, and if so how. And I mean 'you', not me. I have just passed my 75th birthday during the days of this conference, and other people too have carried much of the burden for many years. Peter Dederichs has taken over as chairman of Psi-k and the rest of the committee are also listed on the usual website <http://psi-k.dl.ac.uk> with whom you can discuss the matter. It is clear that there will be no more funding of the activities as a whole, and it will be necessary to make different applications in different ways to support different bits of them. It will mean more work because bureaucracy is increasing, as is the degree of competition for funds.

But on the plus side the importance of our work is increasingly recognised, particularly by experimentalists; the effectiveness of our organising is greatly admired, and our degree of harmonious cooperation across Europe even envied. That is a sound basis for a continuing Psi-k.

There are of course various programmes of various organisations that one might apply to for some funding. For example the ESF has not ruled us out from applying to them: just that our chances of success are zero on the old basis. Then there is COST, and the several subdivisions of the EU. However when reading some of their detailed descriptions, it has seemed to me at first sight that what we were doing was exactly what they said they wanted, but then more detailed study gave an impression as if they had been written specifically to exclude us! To believe that would of course be paranoia, but the truth is that the way the EU and other European organisations work is that groups of 'experts', often self appointed, manouver to 'advise' on what should be done, and hey presto there appear some 'needs' in the final document which they are ideally set up to deliver. And remember that delivery is what EU management is all about. I once attended a 2-day course on how these things work: it was an eye opener for a political simpleton such as me. Maybe the time has come for Psi-k to muster its expertise and join the scrum of advisers.

I want to mention one action going on now. I complained above that there is no niche for us as an infrastructural organisation in Euro-thinking, but there are steps afoot that hopefully may change that in some future Framework several years hence. An application has been made to the ESF (and just been granted at the time of writing this) to organise what the ESF calls a Forward Look on the need for European 'cyber infrastructure', with Psi-k as prime example of what can be achieved. This will be a substantial booklet, produced after consulting (i.e. trying to get on board) various interests through a series of workshops. The report can then be pushed under the noses of officials etc. as a policy proposal. Another aspect of this is trying to get such ideas included in any plans for any prospective European supercomputer.

I also feel very positive about another development this past year, which is the growing cooper-

ation between Psi-k, Juelich, Daresbury and CECAM. In fact we have been successful in getting with them a joint Marie Curie grant for training activities in our field. I see this cooperation as perhaps helping to give Psi-k some degree of ongoing continuity. Remember, we are just a bunch of individuals who dreamt up this name of Psi-k for themselves and whose funding is running out, whereas Juelich, Daresbury and CECAM are legally constituted organisations that have been around for decades. Of course Daresbury has been the 'home' for Psi-k organisationally since the beginning, with Psi-k growing out of the British CCP9 (Collaborative Computing Project) that started about 1978. With suggestions for a European supercomputer in the air, maybe we can help Daresbury and Juelich brush up their Euro credentials by co-organising training events and workshops with them. Moreover CECAM is the only European organisation in our field and hence a natural forum for us to interact with our sister organisation SIMU (or MolSimu) on Molecular Dynamic Simulation. Thus some Psi-k members are helping CECAM broaden its European base. There is no wish for CECAM to take over Psi-k – CECAM wants to remain a small lean outfit – but we can all be stronger by working together.

Volker Heine
Vice-chairman, ESF Psi-k Programme

5 General Workshop/Conference Announcements

5.1 DFTEM Conference

SECOND CIRCULAR

DFTEM 2006

“bringing together two communities: DFT + TEM”

21 - 23 April, 2006 – Vienna, Austria

<http://www.physics.at/dftem2006>

The Conference: April 21-23, 2006

This three-day conference will focus on Density Functional Theory (DFT) and Transmission Electron Microscopy (TEM) with the intention of bringing together these two communities. The conference is dedicated to Karlheinz Schwarz (DFT) and Bernard Jouffrey (TEM) on the occasion of their respective birthdays, which we will celebrate at the conference dinner. The conference will follow two days of separate workshops for the two fields.

The Workshops: April 19 & 20, 2006

12th WIEN2k Workshop

This WIEN workshop deals with density functional (DFT) calculations of solids using the (full-potential) Augmented Plane Wave plus Local Orbitals (APW+lo) method as embodied in the WIEN2k code (<http://www.wien2k.at>) and related topics.

2nd CHIRALTEM Workshop

The CHIRALTEM collaboration (www.chiraltem.physics.at) has recently demonstrated that circular dichroism can be measured with EELS in a TEM, contrary to common belief. This new technique opens the way to the study of site and element specific magnetic moments in the TEM, thus extending to the nanoscale the well established XMCD or PEEM applied on a synchrotron. During the workshop the know-how accumulated in the last two years by the international collaboration will be disseminated to the interested community. A limited number of grants (max. Euro 300,-) is available for young researchers (<35 years). Applications by sending an email to dftem@physics.at including a cover letter and a CV are invited.

Fees + Registration

Workshops:	EUR 100
Conference:	EUR 250
Conference and Workshop:	EUR 300 (available until December 24, 2005)
Conference and Workshop Student:	EUR 200 (when registering until December 24, 2005; proof of the student status is required)

Registration will be possible on the conference web site: www.physics.at/dftem2006. For information on available accommodation please also see our web site.

Registration starts	August 28th, 2005
End of early registration period	December 24th, 2005
Deadline for abstract submission	January 31st, 2006

Invited Speakers

Ole K. Andersen , MPI Stuttgart, Germany	Lucia Reining , École Polytechnique, France
Peter E. Blöchl , Clausthal University of Technology, Germany	Matthias Scheffler , FHI Berlin, Germany
Gianluigi Botton , McMaster University, Hamilton, Canada	Virginie Serin , CENES, France
Helmut Eschrig , IFW Dresden, Germany	Eric L. Shirley , NIST, USA
Frank de Groot , Universiteit Utrecht, Netherlands	David Singh , Oak Ridge NL, USA
Börje Johansson , Uppsala University, Sweden	Susanne Stemmer , UC Santa Barbara, California, USA
Klaus Leifer , Uppsala University, Sweden	Isao Tanaka , Kyoto University, Japan
Georg Madsen , University of Aarhus, Denmark	Samuel B. Trickey , University of Florida, Gainesville, Florida, USA
Manu Perez-Mato , Univ. de Pais Vasco, Bilbao, Spain	John J. Rehr , University of Washington, Seattle, USA

Scientific Contributions

Scientific contributions in the form of posters and oral communications are welcome. The scientific board will decide on the form of presentation. Poster boards are 2 meters high and 1 meter in width. For all contributions an abstract must be submitted before the deadline January 31st, 2006.

Refereed Conference Proceedings

A conference book will be available at the conference including extended abstracts of all talks and posters presented. All abstracts should be prepared in LaTeX using the template available from the conference website and should be submitted electronically using our abstract submission system. Abstracts in WORD format are also accepted, but must not contain any graphics and should be sent by email to dftem@physics.at.

Organizing Committee

* Claudia Ambrosch-Draxl, Univ. of Graz, Austria * Peter Blaha, TU Wien, Austria * Clemens Först, MIT, USA * Cécile Hébert, TU Wien, Austria * Eva Huber, Amici and IAST Austria * Kerstin Hummer, Uni Wien, Austria * Kevin Jorissen, Universiteit Antwerpen, Belgium * Dieter Kvasnicka, TU Wien, Austria * Joachim Luitz, IAST Austria * Pavel Novak, Czech Academy of Sciences, Czech Republic * Peter Schattschneider, TU Wien, Austria * Jorge O. Sofo, Pennsylvania State University, USA * Michael Stöger-Pollach, TU Wien, Austria * Marc Willinger, FHI Berlin, Germany

Vienna

Vienna is the city of the Habsburgs, including Sissi and Franz Josef, of Sigmund Freud and of the Lipizzaners. It is the city of famous scientists like Erwin Schrödinger, Wolfgang Pauli, Ernst Mach, Ludwig Boltzmann and today's scientists like Anton Zeilinger. Vienna hosts several hundred museums, many of them featuring famous artists like Klimt and Schiele. Every evening there are concerts and performances, operas and musicals in the Vienna state opera, the Konzerthaus, the Musikverein, the Knstlerhaus, many theaters and other places. It is easy to spend many days full of new impressions in Vienna. The weather in Vienna in April averages between 6 and 15 °Celcius, 6 hours of sunshine and 40 mm precipitation (13 wet days). So you better bring your umbrella.

Contact

DFTEM 2006	dftem@physics.at
c/o IAST Austria	www.physics.at/dftem2006
Wohlmuthgasse 18	
A-3003 Gablitz/AUSTRIA	
Fax +43-2231-612544	

5.2 QUANTUM MONTE CARLO IN THE APUAN ALPS II

The Towler Institute, Vallico Sotto, Tuscany, Italy

Sat 22nd July - Sat 29th July 2006

www.tcm.phy.cam.ac.uk/~mdt26/tti/tti.html

Following last year's successful informal workshop (detailed report available on the above website) the Cambridge University Theory of Condensed Matter group is organizing a second International Workshop to discuss the development and application of the continuum quantum Monte Carlo method in condensed matter physics and quantum chemistry. The conference will take place in our 15th Century Tuscan monastery in the Apuan Alps. The normal format for these events involves formal presentations being restricted to the mornings, with the afternoons and evenings left free for relaxed discussion whilst participating in mountain walks and other healthy outdoor activities.

This year's expanded conference will involve up to 25 people, all accommodated on site. People who feel they would like to contribute and wish to attend the event should contact Mike Towler (mdt26@cam.ac.uk) for further details.

Confirmed speakers so far: Richard Needs, Cyrus Umrigar, Lubos Mitas, Alan Aspuru-Guzik, Ian Snook, Paolo Umari, Jeff Grossman, Dario Bressanini, Matthew Foulkes, Neil Drummond, Pablo Lopez Rios, Alexander Badinski, Andrea Ma, Matthew Brown, Idoia de Gurtubay, Nick Hine, Ryo Maezono, John Trail, Graham Spink, Nicole Benedek, Mike Towler.

5.3 Summer School : QUANTUM MONTE CARLO AND THE CASINO PROGRAM

The Towler Institute, Vallico Sotto, Tuscany, Italy

Sun 30th July - Sun 6th August 2006

www.tcm.phy.cam.ac.uk/~mdt26/tti/tti.html

August 2006 will see the first Summer School "Quantum Monte Carlo and the CASINO program" hosted by members of the Cambridge University Theory of Condensed Matter Group in their monastery in the Tuscan Apuan Alps. This course is designed for young scientists with no previous experience in quantum Monte Carlo methodology, though anyone interested is welcome to take part.

Many-body quantum theory provides the key ideas for understanding the behaviour of materials at the level of the electrons which bind the atoms together. Describing the complex behaviour of materials at the atomic level requires a sophisticated description of the correlated motion of the electrons, which can be achieved using ab initio computational methods. The quantum Monte Carlo method has many attractive features for probing the electronic properties of real systems. It is an explicitly many-body method which takes electron correlation into account from the outset. It is capable of giving highly accurate results while at the same time exhibiting a very favourable scaling of computational cost with system size. Over the last 15 years, the Cambridge group have been researching QMC methods and we have created a powerful, general computer program - CASINO - to carry them out. The school will focus both on basic theory and on more advanced practical techniques, and will include a thorough introduction to the CASINO program.

Instructors will include a selection from the authors of the CASINO program (Prof. Richard Needs, Dr. Mike Towler, Dr. Neil Drummond, and Dr. Pablo Lopez Rios) and others.

The monastery is a delightful 15th century building with an attached church which is used as a lecture theatre. It is fully equipped with state of the art presentation and computer technology. All accommodation is on-site and time will be set aside for mountain walking, caving, swimming in thermal baths, eating in hearty mountain restaurants, and similar activities.

The cost of the school for one week including accommodation will be around 400 GBP. Participants would need to arrange a flight to Pisa airport from where onward transportation will be arranged.

Interested parties should contact Mike Towler (mdt26@cam.ac.uk) for registration and further details.

5.4 NIC Winter School 2006

”Computational Nanoscience: Do It Yourself!”

14 - 22 February 2006

John von Neumann Institute for Computing (NIC)

Forschungszentrum Juelich, Germany

www.fz-juelich.de/wscn

1. Scope

This NIC Winter School focuses on the application of modern electronic structure calculations and dynamical simulation techniques covering aspects of solid state and surface science, chemical reactions and dynamics, as well as the structure and properties of large molecules and clusters. This School about ”electronic structure at work” is tailored for PhD students and Postdocs with a solid background in basic quantum mechanics coming from physics, chemistry, material science and related disciplines.

2. Participation

In the series of NIC Winter Schools this School is the first with hands-on training, i.e. it combines lectures in the morning, which elucidate the theoretical concepts and numerical procedures, with practical sessions in the afternoon. There will be simulation labs with focus on

A - solids, surfaces, magnetism (FLEUR, KKR-GF)

B - dynamics, reactions, fluctuations (CPMD)

C - molecules, clusters, structures, and spectra (TURBOMOLE)

Therefore, the number of participants has to be restricted to about 40. The participants will be selected by the programme committee on the basis of the scientific background of the applicants.

The application should include

- a short CV
- a short description of the work of the group, in which the applicant is involved
- a short description of his own part of the work
- a letter of recommendation of his supervisor
- a statement on the preferred topic (first and second preference) for the practical sessions.

and should be sent to the School secretary

Bettina Scheid
Forschungszentrum Juelich
Zentralinstitut fuer Angewandte Mathematik
52425 Juelich
Phone: +49-2461-61-6402
Fax: +49-2461-61-6656
Email: b.scheid@fz-juelich.de

before November 25, 2005.

The programme committee will decide in the week 28 November - 2 December on acceptance or rejection of the applications and will immediately inform the applicants by e-mail.

