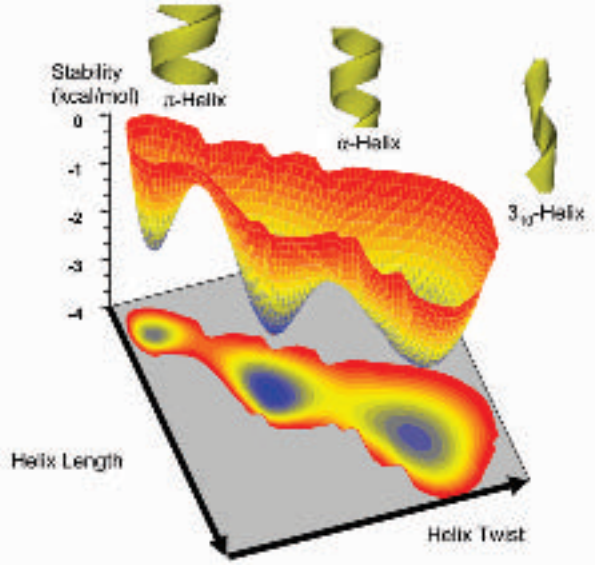
Towards Atomistic Materials Design (Psi-k)

An ESF scientific programme



This programme concerns the rapidly developing field of computer simulation and focuses on the understanding of real materials and the design of new materials with improved properties and functionalities. The calculations are referred to as 'ab initio' or 'first principles' calculations because they use no adjustable parameters to solve the basic equation of quantum mechanics: the Schrödinger equation for the interacting electron system in a solid. These calculations can be applied to all condensed matter systems, ranging from metals and semiconductors to nanostructures, materials in the Earth's core or biological systems such as proteins.

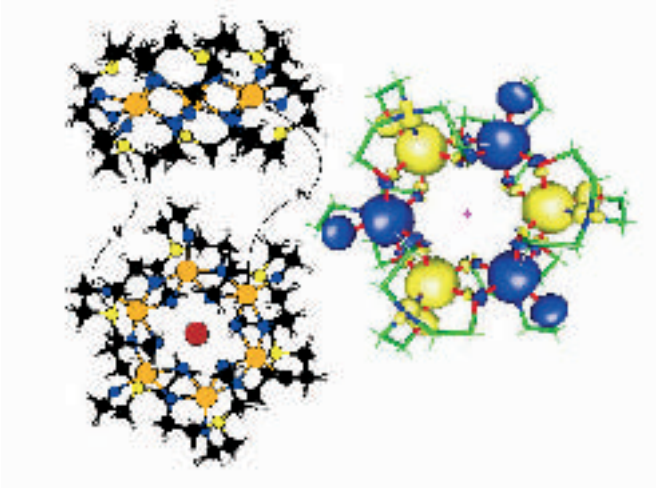
Psi-k aspires to encompass the whole ab-initio community of Europe, which, as a rough estimate, consists of about 2000 scientists, including PhD and master students. At present, Europe is the world's leader in the field, ahead of the US and Japan.

The programme is organised around 15 topical working groups. In order to deal with the sophisticated methodology, the rapid growth in applications and to train young researchers in the field, the programme organises each year approximately 17 workshops, hands-on computer courses and summer schools.

The European Science Foundation acts as a catalyst for the development of science by bringing together leading scientists and funding agencies to debate, plan and implement pan-European initiatives.

Introduction

It is now well established that on the nanoscale, i.e. on the scale of an individual atom, all physical properties are governed by the laws of quantum mechanics, which replace the classical mechanics valid for macroscopic systems. The quantum mechanical equations are not only important for atomistic problems, but also determine the macroscopic behaviour of materials such as the elastic, dielectric or optical properties. It is only recently that the extremely complicated equations involving a sufficiently large number of atoms can be solved on powerful computers, so that important properties can be calculated ab initio from the underlying laws of quantum mechanics without adjustable parameters. Naturally, this has revolutionised electronic structure research since laboratory experiments cannot easily 'see' or manipulate individual atoms. Theory is now able to supplement and, in certain cases, even replace traditional experiments. Therefore the field of ab initio calculations is rapidly expanding and applied to a large spectrum of problems in condensed matter physics, chemistry, material science and even biology, is a spectrum which is continuously broadening. The foundation of this field was laid by Walter Kohn, for which he was awarded the 1998 Nobel Prize in Chemistry.



The structure (left) and spin density distribution (right) of a molecular magnet, i.e. a «ferric wheel» molecule with six Fe atoms. The right figure illustrates the antiferromagnetic coupling of the Fe-moments (Andrei V. Postnikov, Jens Kortus and Mark R. Pederson, Ψ_k-Newsletter 61, p. 151 (2004)).

Today Europe is the world leader in this field, ahead of the USA and Japan. However, the research in Europe is more fragmented than in those countries and in need of a long-term networking infrastructure to foster better communications and cooperations. Such networking is not only required by researchers at isolated locations, often in smaller countries, but also by the large research centres, to maintain world leadership. This important task is the aim of the present ESF Psi-k Programme, which serves the whole European ab initio community in condensed matter.