All interested persons are invited to submit their application in electronic form.

3. Poster Presentations

All participants are kindly invited to present a poster on topics in their working group or on their own work during the School. We would like to prepare a book of poster abstracts prior to the School and therefore ask you to send us a one-page abstract.

4. Fees and Grants

Participation fee: 100,- Euro

The fee includes meals, social events, and the lecture notes, it is highly subsidized. Participants are asked to bear travel and accommodation costs themselves (for accommodation details see the School's web server). There is a limited number of grants available from the ESF Psi-k Network for further support.

We hope to see you in Juelich,

Stefan Bluegel, Institute for Solid State Physics, Forschungszentrum Juelich

Johannes Grotendorst, NIC, Forschungszentrum Juelich

Dominik Marx, Chair of Theoretical Chemistry, Ruhr-Universitaet Bochum

5.5 Spring School 2006: Computational Methods in Condensed Matter Physics

March 6-17, 2006

Forschungszentrum Juelich, Germany

We would like to draw your attention to the

Spring School 2006: Computational Methods in Condensed Matter Physics (DFT, Correlated Electrons, Monte Carlo, Soft Matter, Biophysics, Supercomputing)

which will take place on March 6-17, 2006 at the Forschungszentrum Juelich, Germany.

The Forschungszentrum Juelich has a long tradition in organizing these spring schools, which covered over the years a large spectrum of active subjects in condensed matter research. The lectures focus on students, particularly PhD students in physics and related areas, such as chemistry and material science.

There is no conference fee and the book which goes with the lectures is free of charge. Low-cost accomodation has been arranged for at the youth hostel in Aachen. The fee is 320 Euro including breakfast and dinner.

Deadline for Registration: December 22, 2005

More information can be found at

<http://www.fz-juelich.de/iff/fs2006>

With best regards,

Erik Koch and Stefan Bluegel

5.6 Nano2006 International Conference and School on "Counting Statistics"

Lancaster University, UK

January 7-11, 2006

We would like to draw your attention to the International Conference "Nanoelectronics 2006: Novel Nanomaterials, Quantum Transport, and Noise of Electrons and Photons" and the School on "Counting Statistics", to be held at Lancaster University, UK, on January 7-11, 2006.

A complete description of the conference and registration information can be found at <http://www.lancs.ac.uk/users/esqn/nano2006/>

The Organizers

Gerrit Bauer, Carlo Beenakker, Vadim Cheianov, Henning Schomerus

5.7 ICCSA 2006

International Conference on Computational Science and its Applications

Technical Session on

”Frontiers in High Performance Computing in Materials Science”

Call for Papers

<http://www.iccsa.org/>

8-11 May 2006, Glasgow, UK

Materials Science is increasingly concerned with modelling larger systems and time dependent processes. This pushes forward the need for high performance computing. Challenges lie in producing parallel codes, codes which scale well with the number of atoms and ways of implementing time dependence. This session will include topics such as density functional theory, Monte Carlo and molecular dynamics simulations.

Call for Papers

You are invited to submit a full paper of 6 to 10 pages (Letter or A4 paper) for oral presentation or a short paper (3 to 6 pages) for poster presentation.

Submitted papers have to be original, containing new results that were not previously published. Full version of accepted papers will appear in the Springer-Verlag Lecture Notes in Computer Science (LNCS) volumes.

For full details see the ICCSA 2006 website.

<http://www.iccsa.org/>

Please note that if your paper is accepted to the conference, it will be necessary to register and present a paper in order for it to appear in LNCS printed proceedings.

5.8 5th Workshop "Hands-on-FPLO"

First Announcement

IFW Dresden, Germany

May 22-24, 2006

This workshop will be connected with the 2nd FPLO users and developers meeting.

FPLO is a high-precision local-orbital DFT code for lattices. It comprises a fully relativistic version, a CPA solver, LSDA+U and DLM methods and a number of other useful features. For further details see

<http://www.fplo.de>

Participation will be free of charge for licence holders of fplo-5. A final announcement with details of the program and registration form will be distributed at the end of January.

Please note that places are restricted and that we will follow a first-come-first served policy. You are welcome to pre-register by email to m.richter@ifw-dresden.de.

Manuel Richter

6 General Job Announcements

Ph. D. Position

Tyndall National Institute, Cork, Ireland

<http://www.tyndall.ie>

A Ph. D. position is available within the European Union sponsored Research and Training Network "NANOCAGE" in the area of electronic structure theory or quantum chemistry, with registration for Ph. D. study at University College Cork. The successful applicant will work with the partners in the network including: Nanoscience Group, University of Nottingham, Institut für Schichten und Grenzflächen, Forschungszentrum Jülich GmbH Fullerene Group, Queen Mary, University of London.

Ab initio methods, primarily density functional calculations, will be applied to the study of fullerenes "endohedrally doped" with metal atoms, and their interactions with surfaces.

The objectives of the network are:

1. To ascertain the effects of chemisorption on the properties of encapsulates in a variety of endohedral fullerenes;
2. To probe whether chemisorption induces changes in the position of the encapsulated atom(s);
3. To probe the electronic spin state of caged atoms in endofullerenes;
4. To determine the intramolecular vibrational modes of chemisorbed endofullerenes

Further project details are available at

<http://www.nottingham.ac.uk/~ppzpj/nanocage/>

The successful applicant will be primarily based at the Computational Modelling Group at the Tyndall National Institute, and will spend time visiting the other labs within the network. Interested applicants are encouraged to contact

Dr. J. Andreas Larsson (alarsson@tyndall.ie)

or

Dr. Jim Greer (jgreer@tyndall.ie)

Tyndall National Institute,
Lee Maltings, Prospect Row,
Cork, Ireland

WWW: <http://www.tyndall.ie/research/computational-modelling-group/>

Permanent Position

IPCMS, University of Strasbourg, France

The IPCMS (site web) seeks candidates for a permanent position in the area of theoretical modeling of surfaces and nanostructures. Applicants will take part to a national contest aimed at selecting CNRS (<http://www.cnrs.fr>) permanent researchers upon evaluation operated by a national committee.

The selection process will take place in two different steps (November/December 2005 and May/June 2006). This selection will be based on past accomplishments, validity of the research project and an oral presentation. It has to be intended that the IPCMS will play an important role in the selection and the support of those candidates best fitting within its research lines. In case of successful application, the candidate will be hired to work in close contact with theoreticians and experimentalists already established within the IPCMS.

The required background encompasses previous knowledge and experience in density functional calculations (DFT) of surfaces and/or clusters. Accomplished research work in the field of structural and dynamical characterization of surfaces is highly desirable. We look forward to selecting candidates willing to a) elaborate a theoretical treatment of STM images and spectroscopy data, b) gather information on structural, electronic and magnetic properties of small objects deposited on surfaces and c) develop realistic effective interatomic potential schemes for metallic and oxide surfaces.

For more information, please contact Hervé Bulou (Herve.Bulou@ipcms.u-strasbg.fr) or Carlo Massobrio (Carlo.Massobrio@ipcms.u-strasbg.fr).

Postdoctoral Position

”Ab initio studies of phase separation processes”

**Laboratoire des Colloides, Verres, et Nanomateriaux
Montpellier, France**

A postdoctoral position for 12 months (with possible extension to 24 months) is open in the Laboratoire des Colloides, Verres, et Nanomateriaux in Montpellier. This work is done in collaboration with the LCLT (Laboratoire d'études du Comportement a Long Terme des materiaux de conditionnement) and LEBV (Laboratoire d'études de Base sur les Verres) of the CEA. The goal of the research is to use ab initio methods to investigate the process of demixing of silicate melts containing impurities such as molybdenum.

Competences: ab initio methods (such as Car-Parrinello, VASP, ...), Monte Carlo methods (grand canonical ensemble simulations, calculation of free energies, ...), structure of liquids.

Interested applicants should sent a Curriculum Vitae to

Dr. Simona ISPAS or Pr. Walter KOB

email: simona.ispas@lcvn.univ-montp2.fr

Laboratoire de Colloides, Verres et Nanomateriaux, cc 069

Universite Montpellier 2

34095 Montpellier Cedex 05

Tel: +33 (0)4 67 14 49 79

Fax: +33 (0)4 67 14 34 98

FRANCE

and to

Dr. Jean-Marc DELAYE

email: jean-marc.delaye@cea.fr

Laboratoire d'études du Comportement à Long Terme des materiaux de conditionnement

CEA Marcoule, BP17171, 30207 Bagnols-sur-Ceze cedex, France

Tel: +33 (0)4 66 79 17 94

Fax: +33 (0)4 66 79 66 20

Salary: 1940 Euro to 2100 Euro/month depending on qualifications

Deadline: 1st of December 2005 or until the position is filled.

Postdoctoral Fellowship in Condensed-Matter Atomistic Modelling

Commissariat à l'Energie Atomique, Saclay, France

Applications are invited for a post-doctoral position based in Saclay, near Paris, within the atomistic simulation group of the Thermodynamics and Thermochemistry Modelling Laboratory. Our lab consists of 15 researchers with national and international collaborations and conducts applied research in the fields of advanced nuclear fuels, materials for advanced nuclear reactors, nuclear waste storage. This position is for a one-year term, extendable by one year. The appointment will be available from January, 2006.

The research will consist in contributions to two different projects using ab initio simulation. The first project is part of the PRECCI program of CEA and EDF (Long Term Evolution of Irradiated Fuel Containers) and focuses on chemical reactions involving actinides in geological storage conditions; electronic structure calculations using ab initio methods will be used to investigate the evolution of uranium speciation during leaching of uranium dioxide by ground water. The second project is a collaborative effort and investigates phase diagram of metallic alloys for nuclear fuels and fuel-cladding compatibility issues; the post-doctoral fellow will contribute with thermodynamical properties computed from first principles. A PhD in quantum chemistry and experience of ab initio (DFT) computational work are essential. Some knowledge of actinide chemistry will definitely be a plus.

Net salary is in the range EUR 25,000 to EUR 30,000 and CEA offers a number of additional benefits.

Informal enquiries about the post and how to apply can be made to Dr P Zeller by e-mail (pzeller@cea.fr). They should include a full CV and list of publications.

http://www.cea.fr/fr/travail/Doc_postDoc.htm

http://www-instn.cea.fr/html/F_cfr/acc_cfr.htm

Post-Doctoral Research Position

”Minerals for encapsulation of high-level nuclear waste: simulating damage and durability”

University of Cambridge, United Kingdom

A three-year position exists for a post-doctoral researcher to join our existing group working on ceramics for nuclear waste encapsulation on a new NERC-funded collaboration between the Departments of Earth Science at the University of Cambridge (Emilio Artacho, Martin Dove, Simon Redfern), and Materials Science at Imperial College (Robin Grimes). The aim of the project, entitled ”Minerals for encapsulation of high-level nuclear waste: simulating damage and durability”, is to use atomic scale computer simulation to build an understanding of the long-term durability of ceramic phases proposed for high-level nuclear waste encapsulation, with the goal of developing improved methods of high-level waste encapsulation. We envisage that the first part of the work will focus on developing methods to understand transport of ions in damaged material. This will involve investigating suitable simulation methodologies, developing appropriate interatomic potentials, running large-scale simulations to generate damaged material, and implementing the methodologies for studying diffusion.

The project will involve running a variety of condensed matter simulation methods, including:

- 1) Very-large-scale computer simulations of radioactive decay processes within oxides, the choice being based on practical candidate materials.
- 2) Running simulations of diffusion of radioactive atoms through damaged materials to investigate long-term ability to contain these atoms in real storage materials.
- 3) Developing quantum mechanics methods to understand the role of energy lost through interactions with electrons.

The researcher will be based in Cambridge but will be expected to visit Imperial College regularly, and will

- a) have a PhD (or about to receive a PhD) in condensed matter physics/chemistry or materials science
- b) have experience in simulations of condensed phases, including some experience/interest in classical molecular dynamics, Monte Carlo methods, developments of model potentials, ab initio methods
- c) have experience of computing, including use of high-capability computers, programming, and scripting.

Salary in the range GBP 22,289 to GBP 24,352

Applicants should send CV and e-mails of 2 referees, as soon as possible to:

Professor Simon Redfern (e-mail: satr@cam.ac.uk)

Department of Earth Sciences

Downing Street

Cambridge, CB2 3EQ

UK

Post-Doc Position in Computational Nano-Science

University of Copenhagen, Denmark

A Post-Doc position in computational nano-science is available at the Nano-Science Center at Copenhagen University with starting date spring 2006. The project is funded by by the Danish Research Agency's Programme Commission on Nanoscience, Biotechnology and IT (NABIIT), and is a collaboration between DIKU (Department of Computer Science, University of Copenhagen), DTU (Technical University of Denmark), the Nano-Science Center at the University of Copenhagen, MESH-Technologies A/S and Atomistix A/S.

The topic of the project is to develop first principles methods for calculating the optical properties of molecules and crystals. The developed methods will be coupled with grid technology software to generate large databases of theoretical results. A chemi-informatics group will use this database for finding candidate systems with tailored optical properties.

Candidates should have a PhD degree in chemistry or physics, with a strong background in quantum chemistry or electronic structure theory. Knowledge of time-dependent density functional theory or GW approximation is an advantage. Terms of appointment and payment are as for assistant professors. The annual salary is determined by a standard seniority-based scale starting at DKK 285,669 plus a supplement of DKK 43,723. Both amounts are pensionable with 16.8%. It corresponds to a gross value of approximately US\$ 69,320.

Further information is available from

Kurt Stokbro, Nanoscience Center, Universitetsparken 5d, Dk-2100 Copenhagen O, Denmark,
Phone: +45 35320637/22830537, Email: ks@nano.ku.dk.

Applications with enclosures should be submitted to Kurt Stokbro at the address given above. Applications must include a short application letter describing research interests, curriculum vitae with the name of 3 references, and documentation (including marks) of a completed degree. The application must be received no later than December 15, 2005 at 12.00.

About the Nano-Science Center: *The Nano-Science Center at the University of Copenhagen constitutes an interdisciplinary research and educational effort with the long term goal of merging nano-scale biology, chemistry and physics into a new scientific discipline: Nano-science. The institute currently employs 50 researchers and is rapidly expanding. The successful candidate will be part of the nano-science theory group which currently consists of 3 senior researchers, 4 post. Docs, 3 PhD students and several master students with focus on studying electrical and mechanical properties of nanostructures. The group collaborates with other academic institutions in the Copenhagen area and Atomistix A/S on developing new methods and formalisms for modelling the properties of nanoscale systems.*

Ph. D. Position

Department of Physical Chemistry, University of Geneva, Switzerland

A Ph. D. position sponsored by the Swiss National Science Foundation grant "Modelling complex systems using embedded cluster approach: Methodology and Applications" is available from April 1, 2006.

The whole project involves the following issues relevant to the orbital-free embedding formalism [Wesolowski and Warshel, J. Phys. Chem. vol. 97, (1993) 8050]:

- a) Mathematical properties of the kinetic energy functional.
- b) Development and testing approximations to the bi-functional of the non-additive kinetic energy.
- c) Code development (ADF and/or deMon2K).
- d) Computer simulation studies of electronic properties of atoms and molecules in solids and liquids.

The successful applicant:

- i) Will register as a PhD student at University of Geneva (4 years program).
- ii) Will be involved in teaching activities (teaching assistant).
- iii) Should have solid basis in physical chemistry (physics- or theoretical chemistry background).
- iv) Should have previous experience with quantum chemistry or solid state physics computer simulations.

Interested applicants are encouraged to contact: Dr. Tomasz A. Wesolowski
(Tomasz.Wesolowski@chiphys.unige.ch), <http://lcta.unige.ch/~tomek>.

Two Ph. D. Positions in Computational Materials Science University of Munich, Germany

Two Ph. D. positions in computational materials science are available at the University of Munich, Germany. The first project will investigate magnetism and charge ordering phenomena at transition metal oxide interfaces. The second project is on the adsorption of water at iron oxide surfaces.

Candidates are expected to have background in condensed matter theory, materials science and preferably experience with large scale electronic structure calculations and/or strongly correlated materials as well as the ability to work in an international team and collaborate with experimentalists. Excellent computing resources are available at the Leibniz Rechenzentrum.

To apply please send your curriculum vitae, list of publications together with a short description of research experience and interests and two references via email (or normal mail) to:

Dr. Rossitza Pentcheva or Prof. Dr. Wolfgang Moritz

Department of Earth and Environmental Sciences

Section Crystallography

Ludwig-Maximilians-University

Theresienstr. 41

80333 Munich Germany e-mail: Rossitza.Pentcheva@lrz.uni-muenchen.de

e-mail: W.Moritz@lrz.uni-muenchen.de

<http://www.krist.geo.uni-muenchen.de>

**Research Associate Positions:
Quantum Simulations of Complex Molecular Systems
Center for Theoretical Chemistry, University of Bochum, Germany**

Applications are invited for two research associate positions (full BAT-IIa salary including all benefits) that are expected to becoming available in February or Spring 2006.

The ideal candidates would have significant experience in path integral MC/MD methods, electronic structure theory and computer simulation; a PhD in theoretical chemistry, physics or related field is required.

One position is devoted to developing and applying dynamical ab initio path integral Car-Parrinello techniques to compute IR spectra of complex molecular quantum systems (see e.g. Science 309 (2005) 1219). The other position is focused on applying and improving our novel ab initio Quantum Monte Carlo technique. Both projects will strongly benefit from collaborations with experimental groups. In addition, you are most welcome to get involved in other challenging research projects including both method development and large-scale applications. Information on the techniques used and developed at CTC are accessible via www.theochem.rub.de/go/cprev.html.

The Center for Theoretical Chemistry at RUB offers an exciting interdisciplinary environment with excellent working conditions including several high-performance parallel platforms in house adding up to about two TeraFlop/s, see www.theochem.rub.de/go/jobs.html.

Candidates should send a detailed resume including an outline of their research achievements and interests as well as contact information for academic references to

Professor Dominik Marx
Lehrstuhl fuer Theoretische Chemie
Ruhr-Universitaet Bochum
44780 Bochum, Germany
Email: office@theochem.rub.de

Consideration of candidates will begin immediately and continue until the position is filled. The University particularly welcomes applications from women.

CRISP Postdoctoral Fellowship
Center for Research on Interface Structure and Phenomena
(CRISP)
Yale University, USA

The Center for Research on Interface Structure and Phenomena (CRISP) at Yale, an NSF Materials Research Science and Engineering Center (MRSEC), has established a new interdisciplinary research position at the postdoctoral level. The focus is on performing theoretical studies of the structural, mechanical, chemical, and electronic properties of complex oxides and their interfaces by both applying state-of-the-art methods and developing novel approaches for dealing with electronic correlations. In addition, the theoretical effort will connect with parallel experimental efforts within the MRSEC.

The candidate should have a Ph.D. in materials physics or a related field and have prior experience with first principles calculations of material properties. For further information, please contact Prof. Sohrab Ismail-Beigi (sohrab.ismail-beigi@yale.edu) or Prof. John Tully (john.tully@yale.edu). A curriculum vitae and three letters of recommendation should be sent to CRISP@yale.edu, or to CRISP, Yale University, 401 Becton Center, P.O. Box 208284, New Haven, CT 06520-8284. Recommenders should send letters directly under separate cover. The deadline for receipt of all material is December 20, 2005.

Yale is an affirmative action/equal opportunity employer and encourages applications from qualified women and minority group members.

Tenure-Track Faculty Positions

University of Vermont, Burlington, USA

The Physics Department of the University of Vermont invites applications for two tenure-track positions, contingent on funding, starting September 2006. One position is in experimental nanoscale physics and is tenure-track at the Assistant Professor level; the other is in computational condensed matter physics and is either at the Associate level (tenure-track) or full Professor level (tenured), depending upon qualifications. A doctorate in Physics or a closely related field, as well as postdoctoral experience, is required. Successful candidates must be committed to excellence in teaching at the undergraduate and graduate levels and are expected to initiate research in their field of specialization. Start-up funds will be available.

Candidates can apply online at www.uvmjobs.com and attach to their application a curriculum vitae, representative publications, a statement of research and teaching interests, and the names and contact information for three references.

The Department is committed to increasing faculty diversity and welcomes applications from women and underrepresented ethnic, racial and cultural groups and from people with disabilities. Minority and women candidates are strongly encouraged to apply.

The deadline for applications is 15 December 2005.

See www.uvm.edu/physics or contact Denise.Fontaine@uvm.edu for more information. The University of Vermont is an AA/EO employer.

Postdoctoral Positions in University of California, Davis

Two postdoctoral positions in theoretical condensed matter physics are available immediately at Physics Department of University of California, Davis.

This project is part of a research program that focuses on new methods for calculating electronic structure and electron-phonon interactions in strongly correlated materials. Successful candidates should hold a PhD or equivalent degree in physics. Experience with density functional calculations, Quantum Monte Carlo, numerical methods and programming using Fortran, Java and/or C++ is highly desired.

Interested candidates should email their resumes and contact emails of at least two references to Sergey Savrasov at savrasov@physics.ucdavis.edu.

For additional information, please visit our web site <http://www.physics.ucdavis.edu/>

**POSTDOCTORAL OR RESEARCH ASSOCIATE POSITION
IN NREL'S SOLID STATE THEORY GROUP:
"THEORY OF NANOSTRUCTURES AND ALLOY THEORY"**

National Renewable Energy Laboratory (NREL)

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

NREL's Solid State Theory Group is looking to fill a Postdoctoral or a Research Associate position (depending on qualifications). The research areas include theory of nanostructures, alloy theory and defect physics in solids. The positions are for up to 3 years. The salary range is US\$48,000 - US\$62,000 per year, depending on seniority, qualification and experience. Applicants are expected to have a strong background in solid-state theory. The positions are with Alex Zunger, Solid State Theory Group Leader. The start date is between April 2006 and September 2006. Applications are being considered now. For more details about ongoing work, see

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

The Solid State Theory Group currently consists of ten Ph.D.'s in condensed matter theory and interacts with a broad range of experimentalists. The group has outstanding computational facilities, an excellent basic-research atmosphere, and is located in the beautiful Rocky Mountains. Consult our web page for additional information on the group, its history, research subjects, publications, current and past personnel and facilities.

Interested candidates should send no later than Jan, 1, 2005 curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two to three references addressed to:

Alex Zunger
Solid State Theory Group
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401

Clarification or further details can be obtained via email to
alex_zunger@nrel.gov .

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

Postdoctoral Position
CEA, Grenoble, France

Multiscale simulation of diffusion in SiGe

The subject of this postdoctoral study is to understand the diffusion processes in SiGe using an atomistic multilevel approach, combining ab initio and kinetic Monte Carlo calculations. This work will take place in CEA-Grenoble within the simulation laboratory of the fundamental research department. The funding is provided by the French National Research Agency (ANR) through the OSiGe_Sim project. This project brings together three academic laboratories, as well as an applied-research and an industrial modeling groups. It concerns modeling of oxidation, stress and diffusion processes in SiGe nano-devices.

This research is in the framework of multiscale simulations applied to nanoelectronics issues. Ab initio calculations will be performed in order to determine the diffusion mechanisms in SiGe, using vacancies and interstitials scenarios. Kinetic Monte Carlo will then be used to simulate the whole diffusion process under equilibrium and non-equilibrium for different Ge concentration, temperature, and stress conditions.

For more details about ongoing work, see the web page of the laboratory

http://www-drfmc.cea.fr/sp2m/L_Sim/

The position is for one year, renewable upon mutual agreement to a second year. The net salary range is 2,000 EURO - 2,400 EURO per month, depending on seniority, qualification and experience. The start date is between March 2006 and June 2006. Applications are being considered now. The applicant must have strong skills in quantum physics, atomistic simulations and solid state physics, licensed by a PhD in the domain.

Interested candidates should send no later than January 2006 curriculum vitae, list of publications (including preprints of unpublished papers if possible), and arrange for two to three references addressed to:

Pascal Pochet
DRFMC/SP2M/L_Sim
CEA Grenoble, cedex 9
F-38054 Grenoble, France

Further details can be obtained via email to pascal.pochet@cea.fr.

Postdoctoral Position
CEA, Grenoble, France

Wavelets and order N method (BigDFT)

One postdoctoral position based at the atomistic Simulation group (L_Sim, CEA-Grenoble) is available to carry out research in electronic structure calculations. This position is funded by the European project BigDFT (http://www-drfmc.cea.fr/sp2m/L_Sim/BigDFT).

The subject is to apply wavelet techniques within linear scaling electronic structure calculations. The work involves implementing new methodologies to use wavelet functions in the ABINIT program (<http://www.abinit.org>).

Applicants are expected to have a strong background in electronic structure calculations, as well as a programming experience (Fortran 95). A background in mathematics (wavelet) would be appreciated.

The position is available immediately and the duration is for one year, renewable upon mutual agreement to a second year. The net salary range is 2,000 EURO - 2,400 EURO per month, depending on seniority, qualification and experience.

Interested candidates should send curriculum vitae, list of publications and arrange for two references addressed to:

Thierry Deutsch
SP2M/L_Sim
17 avenue des Martyrs, Cedex 9
38054 Grenoble, France
e-mail: Thierry.Deutsch@cea.fr
Phone: +33 4 38 78 34 06
Fax: +33 4 38 78 51 97
Web: http://www-drfmc.cea.fr/SP2M/L_Sim

Open Position at ETH Zurich, Switzerland

We expect an opening of a postdoc position in the "Theory of Minerals at Extreme Conditions" group at the Laboratory of Crystallography, ETH Zurich, starting approximately from June 2006. We seek a highly motivated researcher, ideally with a good background in high-pressure physics and/or ab initio simulations. Additional experience with computational methods is an advantage. The length of appointment is 3 years (extension is possible), with starting salary around 75,000 SFr (ca 60,000 USD), depending on experience.

The job is related to the application of the crystal structure prediction methodology (and the corresponding computer code) developed by our group. This novel methodology allows one to predict stable crystal structures at any pressure just from the knowledge of the chemical composition and is thus a very powerful tool to investigate matter at extreme conditions. The offered job will involve systematic application of this methodology to study minerals at high pressure, as well as other systems of fundamental and applied interest. Much of this work will be done in collaboration with experimentalists. Our group has world-class supercomputing facilities and a very dynamic research programme.

Applicants should submit (preferably by e-mail) a letter of application, CV with a list of publications, and the names and addresses of at least two referees to: Dr. Artem R. Oganov, Senior Researcher and Lecturer; Group Leader Laboratory of Crystallography, Department of Materials, ETH Hoenggerberg, Wolfgang-Pauli-Strasse 10, HCI G 515, Zurich CH-8093, Switzerland. E-mail: a.oganov@mat.ethz.ch.

Artem R. Oganov

Vice-chairman, Special Interest Group "Mineralogical Crystallography"

<http://www.lcm3b.uhp-nancy.fr/ecasig5/>

Dr. Artem R. Oganov, Senior Researcher and Lecturer;

Group Leader Laboratory of Crystallography, Department of Materials, ETH Hoenggerberg, Wolfgang-Pauli-Strasse 10, Zurich CH-8093, Switzerland

Tel.: +41-(0)44-632-3752; Fax: +41-(0)44-632-1133

Personal web-page: <http://olivine.ethz.ch/~artem>

Group page: <http://www.crystal.mat.ethz.ch/research/ExtremeConditions>

Postdoctoral Research Assistant

Imperial College London and City University London, UK

Applications are invited for the post of a Postdoctoral Research Assistant funded by EPSRC to work on a project carried out jointly at Imperial College London and City University London under the leadership of Professor D.M. Edwards and Professor J. Mathon. The successful candidate will undertake research into theory of quantum transport of charge and spin in magnetic nanostructures. The main aim of the project is to investigate theoretically coherent spin-dependent tunneling and the use of spin-polarized current to switch magnetization and move domain walls.

The theoretical research to be undertaken is a part of a large research programme into spintronics at finite temperature carried out by the consortium of eight UK universities (Cambridge, City, Durham, Exeter, Glasgow, Imperial, Leeds and Rutherford Appleton Laboratory). The whole joint programme is funded by EPSRC and the successful candidate will have the benefit of being able to interact and collaborate with other PDRAs and researchers at all the member institutions.

A PhD in a relevant area of theoretical physics or materials modelling is required and experience in using/modifying/developing electronic structure codes is highly desirable.

The research programme of the Imperial/City theory node, which underpins the experimental effort of all the other members of the consortium, will be demanding and this is reflected in the salary of the PDRA. This will be in on a RA1A scale with a starting salary of up to £30,384 inclusive of London allowance and is available for up to 36 months starting as soon as possible after January 1st 2006.

Informal enquires should be addressed to either Prof. J. Mathon at j.mathon@city.ac.uk or Prof. D.M. Edwards at d.edwards@ic.ac.uk.

Ph.D. Position

”Quantum coherence in superconducting circuits”

Department of Physics and NanoScience Centre, University of Jyvaskyla, Finland

A Ph.D. position in the field of quantum coherence in superconducting circuits is available starting 2006 in the Quantum Engineering/Nanophysics group of the Department of Physics and NanoScience Centre, University of Jyvaskyla, Finland. Our research currently focuses on the physics of various Josephson junction devices and their use as superconducting quantum bits.

The research is experimental, but involvement in more theoretical problems is also possible. The successful candidate will learn a broad range of nanofabrication techniques and low-temperature measurement methods, and is expected to develop her/his skills in these directions while contributing significantly to the research done in the group.

Applications are invited immediately. The position will be filled as soon as a suitable candidate is identified. To apply, please send the following materials by e-mail to Dr. S. Paraoanu (paraoanu@phys.jyu.fi): CV, copies of official transcripts, statement of purpose, and the names and contact information of (at least) two persons who can provide letters of recommendation. Applicants must have a M.Sc. degree in physics. Results from standardized tests (TOEFL, GRE) are not requested but can be mentioned if they were taken. M.Sc. thesis could be also submitted.

Postdoctoral and Ph.D. Positions in Computational Materials Physics The COMP Group

Laboratory of Physics, Helsinki University of Technology

<http://www.fyslab.hut.fi/comp>

Following its reselection as a national Centre of Excellence in Computational Nanoscience, from January 2006, postdoctoral and Ph.D. positions are available in the COMP Group at HUT, Finland. The group is led by Professor Risto Nieminen, and consists of over 60 researchers forming six focused research groups. Projects are available in several of COMP's subgroups, and candidates are encouraged to explore the online project descriptions or contact subgroup leaders directly for more information:

- Biological Physics (BIO) - Ilpo Vattulainen
- Complex Systems and Materials (CSM) - Mikko Alava
- Electronic Properties of Materials (EPM) - Risto Nieminen and Martti Puska
- Quantum Many-body physics (QMP) - Ari Harju
- Multiscale Statistical Physics (MSP) - Tapio Ala-Nissil
- Surfaces and Interfaces at the Nanoscale (SIN) - Adam Foster

Applicants should send any project preferences, along with a CV including a publication list and the name of two potential referees to: risto.nieminen@hut.fi or Prof. R. M. Nieminen, Laboratory of Physics, Helsinki University of Technology, PO Box 1100, 02015, Finland

Tenured Full Professorship in Computational Materials Science

An opening of a permanent position at the Institute of Solid State Physics, Faculty of Physics at the Vienna University of Technology (Technische Universitaet Wien)

The applicant is required to have outstanding academic credentials and a proved track record of scientific accomplishments in the field of "Computational Materials Science", preferably in the area of quantum criticality, magnetism and superconductivity. In addition to extensive experience in applications of well-established methods, she/he should have demonstrated potential for developing new numerical methods to treat these topics. Strong interest in the ongoing experimental work and an active participation in strengthening the research activities of the institute are expected. Teaching duties include both mandatory courses of the physics core curriculum and elective courses.

Willingness to develop collaborations with other research groups working in the field of "Condensed Matter Physics" at the Vienna University of Technology is essential.

The applicants must meet the requirements:

1. an Austrian or equivalent foreign terminal academic degree in the field under consideration,
2. an outstanding academic track record in research and teaching,
3. pedagogic and didactic skills,
4. leadership abilities,
5. international working experience in the field of research.

Application deadline: January 31, 2006.

The Vienna University of Technology is committed to increase female employment in leading scientist positions. Qualified female applicants are expressly encouraged to apply and will be given preference when equally qualified.

Applications including a detailed curriculum vitae, description of scientific objectives, list of publications, and copies of the five most outstanding publications of the applicant should be sent to the Dean of the Faculty of Physics, (Univ.-Prof. Dr. Gerald Badurek), Getreidemarkt 9, A-1060 Vienna, Austria. In addition a CD-ROM with the complete application records must be attached.

Additional note by Prof. Volker Heine, Chairman of the International Scientific Advisory Board of the Computational Materials Science (CMS) Centre in Vienna.

This Centre is a joint venture between the two universities in Vienna, namely the University of Vienna and the Vienna Technical University, with its webpage at

<http://www.cms.tuwien.ac.at/>

It includes faculty members from both universities drawn from institutes of physics, theoretical physics, materials physics, and physical chemistry.

The Board would like candidates to know of the existence of this Centre in Vienna which the Board considers outstanding in quality, breadth and size by world standards.

7 Abstracts

Vanadium oxides on aluminium oxide supports. 2. Structure, Vibrational Properties and Reducibility of V_2O_5 Clusters on $\alpha\text{-Al}_2O_3(0001)$

V. Brázdová, M. V. Ganduglia-Pirovano and J. Sauer
*Humboldt Universität zu Berlin, Institut für Chemie,
Unter den Linden 6, D-10099 Berlin, Germany*

Abstract

The structure, stability and vibrational properties of isolated V_2O_5 clusters on the $\alpha\text{-Al}_2O_3(0001)$ surface have been studied by density functional theory and statistical thermodynamics. The most stable structure does not possess vanadyl oxygen atoms. The positions of the oxygen atoms are in registry with those of the alumina support and both vanadium atoms occupy octahedral sites. Another structure with one vanadyl oxygen atom is only 0.12 eV less stable. Infrared spectra are calculated for the two structures. The highest frequency at 922 cm^{-1} belongs to a V–O stretch in the V–O–Al interface bonds, which supports the assignment of such a mode to the band observed around 941 cm^{-1} for vanadia particles on alumina. Removal of a bridging oxygen atom from the most stable cluster at the V–O–Al interface bond costs 2.79 eV. Removal of a (vanadyl) oxygen atom from a thin vanadia film on $\alpha\text{-Al}_2O_3$ costs 1.3 eV more, but removal from a $V_2O_5(001)$ single crystal surface costs 0.9 eV less. Similar to the $V_2O_5(001)$ surface, the facile reduction is due to substantial structure relaxations that involve formation of an additional V–O–V bond and yield a pair of $V^{IV}(d^1)$ sites instead of a $V^{III}(d^2)/V^V(d^0)$ pair.

(J. Phys. Chem. B **109**, xxxx (2005) in press)

Contact person: M. Veronica Ganduglia-Pirovano (vgp@chemie.hu-berlin.de)

Vanadium oxides on aluminium oxide supports. 1. Surface termination and reducibility of vanadia films on α -Al₂O₃(0001)

T. K. Todorova, M. V. Ganduglia-Pirovano and J. Sauer
*Humboldt Universität zu Berlin, Institut für Chemie,
Unter den Linden 6, D-10099 Berlin, Germany*

Abstract

Using density functional theory and statistical thermodynamics we obtained the phase diagram of thin V_nO_m films of varying thickness (\sim 2–6 Å, 1–6 vanadium layers) supported on α -Al₂O₃(0001). Depending on temperature, oxygen pressure and vanadium concentration, films with different thickness and termination may form. In ultra-high vacuum (UHV), at room-temperature and for low vanadium concentrations, an ultra-thin (1 × 1) O=V terminated film is most stable. As more vanadium is supplied, the thickest possible films form. Their structures and terminations correspond to previous findings for the (0001) surface of bulk V₂O₃ [Kresse *et al.*, Surf. Sci. **2004**, 555, 118]. The presence of surface vanadyl (O=V) groups is a prevalent feature. They are stable at least up to 800 K in UHV. Vanadyl oxygen atoms induce a V_{2p} core-level shift of about 2 eV on the surface V atoms. The reducibility of the supported films is characterized by the energy of oxygen defect formation. For the stable structures the results vary between 4.11 and 3.59 eV per $\frac{1}{2}$ O₂. In contrast, oxygen removal from the V₂O₅(001) surface is much easier (1.93 eV). This provides a possible explanation for the lower catalytic activity of vanadium oxides supported on alumina compared to crystalline vanadia particles.

(J. Phys. Chem. B **109**, xxxx (2005) in press)

Contact person: M. Veronica Ganduglia-Pirovano (vgp@chemie.hu-berlin.de)

Ag- and W-Induced Magnetic Moment in 3d Multilayer

Nicolas Jaouen, Fabrice Wilhelm, Andrei Rogalev

E.S.R.F., 38043 Grenoble, France

Jean-Marc Tonnerre

Laboratoire de Cristallographie, C.N.R.S., 38042 Grenoble, France

Tarnjit K. Johal, Gerrit van der Laan

Daresbury Laboratory, Warrington WA4 4AD, U.K.

Abstract

The information of the W- and Ag-induced magnetic moments in Fe/W and NiFe/Ag multilayers was determined separately from the huge 3d magnetic moments with X-ray magnetic circular dichroism. Moreover, their spatial distribution has been extract from X-ray resonant magnetic scattering experiments. It was found that both W and Ag atoms are magnetically polarized and that this polarization extends through all the W and Ag layers, respectively. However, although W is found to be oscillating, the Ag polarization is exponentially decreasing from the interface.

Published in IEEE TRANSACTIONS ON MAGNETICS **41**, 10, 3334–6.

Manuscript available from g.van_der_laan@dl.ac.uk

Spin and Orbital Moments of Ultra-Thin Fe Films on Various Semiconductor Surfaces

Jill S. Claydon, Daxin Niu, Yongbing Xu

The Department of Electronics, University of York, York YO10 5DD, U.K.

Neil D. Telling, Ian W. Kirkman, Gerrit van der Laan

Daresbury Laboratory, Warrington WA4 4AD, U.K.

Abstract

The magnetic moments of ultrathin Fe films on three different III-V semiconductor substrates, namely GaAs, InAs and $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$ have been measured with X-ray magnetic circular dichroism at room temperature to assess their relative merits as combinations suitable for next-generation spintronic devices. The results revealed rather similar spin moments and orbital moments for the three systems, suggesting the relationship between film and semiconductor lattice parameters to be less critical to magnetic moments than magnetic anisotropy.

Published in IEEE TRANSACTIONS ON MAGNETICS **41**, 10, 3325–7.

Manuscript available from g.van_der_laan@dl.ac.uk

XPS and XMCD Study of Fe₃O₄/GaAs Interface

Yongxiong Lu, Jill S. Claydon, Ehsan Ahmad, Yongbing Xu

Department of Electronics, The University of York, York, YO10 5DD, U.K.

Sarah M. Thompson

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

Karen Wilson

Department of Chemistry, The University of York, York, YO10 5DD, U.K.

Gerrit van der Laan

Daresbury Laboratory, Warrington, WA4 4AD, U.K.

Abstract

Ultrathin Fe oxide films of various thicknesses prepared by post-growth oxidation on GaAs(100) surface have been investigated with X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), and X-ray magnetic circular dichroism (XMCD). The XPS confirms that the surfaces of the oxide are Fe₃O₄ rather than Fe₂O₃. XAS and XMCD measurements indicate the presence of insulating Fe divalent oxide phases (FeO) beneath the surface Fe₃O₄ layer with the sample thickness above 4 nm. This FeO might act as a barrier for the spin injection into the GaAs.

Published in IEEE TRANSACTIONS ON MAGNETICS **41**, 10, 2808–10.

Manuscript available from g.van_der_laan@dl.ac.uk

Electronic Structure and Exchange Coupling of Mn Impurities in III-V Semiconductors

Thomas C. Schulthess¹, Walter M. Temmerman², Zdzislawa Szotek²,
William H. Butler³, G. Malcolm Stocks⁴

¹*Computer Science and Mathematics Division, Oak Ridge National Laboratory,
Oak Ridge, Tennessee 37831-6164, USA*

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

³*Center for Materials for Information Technology, University of Alabama,
Tuscaloosa, Alabama 35487-0209, USA*

⁴*Metals and Ceramics Division, Oak Ridge National Laboratory,
Oak Ridge, Tennessee 37831, USA*

Abstract

Dilute magnetic semiconductors are without doubt amongst the most interesting classes of new magnetic materials. However, the nature of their electronic structure and magnetic exchange is far from understood, and important discrepancies exist between widely used phenomenological models and first principles electronic structure descriptions. Here we apply the ab initio self-interaction corrected local spin density method to study the electronic structure of Mn doped III-V semiconductors. For (GaMn)As, our results with $(d^5 + h)$ configuration agree with the Zener model description and predict p - d exchange that is in good agreement with experiment. The ground state in (GaMn)N and (GaMn)P is the d^4 configuration with no intrinsic carriers. If, however, holes are introduced extrinsically, carrier mediated exchange is possible, but the p - d exchange is predicted to be lower in p-type GaN, as compared to GaP and GaAs. Nevertheless, due to the smaller lattice constant, the estimated Curie temperature is higher than in (GaMn)As, at comparable doping levels.

(Nature Materials **4**, 838-844 (2005))

Contact person: Thomas C. Schulthess (schulthesstc@ornl.gov)

Interface-Controlled Ferroelectricity at the Nanoscale

Chun-Gang Duan,^{1,2,3} Renat F. Sabirianov,^{2,3} Wai-Ning Mei,^{2,3}
Sitaram S. Jaswal,^{1,3} and Evgeny Y. Tsymbal^{1,3}

¹*Department of Physics and Astronomy, University of Nebraska-Lincoln,
Lincoln, Nebraska 68588*

²*Department of Physics, University of Nebraska at Omaha,
Omaha, Nebraska 68182*

³*Center for Materials Research and Analysis, University of Nebraska-Lincoln,
Lincoln, Nebraska 68588*

Abstract

Recent experimental results demonstrate that in thin films ferroelectricity persists down to film thickness of a few unit cells. This finding opens an avenue for novel electronic devices based on ultrathin ferroelectrics, but also raises questions about factors controlling ferroelectricity and the nature of the ferroelectric state at the nanoscale. Here we report a first-principles study of KNbO_3 ferroelectric thin films placed between two metal electrodes, either SrRuO_3 or Pt. We show that the bonding at the ferroelectric-metal interface imposes severe constraints on the displacement of atoms, destroying the bulk tetragonal soft mode in thin ferroelectric films. This does not, however, quench local polarization. If the interface bonding is sufficiently strong the ground state represents a ferroelectric double-domain structure, driven by the intrinsic oppositely-oriented dipole moments at the two interfaces. Although the critical thickness for the net polarization of the KNbO_3 film is finite—about 1 nm for Pt and 1.8 nm for SrRuO_3 electrodes—local polarization persists down to the thickness of a unit cell.

(Preprint: <http://arxiv.org/ftp/cond-mat/papers/0510/0510592.pdf>)

Contact person: Evgeny Y. Tsymbal, e-mail: tsymbal@unl.edu

Role of Embedded Clustering in Dilute Magnetic Semiconductors: Cr doped GaN

X. Y. Cui,¹ J. E. Medvedeva,² B. Delley,³ A. J. Freeman,²,
N. Newman⁴, C. Stampfl¹

¹*School of Physics, The University of Sydney, Sydney 2006, NSW Australia*

²*Physics and Astronomy Department, Northwestern University,*

Evanston, IL 60208-3112

³*Paul Scherrer Institut WHGA/123 CH-5232 Villigen PSI, Switzerland*

⁴*Chemical & Materials Engineering Department, Arizona State University,*

Tempe, AZ 85287-6006

Abstract

Results of extensive density functional studies provide direct evidence that Cr atoms in Cr:GaN have a strong tendency to form embedded clusters, occupying Ga sites. Significantly, for larger than two-Cr-atom clusters, states containing antiferromagnetic coupling with net spin in the range 0.06-1.47 μ_B /Cr are favored. We propose a picture where various configurations coexist and the statistical distribution and associated magnetism will depend sensitively on the growth details. These findings elucidate various hitherto puzzling experimental results – such as the observed strong dependence of the magnetization on the Cr concentration, growth temperature and annealing – and represents significant progress towards understanding the intrinsic complex nature of the distribution and magnetism in TM-doped DMS.

Physical Review Letters, in press

Contact person: Dr. Carl Cui, carlc@physics.usyd.edu.au

Impurity scattering and quantum confinement in giant magnetoresistance systems: a comparative study

Peter Zahn¹, Jörg Binder², and Ingrid Mertig¹

¹*Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg,
D-06099 Halle, Germany*

²*Institut für Theoretische Physik, Technische Universität Dresden,
D-01062 Dresden, Germany*

Abstract

Ab initio calculations for the giant magnetoresistance (GMR) in Co/Cu, Fe/Cr, and Fe/Au multilayers are presented. The electronic structure of the multilayers and the scattering potentials of point defects therein are calculated self-consistently. Residual resistivities are obtained by solving the quasi-classical Boltzmann equation including the electronic structure of the layered system, the anisotropic scattering cross sections derived by a Green's function method and the vertex corrections. Furthermore, the influence of scattering centers at the interfaces and within the metallic layers is incorporated by averaging the scattering cross sections of different impurities at various sites. An excellent agreement of experimental and theoretical results concerning the general trend of GMR in Co/Cu systems depending on the type and the position of impurities is obtained. Due to the quantum confinement in magnetic multilayers GMR can be tailored as a function of the impurity position. In Co/Cu and Fe/Au systems impurities in the magnetic layer lead to high GMR values, whereas in Fe/Cr systems defects at the interfaces are most efficient to increase GMR.

(Accepted for Phys. Rev. B, Dec 2005)

Contact person: zahn@physik.uni-halle.de

Influence of interface structure on the bias dependence of tunneling magnetoresistance

Christian Heiliger, Peter Zahn, Bogdan Yu. Yavorsky, and Ingrid Mertig
*Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg,
D-06099 Halle, Germany*

Abstract

Ab initio calculations for the tunneling magnetoresistance (TMR) in planar Fe/MgO/Fe junctions are presented. The electronic and magnetic structure of the junctions are calculated self-consistently in the framework of density functional theory. The bias dependence of the tunneling conductance and the magnetoresistance is calculated in the limit of coherent tunneling. Positive and negative TMR ratios are obtained as a function of interface structure and even a sign reversal of TMR as a function of bias was found in agreement with experiments.

(Accepted for Phys. Rev. B (RC), Dec 2005)

Contact person: c.heiliger@physik.uni-halle.de, zahn@physik.uni-halle.de

Fullerene in a metal-organic matrix: design of the electronic structure

Sébastien Hamel, Vladimir Timoshevskii, and Michel Côté
*Département de Physique et Regroupement Québécois
sur les Matériaux de Pointe (RQMP), Université de Montréal,
Case Postale 6128, Succursale Centre-ville,
Montréal, Québec, H3C 3J7 Canada*

Abstract

We present a theoretical study of a new hybrid compound, where the C_{60} molecules are encapsulated in a recently discovered metal-organic frameworks (MOF). Being placed in a rigid skeleton, the fullerene molecules form a cubic crystal, while the intermolecular distance of the fullerenes is tuned by the choice of appropriate organic linkers of the MOF structure. The resulting C_{60} crystal shows a density of conduction states considerably higher than any of the fullerene crystals considered so far, which is a key factor influencing the transition temperature of the superconducting state. This constitutes a new approach of tuning the density of states of a fullerene crystal.

Published in: Phys. Rev. Lett. **95**, 146403 (2005)

Contact person: Michel Ct (Michel.Cote@umontreal.ca)

First-principles kinetic Monte Carlo simulations for heterogeneous catalysis, applied to the CO oxidation at RuO₂(110)

Karsten Reuter and Matthias Scheffler
*Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, D-14195 Berlin, Germany*

Abstract

We describe a first-principles statistical mechanics approach enabling us to simulate the steady-state situation of heterogeneous catalysis. In a first step density-functional theory together with transition-state theory is employed to obtain the energetics of all relevant elementary processes. Subsequently the statistical mechanics problem is solved by the kinetic Monte Carlo method, which fully accounts for the correlations, fluctuations, and spatial distributions of the chemicals at the surface of the catalyst under steady-state conditions. Applying this approach to the catalytic oxidation of CO at RuO₂(110), we determine the surface atomic structure and composition in reactive environments ranging from ultra-high vacuum (UHV) to technologically relevant conditions, i.e. up to pressures of several atmospheres and elevated temperatures. We also compute the CO₂ formation rates (turnover frequencies). The results are in quantitative agreement with all existing experimental data. We find that the high catalytic activity of this system is intimately connected with a disordered, dynamic surface “phase” with significant compositional fluctuations. In this active state the catalytic function results from a self-regulating interplay of several elementary processes.

(submitted to: Phys. Rev. B)

Contact person: Karsten Reuter (reuter@fhi-berlin.mpg.de)

Quantum size effect in Pb(100) films: the role of symmetry and implication for film growth

Dengke Yu¹, Matthias Scheffler¹, and Mats Persson^{1,2}

¹ *Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195, Berlin, Germany*

² *Department of Applied Physics, Chalmers University of Technology, SE-412 96, Göteborg, Sweden*

Abstract

We show from density-functional calculations that Pb(100) thin films exhibit quantum size effect with a bilayer periodicity in film energies, film relaxations, and work functions, which originate from different symmetry of the stacking geometry of odd and even layer films. The bilayer periodicity of the film energy is argued to survive on a semiconductor substrate, which should allow the growth of “magically” thick even-layer Pb(100) films. Furthermore, it is found that the quantum well states in a simple metal film can be classified into σ -bonded and π -bonded states, which quantize independently.

(Submitted to Phys. Rev. Lett.)

Contact person: Mats Persson (tfymp@fy.chalmers.se)

Orbital ordering in cubic LaMnO₃ from first principles calculations

H. Zenia^{1,2}, G. A. Gehring¹, and W. M. Temmerman²

¹*Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK*

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

Abstract

We report on first principles Self-Interaction Corrected LSD (SIC-LSD) calculations of electronic structure of LaMnO₃ in the cubic phase. We found a strong tendency to localisation of the Mn e_g electron and to orbital ordering. We found the ground state to be orbitally ordered with a staggered order of $x^2 - z^2$ and $y^2 - z^2$ orbitals in one plane and this order is repeated along the third direction. The difference in energy with a solution consisting of the ordering of $3x^2 - r^2$ and $3y^2 - r^2$ is, however, very small. The system is in the insulating A-type antiferromagnetic ordered state in both cases. The presence of orbital ordering means breaking of the cubic symmetry and without recourse to distortion. The latter may rather be the result of the orbital ordering but the symmetry of this ordering is determined by coupling to the lattice. The strong tendency to localisation of the e_g electron in LaMnO₃ accounts for the survival of local distortions above the structural phase transition temperature.

(Accepted, New Journal of Physics, 2005)

Contact person : h.zenia@sheffield.ac.uk

Periodic DFT Calculations of the Stability of Al/Si Substitutions and Extraframework Zn²⁺ Cations in Mordenite and Reaction Channel for the Dissociation of H₂ and CH₄

L. Benco^{1,2}, T. Bucko¹, J. Hafner¹, H. Toulhoat³

L. Benco¹, T. Demuth¹, J. Hafner¹, F. Hutschka², H. Toulhoat³

¹*Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8, A-1090 Wien, Austria*

²*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dubravska cesta 9, SK-84536 Bratislava, Slovak Republic*

³*Institut Français du Pétrole, F-92852 Rueil-Malmaison Cedex, France*

Abstract

The local stability of Al atoms replacing Si in the zeolite framework is compared for all inequivalent tetrahedral (T) sites in mordenite. For Al/Si substitutions in two T-sites the stable location of the compensating extra-framework Zn²⁺ cation forming a Lewis acid site is determined. In the most stable Zn-MOR structures Zn²⁺ is located in a small ring (5MR, 6MR) containing two Al/Si substitutions. In less stable structures the Al atoms are placed at larger distances from each other and Zn²⁺ interacts with only one Al-site. The simulated adsorption of H₂ and CH₄ shows that adsorption strength decreases with increasing stability of the Zn²⁺ Lewis site. For Zn²⁺ deposited in the 5MR a higher adsorption strength is observed than for the 6MR. The reactivity of a series of stable Zn²⁺ Lewis sites is tested via the dissociative adsorption of H₂ and CH₄. The heterolytic dissociation of the adsorbed molecule on the extra-framework Zn²⁺ cation produces a proton and an anion. The anion binds to Zn²⁺ and proton goes to the zeolite framework, restoring a Brønsted acid site. Because bonding of the anion to Zn²⁺ is almost energetically equivalent for Zn²⁺ in any of extra-framework positions the dissociation is governed by stabilizing bonding of the proton to the framework. Those structures which can exothermically accommodate the proton represent reaction pathways. Due to the repulsion between the proton and Zn²⁺ the most favorable proton-accepting O-sites are not those of the ring where Zn²⁺ is deposited, but O-sites close to the ring. Large differences are observed for neighboring positions in *a*- and *b*-directions and those oriented along the *c*-vector. Finally, among the stable Zn²⁺ Lewis sites not all represent reaction pathways for dehydrogenation. For all of them the dissociation of H₂ is an exothermic process. In structures exhibiting the highest reactivity the Al/Si substitutions are placed at a large distance and the Zn²⁺ cation interacts with O-atoms next to Al in the T4-site of the 5MR. This Lewis site is strong enough to break the C-H bond in the CH₄ molecule.

J. Phys. Chem. B, 109 (2005) 20361

Preprints available from: lubomir.benco@univie.ac.at

A DFT study of molecular and dissociative adsorption of H₂ on active sites in mordenite

L. Benco^{1,2}, T. Bucko¹, J. Hafner¹, H. Toulhoat³ ¹*Institut für Materialphysik and Center for Computational Materials Science, Universität Wien, Sensengasse 8, A-1090 Wien, Austria*

²*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dubravská cesta 9, SK-84236 Bratislava, Slovak Republic*

³*Institut Français du Pétrole, F-92852 Rueil-Malmaison Cedex, France*

Abstract

Adsorption and chemisorption of H₂ in mordenite is studied using ab initio DFT calculations. The geometries of the adsorption complex, the adsorption energies, stretching frequencies and the capacity to dissociate the adsorbed molecule are compared for different active sites. The active centers include a Brønsted acid site, a 3-coordinated surface Al-site, and Lewis sites formed by extra-framework cations: Na⁺, Cu⁺, Ag⁺, Zn²⁺, Cu²⁺, Ga³⁺, and Al³⁺. Adsorption properties of cations are compared for a location of the cation in the five-membered ring. This location differs from the location in the six-membered ring observed for hydrated cations. The five-membered ring, however, represents a stable location of the bare cation. In this position any cation exhibits higher reactivity compared with the location in the six-membered ring and is well accessible by molecules adsorbed in the main channel of the zeolite. Calculated adsorption energies range from 4 kJ/mol to 87 kJ/mol, depending on electronegativity and ionic radius of the cation and the stability of the cation-zeolite complex. The largest adsorption energy is observed for Cu⁺ and the lowest for Al³⁺ integrated into the interstitial site of the zeolite framework. A linear dependence is observed between the stretching frequency and the bond length of the adsorbed H₂ molecule. The capacity of the metal-exchanged zeolite to dissociate the H₂ molecule does not correlate with the adsorption energy. Dissociation is not possible on single Cu⁺ cation. The best performance is observed for the Ga³⁺, Zn²⁺, and Al³⁺ extra-framework cations, in good agreement with experimental data.

J. Phys. Chem. B 109 (2005) 22491

Preprints available from: lubomir.benco@univie.ac.at

Superconductivity in lithium, potassium and aluminium under extreme pressure: A first-principles study

G. Profeta¹, C. Franchini², N.N Lathiotakis³, A. Floris^{3,2}, A. Sanna²,
M.A.L. Marques³, M. Lüders⁴, S. Massidda², E.K.U Gross³ and A. Continenza¹

¹ *CASTI - INFM and Dipartimento di Fisica, Università dell'Aquila,
I-67010 Coppito (L'Aquila) Italy*

² *SLACS INFM and Dipartimento di Scienze Fisiche, Università di Cagliari,
S.P. Monserrato-Sestu km 0.700, I-09124 Monserrato (Cagliari), Italy*

³ *Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14,
D-14195 Berlin, Germany*

⁴ *Daresbury Laboratory, Warrington WA4 4AD, United Kingdom*

Abstract

Extreme pressure strongly affects the superconducting properties of “simple” elemental metals, like Li, K and Al. Pressure induces superconductivity in Li (as high as 17 K), while suppressing it in Al. We report first-principles investigations of the superconducting properties of dense Li, K and Al based on a recently proposed, parameter-free, method. Our results show an unprecedented agreement with experiments, assess the predictive power of the method over a wide range of densities and electron-phonon couplings, and provide predictions for K, where no experiments exist so far. More importantly, our results help uncovering the physics of the different behaviors of Li and Al in terms of phonon softening and Fermi surface nesting in Li.

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Contact person: gianni.profeta@aquila.infn.it

Ab-initio prediction of pressure induced superconductivity in potassium

A. Sanna¹, C. Franchini^{1,2}, A. Floris^{1,3}, G. Profeta⁴, N.N. Lathiotakis³,
M. Lüders⁵, M. A. L. Marques³, E. K. U. Gross³, A. Continenza⁴, and S. Massidda¹

¹ *SLACS-INFN/CNR, Sardinian Laboratory for Computational Materials Science,
Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari,
Cittadella Universitaria, I-09124 Monserrato (CA), Italy*

² *Institut für Physikalische Chemie, Universität Wien and
Center for Computational Materials Science,
Liechtensteinstrasse 22A, A-1090 Vienna, Austria*

³ *Institut für Theoretische Physik, Freie Universität Berlin,
Arnimallee 14, D-14195 Berlin, Germany*

⁴ *CASTI-INFN/CNR, and Dipartimento di Fisica,
Università degli studi dell'Aquila, I-67010 Coppito (L'Aquila) Italy*

⁵ *Daresbury Laboratory, Warrington WA4 4AD, United Kingdom*

Abstract

We report first principles calculations of the superconducting properties of *fcc* potassium under high pressure. Using a completely *ab-initio* method we predict a superconducting phase transition at 18 GPa. A maximum critical temperature of about 2 K is observed around 23 GPa, the pressure at which the crossover between the *fcc* phase and the *K III* structure experimentally occurs. At higher pressure, when the *fcc* phase is experimentally unstable, we find, in the phononically stable range, values of T_c up to 11 K. In order to understand the underlying mechanisms inducing superconductivity in potassium, we study the effect of pressure on the electronic and vibrational properties, showing a progressive phonon softening near the *K* point of the Brillouin zone and a concomitant enhancement of the electron-phonon coupling constant λ . Interestingly, we find that the pressure induced *s-d* charge transfer causes an increasing anisotropy of the superconducting gap Δ . Although similar to dense Li in many respects, K displays interesting peculiar features.

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Contact person: antonio.sanna@dsf.unica.it

Weakly dispersive band near the Fermi level of GaMnAs due to Mn interstitials

A. Ernst, L. M. Sandratskii, M. Bouhassoune, J. Henk

Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

M. Lüders

Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

Abstract

The nature of the weakly-dispersive electronic band near the Fermi level observed in photoemission experiments on the diluted magnetic semiconductor GaMnAs is investigated theoretically. The combination of experimental features appears puzzling. We show that the formation of the band is closely related to the presence of the Mn interstitial impurities. The states forming the band have predominantly minority-spin Mn-3*d* character. The low experimental Mn-3*d* intensity is explained by the low content of the interstitial Mn impurities. The features of the band are robust with respect to the calculational technique (LDA, LDA+U).

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Contact person: aernst@mpi-halle.de

8 SCIENTIFIC HIGHLIGHT OF THE MONTH: "ONETEP: linear-scaling density-functional theory with plane waves"

ONETEP: linear-scaling density-functional theory with plane waves

Peter D. Haynes¹, Chris-Kriton Skylaris², Arash A. Mostofi³ and Mike C. Payne¹

¹*Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, U.K.*

²*Physical and Theoretical Chemistry Laboratory, University of Oxford, U.K.*

³*Department of Materials Science and Engineering, Massachusetts Institute of Technology, U.S.A.*

Abstract

An overview of the ONETEP (Order- N Electronic Total Energy Package) code is presented, focusing on the twin aims of overall linear scaling and controlled accuracy. The method is outlined, including a description of the density-matrix formulation of density-functional theory, and the optimisation procedures for both the density-kernel and the local orbitals or non-orthogonal generalised Wannier functions. Results of applying the method to a variety of systems are presented to demonstrate the accomplishment of the original aims.

1 Introduction

Density-functional theory (DFT) [1, 2] has made a unique impact [3] on science, well beyond the traditional realms of quantum-mechanical simulations into disciplines such as microelectronics [4], biochemistry [5] and geology [6]. This broad multidisciplinary appeal has its origin in the ability of DFT to provide a sufficiently accurate description of electron correlation for many purposes at a computational cost which scales favourably (as the cube of the system size N) compared with correlated wave function methods (which typically exhibit N^5 to N^7 scaling).

The origin of the N^3 asymptotic scaling of DFT can be understood with reference to Fig. 1, which shows one of the solutions $\psi_n(\mathbf{r})$ to the single-particle Kohn-Sham equation

$$\hat{H}_s \psi_n(\mathbf{r}) = \left[-\frac{1}{2} \nabla^2 + V_{\text{eff}}[n](\mathbf{r}) \right] \psi_n(\mathbf{r}) = \varepsilon_n \psi_n(\mathbf{r}). \quad (1)$$

In addition to the potential due to the ion cores, the effective potential $V_{\text{eff}}[n](\mathbf{r})$ describes electron-electron interactions in a mean field manner (via the electron density $n(\mathbf{r})$). As a result, Eq. 1 must be solved self-consistently along with

$$n(\mathbf{r}) = 2 \sum_n f_n |\psi_n(\mathbf{r})|^2, \quad (2)$$

where the occupation numbers $\{f_n\}$ are unity (zero) for states below (above) the chemical potential at absolute zero and the factor of two accounts for spin degeneracy. For small basis sets, Eq. 1 may be solved by direct matrix diagonalisation which scales as N^3 . For large-scale simulations or large basis sets (not least the plane-wave pseudopotential method [7,8], the leading workhorse for DFT calculations) iterative methods [9] are more efficient. In this case, the orthonormality of the Kohn-Sham orbitals $\{\psi_n(\mathbf{r})\}$ must be imposed directly:

$$\int d^3r \psi_m^*(\mathbf{r})\psi_n(\mathbf{r}) = \delta_{mn}. \quad (3)$$

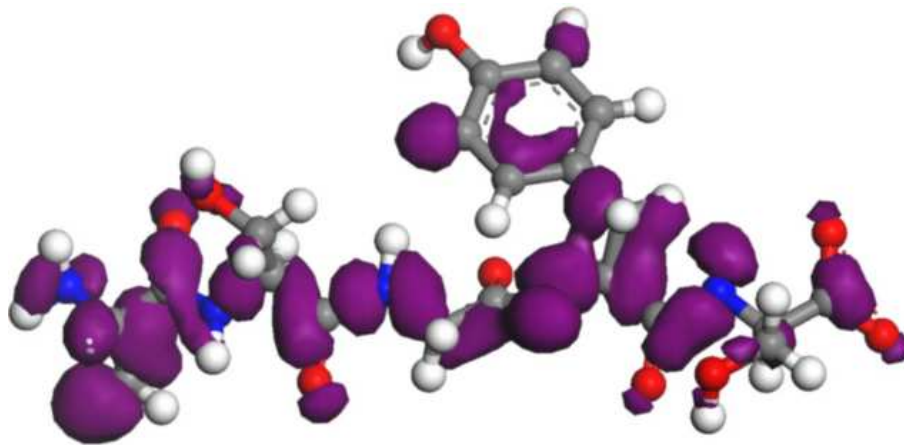


Figure 1: A Kohn-Sham orbital for an oligopeptide molecule: in general, each orbital extends over the entire system.

The number of orbital pairs and thus the number of constraints (3) is proportional to N^2 . As illustrated in Fig. 1, each Kohn-Sham orbital extends over the entire system so that the overlap integral in (3) requires a computational effort which scales linearly with N (in the same manner as the volume of the system increases). Thus the total cost of enforcing the orthonormality constraints scales as N^3 .

While relatively benign compared to other methods, this N^3 scaling still presents a bottleneck which restricts the size of simulations to a few hundred atoms, even with the most powerful supercomputers. In recent years there has therefore been considerable interest in the development of linear-scaling or order- N methods (see the review articles [10,11] and references therein). These offer the potential to revolutionise the scope and scale of first-principles simulations based on DFT to include entire biological molecules and nanostructures containing many thousands of atoms.

While many different computational schemes have been proposed, this article focuses on one more recent method which has been implemented in the ONETEP code [12,13]. The twofold aim of this work has been to develop a general purpose scheme which exhibits true linear scaling and controlled accuracy.

In all proposed order- N schemes the computational effort associated with the dominant part of the calculation (e.g. evaluation of the Hamiltonian matrix elements or application of the Hamiltonian to a trial vector) scales linearly with system-size. However this does not guarantee that the total calculation time will scale so well. For example, while the time for a single self-consistent iteration may scale linearly, various forms of ill-conditioning [14] can cause the number of iterations required to reach convergence to increase with system-size. The aim of true linear scaling thus requires that the total effort to calculate the desired physical properties of a system should scale linearly.

In order to obtain any linear-scaling method, it is necessary to make further approximations that exploit the “nearsightedness” [15, 16] of quantum many-particle systems, in addition to those common to all DFT methods (exchange-correlation functional, finite basis set, discrete Brillouin zone sampling and choice of pseudopotential if appropriate). Pursuing Kohn’s analogy of myopia, this involves deliberately impairing the vision of the simulated quantum system so that the local density is blind to distant perturbations in the potential. As the range of sight is decreased, the calculation will become cheaper, but with a consequent loss of accuracy. Therefore this approximation must be controlled to reduce any error to an acceptable level if the results are to be used with confidence.

The accuracy of a calculation is heavily influenced by the choice of basis set. Linear-scaling methods can be divided into two categories: those which use relatively small basis sets of atomic-like orbitals such as numerical atomic orbitals [17–21], Slater type orbitals [22], localised spherical waves [23], or Gaussian type orbitals [24, 25]; and those which use larger sets of simpler functions such as B-splines or blip functions [26], finite elements [27], or methods based on finite-difference [28] and multigrid [29] techniques. To satisfy the requirement for controlled accuracy, it is necessary to choose a basis set which may be improved systematically, ideally via a single parameter, and which spans the range from minimal atomic sets to plane-wave accuracy.

In Sec. 2 an overview of the ONETEP linear-scaling method is given, and in Sec. 3 an assessment is made of representative results for a variety of systems in the light of the above aims.

2 Overview of the ONETEP method

2.1 Density-matrix formulation

The set of Kohn-Sham orbitals $\{\psi_n(\mathbf{r})\}$ provides a complete description of the fictitious system of non-interacting particles in DFT. An equivalent description may also be given by the single-particle density-matrix $\rho(\mathbf{r}, \mathbf{r}')$,

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_n f_n \psi_n^*(\mathbf{r}) \psi_n(\mathbf{r}'), \quad (4)$$

which possesses the property of idempotency, namely

$$\rho^2(\mathbf{r}, \mathbf{r}') = \int d^3r'' \rho(\mathbf{r}, \mathbf{r}'') \rho(\mathbf{r}'', \mathbf{r}') = \rho(\mathbf{r}, \mathbf{r}'), \quad (5)$$

which requires the orthonormality of the orbitals $\{\psi_n(\mathbf{r})\}$ according to Eq. 3 and the *Aufbau* principle of singly occupying all states up to the chemical potential, which itself follows straightforwardly from the Pauli exclusion principle. The density-matrix is thus the position representation of the projection operator onto the space of occupied states $\hat{\rho}$.

The density $n(\mathbf{r})$ may be obtained from the diagonal elements of the density-matrix,

$$n(\mathbf{r}) = 2\rho(\mathbf{r}, \mathbf{r}), \quad (6)$$

where the factor of two again accounts for spin degeneracy (assuming no spin polarisation). The total energy of the non-interacting system E_s may be obtained via

$$E_s = 2 \text{Tr}(\hat{\rho}\hat{H}_s) \quad (7)$$

and thus the energy of the real interacting system calculated by applying the usual double-counting corrections to the Hartree and exchange-correlation terms. The solution to Eq. 1 may therefore be found by minimising the energy with respect to the density-matrix, subject to the constraints of idempotency (5) and normalisation,

$$2 \int d^3r \rho(\mathbf{r}, \mathbf{r}) = N_e, \quad (8)$$

i.e. the density-matrix corresponds to a system of N_e electrons.

Since the number of occupied states is directly proportional to N and each state extends over the whole system (Fig. 1), the amount of information in the density-matrix defined by Eq. 4 therefore scales as N^2 . Any calculation involving manipulation of this density-matrix will therefore scale quadratically with system-size at best. In order to obtain a linear-scaling method, it is necessary to exploit the nearsightedness of many-body quantum mechanics [15] mentioned above.

Both analytical [30, 31] and numerical [32] studies have demonstrated that, for an insulating system, both the Wannier functions and density-matrix decay exponentially, so that

$$\rho(\mathbf{r}, \mathbf{r}') \sim \exp(-\gamma |\mathbf{r} - \mathbf{r}'|) \rightarrow 0 \text{ as } |\mathbf{r} - \mathbf{r}'| \rightarrow \infty. \quad (9)$$

This means that for any given position \mathbf{r} the density-matrix $\rho(\mathbf{r}, \mathbf{r}')$ differs significantly from zero only for points \mathbf{r}' within a finite volume around \mathbf{r} . Since the decay rate γ depends only on the energy gap between the highest occupied and lowest unoccupied states, this volume is independent of system-size. Thus the total amount of significant information in the density-matrix only scales linearly with N .

In practice this is exploited by writing the density-matrix in separable form:

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_{\alpha\beta} \phi_\alpha(\mathbf{r}) K^{\alpha\beta} \phi_\beta^*(\mathbf{r}'), \quad (10)$$

where the $\{\phi_\alpha(\mathbf{r})\}$, illustrated in Fig. 2, are a set of spatially localised non-orthogonal functions which span a superspace of the Hilbert space of the set of occupied Kohn-Sham orbitals

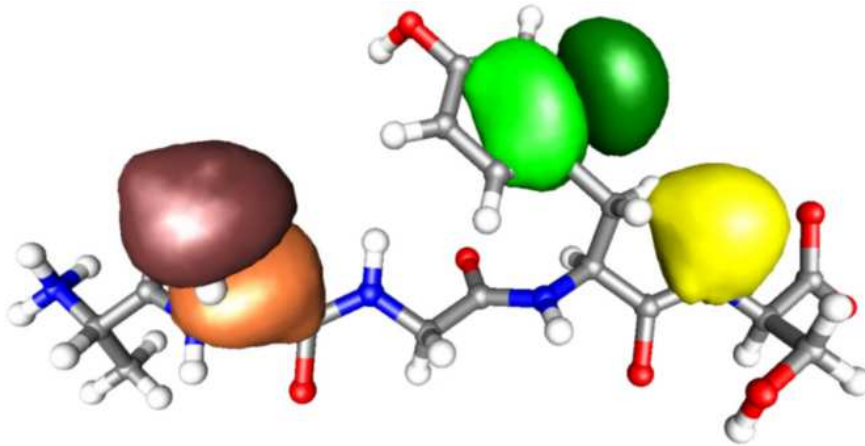


Figure 2: Three localised orbitals (non-orthogonal generalised Wannier functions) generated by ONETEP for the same oligopeptide molecule as Fig. 1.

$\{\psi_n(\mathbf{r}); \varepsilon_n < \mu\}$ and have been called support functions [33] or non-orthogonal generalised Wannier functions (NGWFs) [34] in this work. The matrix $K^{\alpha\beta}$, known as the density-kernel [35] is in fact the representation of the density-matrix in the set of duals of the NGWFs $\{\phi^\alpha(\mathbf{r})\}$ defined by

$$\langle \phi_\beta | \phi^\alpha \rangle = \int d^3r \phi_\beta^*(\mathbf{r}) \phi^\alpha(\mathbf{r}) = \delta_\beta^\alpha. \quad (11)$$

The total amount of information contained in the density-matrix defined by Eq. 10 must of course still scale as N^2 . However the advantage of this form is that it allows the nearsightedness to be exploited with the use of spatial cut-offs.

First, the NGWFs which are exponentially localised are truncated, by allowing them to be non-vanishing only in spherical regions of fixed radii $\{r_\alpha\}$ and centred at positions $\{\mathbf{R}_\alpha\}$. In ONETEP, a number of NGWFs are associated with each atom in the system, so that the regions are centred on atoms and their radii essentially depend only on the atomic species.

Second, the density-kernel is required to be a sparse matrix, by discarding elements $K^{\alpha\beta}$ corresponding to NGWFs centred further apart than some cut-off r_K . Note that since the density-kernel is related directly to the duals of the NGWFs, rather than the NGWFs themselves, the density-kernel cut-off r_K is not simply the sum of the radii $r_\alpha + r_\beta$. This is a consequence of the non-orthogonality of the NGWFs.

The approach adopted in ONETEP of truncating the NGWFs and predetermining the sparsity pattern of the density-kernel contrasts with approaches based on thresholding [36] which are common in methods based on Gaussian basis sets. The former approach has the advantage that the overlap matrix for NGWFs remains strictly positive definite, whereas the latter approach is more flexible and hence potentially more efficient.

Imposing spatial cut-offs on the NGWFs and the density-kernel results in a density-matrix whose information content scales linearly with system-size, an approximation which is controlled by adjusting the $\{r_\alpha\}$ and r_K . In practice, these cut-offs are increased until the desired physical

properties of the system converge.

2.2 Density-kernel optimisation

Most linear-scaling methods fall into two categories, typically along the same lines as the basis set division above. The first is equivalent to optimising the density-kernel only [22, 37–39] for a fixed, but potentially large, set of local orbitals and the second involves both density-kernel and NGWF optimisation [26, 34, 40]. These two approaches are further compared in the next section, while this section concerns the common point of density-kernel optimisation.

Functionally at least, this stage of the calculation proceeds along the lines of an *ab initio* tight-binding [41] calculation and linear-scaling methods for tight-binding [42] may be applicable. While self-consistency may be treated independently of density-kernel and NGWF optimisation [43], the approach in ONETEP is closely related to the ensemble DFT method for metallic systems [44] and performs both density-kernel and NGWF optimisation self-consistently.

To impose the idempotency constraint a combination of two methods is used: a penalty-functional method [45] and the method of Li, Nunes and Vanderbilt [47], and independently Daw [48], based on McWeeny’s purification transformation [35]. The latter has been implemented in both its original non-orthogonal formulation [49] and the Millam and Scuseria variant [50].

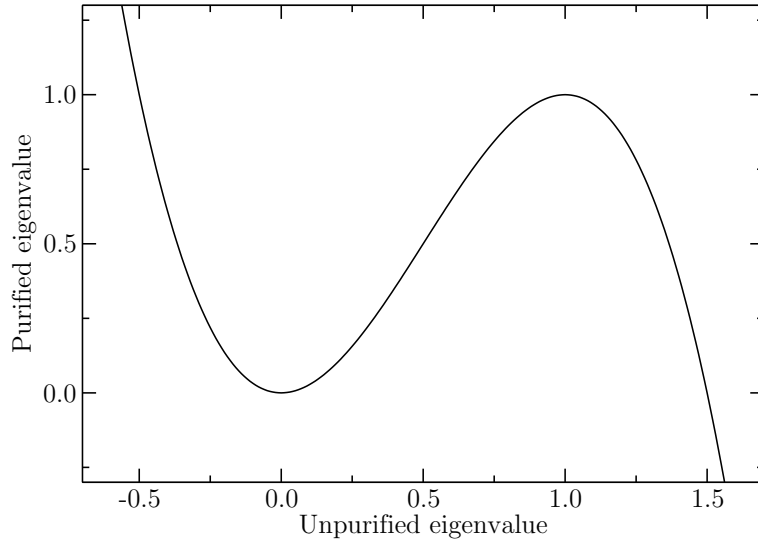


Figure 3: The purification transformation illustrated in terms of its effect on the density-matrix eigenvalues (occupation numbers).

The purification transformation may be defined in terms of an auxiliary matrix $\sigma(\mathbf{r}, \mathbf{r}')$ by:

$$\rho(\mathbf{r}, \mathbf{r}') = 3\sigma^2(\mathbf{r}, \mathbf{r}') - 2\sigma^3(\mathbf{r}, \mathbf{r}'). \quad (12)$$

Clearly $\rho(\mathbf{r}, \mathbf{r}')$ and $\sigma(\mathbf{r}, \mathbf{r}')$ commute and so the transformation is best illustrated as in Fig. 3 in terms of their eigenvalues, which for $\rho(\mathbf{r}, \mathbf{r}')$ are the occupation numbers $\{f_n\}$ of Eq. 4. Under repeated iteration of this transformation, eigenvalues around zero vanish quadratically

and those close to unity converge to the maximum there. Expressing the density-matrix in this way and optimising the auxiliary matrix thus applies the constraint of idempotency, so long as the occupation numbers remain in the interval $\left[\frac{1-\sqrt{5}}{2}, \frac{1+\sqrt{5}}{2}\right]$ where the transformation is stable. Should the calculation become unstable (generally at the start of a calculation) then the globally convergent penalty-functional method is used instead.

The purification transformation may also be derived as the result of a steepest descents minimisation of the positive definite functional $P[\rho]$ given by

$$P[\rho] = \int \int d^3r d^3r' [\rho^2(\mathbf{r}, \mathbf{r}') - \rho(\mathbf{r}, \mathbf{r}')] [\rho^2(\mathbf{r}', \mathbf{r}) - \rho(\mathbf{r}', \mathbf{r})], \quad (13)$$

which gives a quantitative measure of the departure of $\rho(\mathbf{r}, \mathbf{r}')$ from idempotency (for nearly-idempotent density-matrices it is proportional to the mean square deviation of the occupation numbers from zero or unity). $P[\rho]$ may thus be used as a penalty functional, some proportion of which is added to the energy functional to enforce idempotency [45].

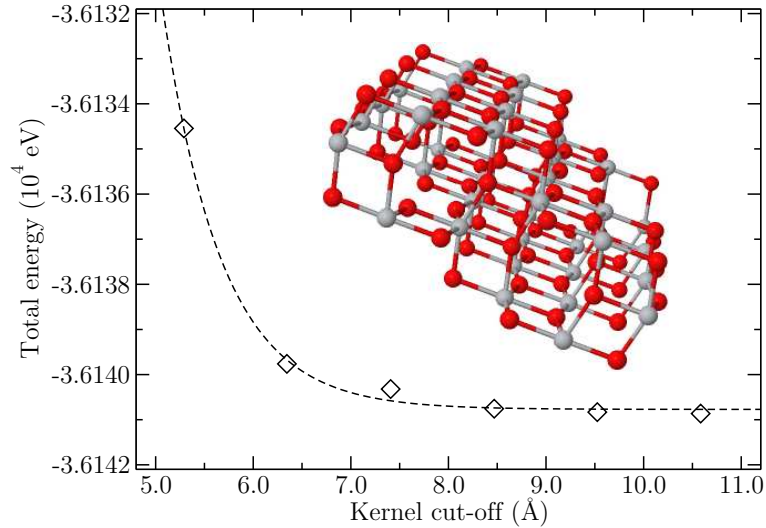


Figure 4: Total energy convergence with respect to density-kernel cut-off r_K for a $\text{Ti}_{38}\text{O}_{76}$ cluster [46].

Figure 4 shows a particular example of how the total energy varies as the density-kernel cut-off r_K is increased, and this behaviour is qualitatively similar to that observed in all insulating systems. Physical properties based on energy differences converge even more rapidly with r_K . For example, in crystalline silicon the errors from truncating the density-kernel to $r_K = 10 \text{ \AA}$ are 0.3% and 0.1% in the lattice parameter and bulk modulus respectively [13].

2.3 NGWF optimisation

Linear-scaling methods which use a fixed set of local orbitals generally use atomic-type functions, typically solutions to the Schrödinger equation for isolated atoms, possibly immersed in a confining potential. The smallest minimal orbital sets allow calculations which are quick but relatively inaccurate. To improve their accuracy, the size of the orbital set is increased, gen-

erating split valence or multiple-zeta sets, with optional polarisation functions to describe the response of the atom to an applied electric field.

The second approach, which is the one adopted in ONETEP, instead optimises these local orbitals in the environment of the system being studied, to generate NGWFs. Thus it is no longer necessary to increase the size of the orbital set to improve transferability. While extra computational effort is required to perform this optimisation, some saving is obtained since the orbital set used is of minimal size, while high accuracy is maintained.

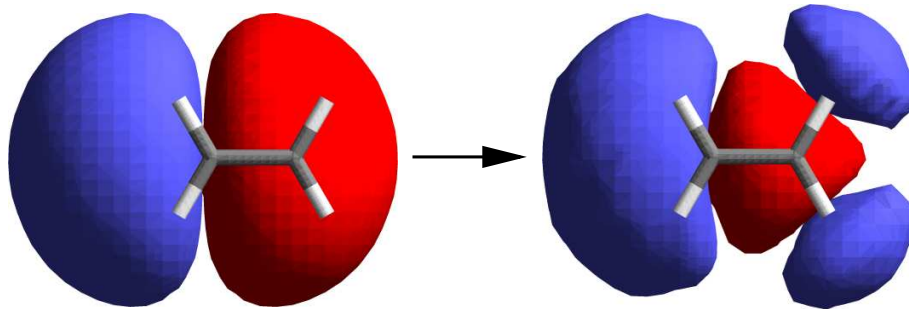


Figure 5: A single NGWF centred on one carbon atom of an ethene molecule before (left) and after (right) optimisation in ONETEP.

Figure 5 illustrates this optimisation for the case of a single orbital centred on the left-hand carbon atom in an ethene molecule. The orbital is initialised to a truncated p_x atomic orbital. After the orbital has been adapted *in situ* to generate the NGWF on the right-hand side of the figure, it is clear that the NGWF now reflects the molecular environment.

In order to perform this optimisation, it is necessary to expand the NGWFs in some underlying basis set of primitive functions. In ONETEP, these are chosen to be periodic cardinal sine (psinc) functions [34, 51], also known as Dirichlet or Fourier Lagrange functions [52, 53]. One such function is illustrated in Fig. 6, and there is one function centred on each grid point of a regular mesh commensurate with the simulation cell.

Since the psinc functions are related to plane-waves by Fourier transform, they enable the kinetic energy to be calculated accurately and efficiently [54, 55] using fast Fourier transforms (FFTs). They are also orthogonal by construction and highly localised, being non-zero at only one grid point (although they do oscillate between grid points). The basis set quality may also be controlled by a single energy cut-off parameter, related to that used for plane-wave basis sets [13]. Thus in ONETEP it is possible to vary the accuracy from that of a minimal atomic-type basis (by performing no NGWF optimisation) to full plane-wave accuracy.

The scheme as described so far involves expanding each NGWF in terms of the psinc basis functions whose centres lie within the truncation volume of that NGWF. This is a small subset of the total psinc basis set, as illustrated schematically in Fig. 7. However the FFTs required to calculate the kinetic energy remain global operations, so that the time to calculate the kinetic energy of a single NGWF scales as $O(N \log N)$, giving an overall scaling higher than N^2 .

To overcome this problem the FFT box technique has been introduced [54], which is illustrated in Fig. 8. A smaller FFT box is associated with each NGWF, which is centred on that NGWF.

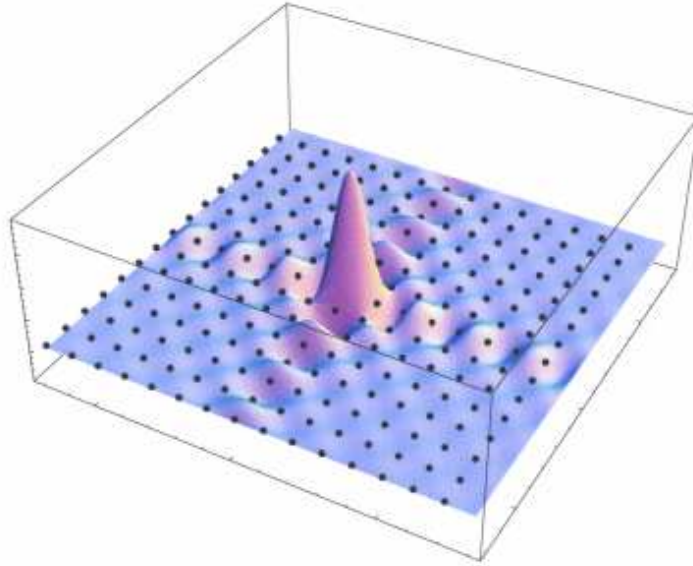


Figure 6: A psinc basis function used to expand the NGWFs in ONETEP.

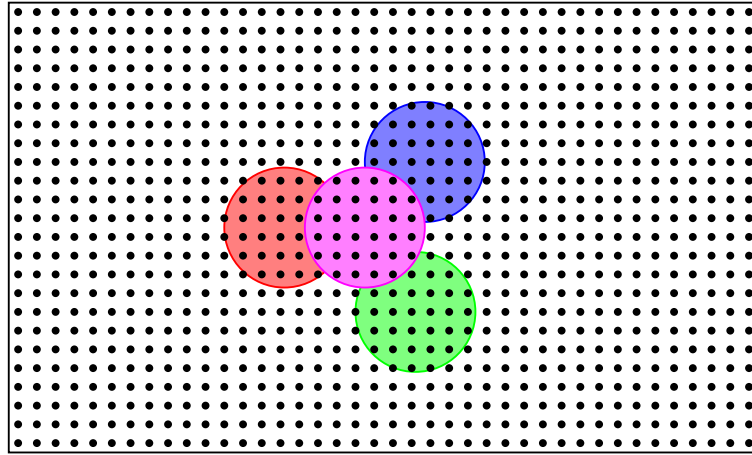


Figure 7: The regular psinc grid covering the whole simulation cell.

The FFT boxes for all NGWFs are of a universal shape and size, and are chosen to be sufficiently large to include the central NGWF and all of its overlapping neighbours. This guarantees the consistent action of operators and the hermiticity of the calculated Hamiltonian.

A psinc basis set may be defined for each FFT box, and each NGWF is now expanded in those functions centred in its truncation volume. In effect, the periodicity of the NGWFs is altered, but since the NGWFs are localised within volumes smaller than the FFT box, this is a very good approximation. Equivalently, since the NGWFs are localised in real-space, their Fourier transforms are broad in reciprocal-space and thus the coarser sampling in reciprocal-space provided by the FFT box compared to the cell remains adequate. The volume of the FFT box is independent of system-size, depending only upon the cut-off radii of the NGWFs, and so the computational effort of an FFT within the FFT box does not increase as the system becomes larger, and linear scaling is recovered.

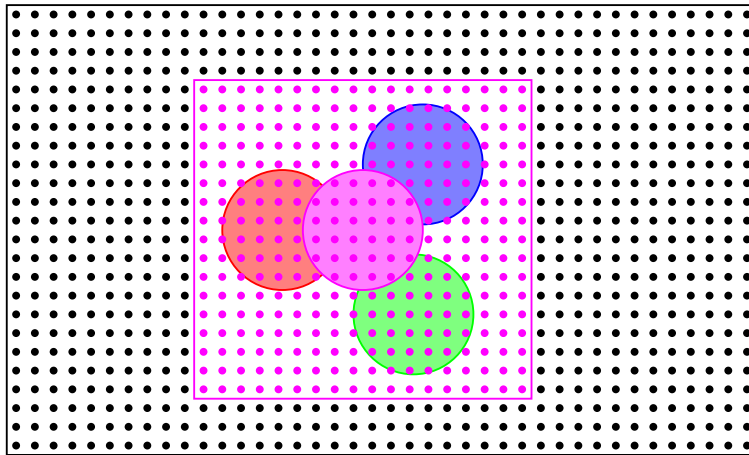


Figure 8: Illustration of the FFT box technique used in ONETEP.

In ONETEP the FFT box is used not only to calculate the kinetic energy, but also to interpolate the NGWFs before the calculation of the density (to avoid aliasing) and to evaluate every term in the Hamiltonian [56].

The FFT box also allows an estimate of the cross-over (the point at which a linear-scaling method is more efficient than traditional cubic-scaling methods). Comparing ONETEP to a traditional plane-wave pseudopotential code shows that both methods spend considerable time performing FFTs. For the traditional code these are performed over the entire simulation cell. In the case of ONETEP, fine grid FFTs in the FFT box dominate the computational effort. Since both methods perform similar numbers of FFTs, the cross-over is expected to occur when the FFT grids are about the same size i.e. the volume of the FFT box and the simulation cell are comparable. The number of atoms that this corresponds to depends upon the nature of the system. ONETEP has a particular advantage for low-dimensional structures such as molecules, polymers, nanotubes and surfaces, since regions of vacuum can be included essentially for free [12]. For solids, the cross-over will be rather higher in the number of atoms.

3 Results and assessment

The ONETEP method has been parallelised, and results are available elsewhere [12, 57]. By construction, the cost of a single self-consistent iteration in the determination of the ground state scales linearly with system-size. However, as pointed out in Sec. 1, this is not sufficient to guarantee that the calculation of physical properties scales linearly with system-size, since the number of iterations required has been observed to increase in some methods.

Figure 9 shows the convergence of the ONETEP method with respect to iterations of the NGWF optimisation procedure. A wide variety of systems with different properties have been chosen: a supercell of crystalline silicon, a hydrogen-bonded formaldehyde-water complex, a (20,0) carbon nanotube, a protein complex and a supercell of the zeolite ZSM5. Both the gain in total energy and the length of the residual vector are plotted. In all cases, the convergence criteria are satisfied within 10-20 iterations, independently of the number of atoms in the system. Thus

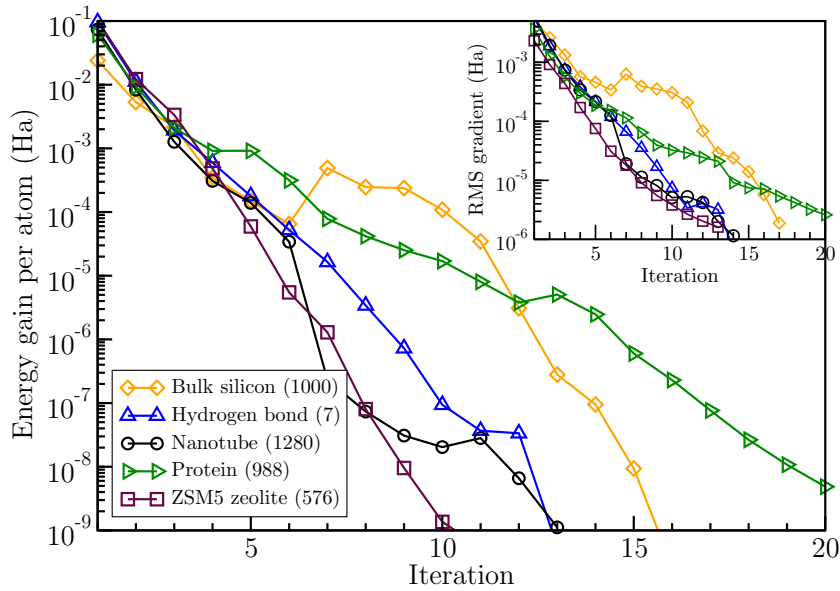


Figure 9: Energy (inset RMS gradient) convergence of the NGWF optimisation for a variety of systems – figures in parentheses in legend indicate number of atoms.

in ONETEP, the total calculation time, not just the time per iteration, scales linearly with system-size. This is believed to result from the choice of an orthogonal basis set and the careful and consistent treatment of all terms in the energy.

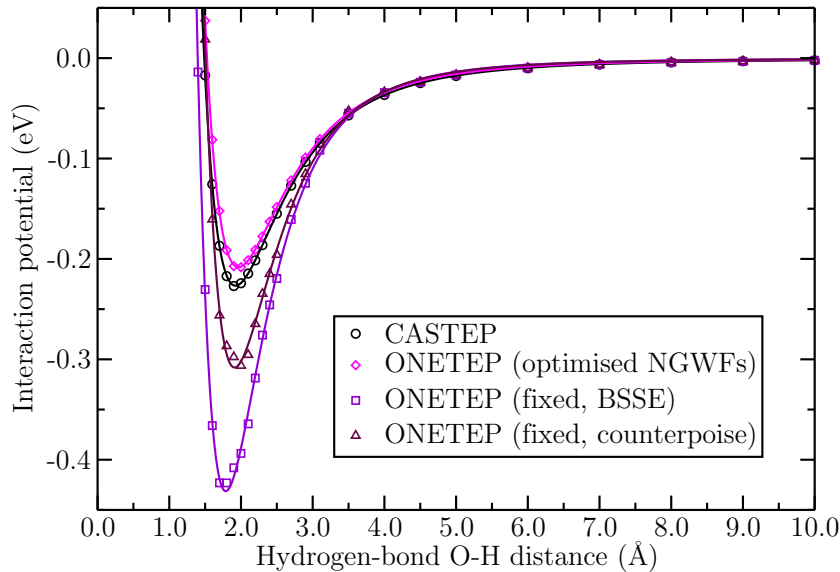


Figure 10: Interaction potentials (negated binding energies) for a hydrogen-bonded water dimer.

The accuracy of ONETEP calculations has been compared with traditional plane-wave pseudopotential and all-electron methods elsewhere [13]. Figure 10 shows the interaction potential for a hydrogen-bonded water dimer as calculated by the CASTEP [58] code and by ONETEP using the same pseudopotential, gradient-corrected exchange-correlation functional [59] and equivalent energy cut-offs for the basis sets [60]. In two of the ONETEP calculations, only the density-

kernel has been optimised, the NGWFs have been fixed as a minimal set of atomic-type orbitals. This calculation exhibits basis set superposition error (BSSE) [61] for which in this system the counterpoise correction [62] is only partially successful. While ONETEP is capable of performing calculations at this level, for weakly bound systems such as this one, high accuracy is required. When the NGWFs are optimised in addition to the density-kernel, no BSSE is observed and the agreement is vastly improved. With fully converged basis sets, the equilibrium bond lengths and binding energies obtained by ONETEP and CASTEP agree to 0.3% and 2% respectively. Together with the results presented in Fig. 4, it can be seen that the accuracy of calculations in ONETEP can be controlled, and that plane-wave accuracy can be achieved routinely. The twin aims of overall linear scaling and controlled accuracy have thus been achieved.

Acknowledgments

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