The activities of Psi-k include:

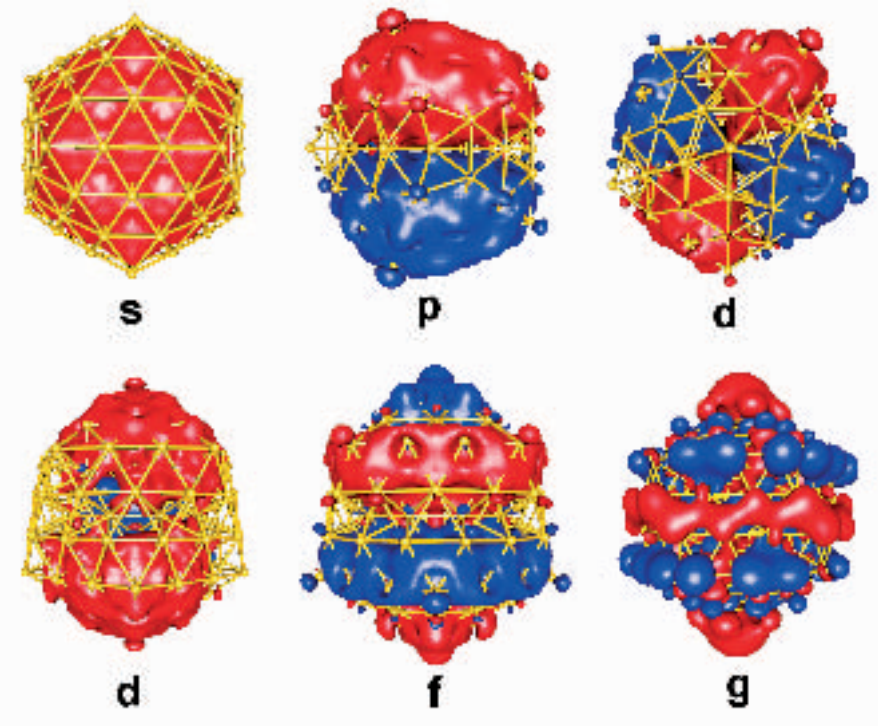
- a bi-monthly electronic newsletter
- approximately 15 topical workshops per year
- on average 3 summer schools or computer tutorials per year
- an international conference (Psi-k 2005) every four to five years
- short visits for in depth consultations and secondments.

Research field

The research field originates from the density functional theory development postulated by Walter Kohn in 1964-65. However, it took more than ten years before the importance of this theory and its tremendous potential for materials-specific research was fully realised. It soon became clear that the accuracy of the solutions of the so-called 'Kohn-Sham' equations would be of great relevance to both research and applications.

In the past, a large part of atomistic calculations was done with empirical models, using pair-wise interaction potentials between atoms or by simulating the bonding of the electrons by glue-models or so-called 'embedded atom potentials'. While these approaches have many advantages, the potentials contain many parameters which are fitted to experimental data. Thus, only the solution of the quantum mechanical Schrödinger equation, describing electrons moving in the field of the nuclei, can overcome this problem, allowing calculations where the nuclear charge characterising the individual atoms is, at least in principle, the only input parameter.

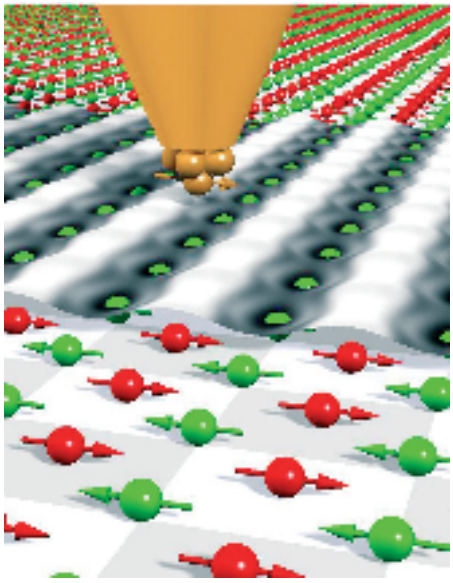
The last two decades have witnessed an enormous progress in the development of density functional theory-based calculations. This was partly because of the availability of faster and cheaper computers, in particular the introduction of fast workstations and PCs. To an even larger extent the progress was achieved by new calculational concepts and strategies, which strongly increased the



The figure shows the one-electron eigenstates of an 147-atom Au cluster, which can be characterized by the angular momentum symmetries of the cluster (Courtesy of Young-Loo Lee, Helsinki University of Technology).

number of atoms that can be handled. At present the activities of the network cover a broad range of problems in condensed matter physics, chemistry and material science.

One can identify two new trends in our work that have become increasingly prominent in the last years and which will characterise our activities in the foreseeable future. One is to apply our methods to *new materials*, such as *biological systems* and *nanostructures* where a real understanding of the atomistic properties can be provided only by the solution of the quantum mechanical Schrödinger equation. For example, the study of *transport* in nanostructures, of relevance for information technology, necessitates a realistic description – by the ab initio methods – of tunnel junctions, molecular systems and nanotubes. The second important trend is the development of ab initio methods for systems with *strong electron-electron correlations*. The experience with density functional theory calculations has exposed serious shortcomings of the 'local density approximation' in systems where the motion of the electrons is strongly correlated. Three of our working groups are addressing this problem. Thus, at present, the Psi-k Programme is expanding its research both in width and depth.

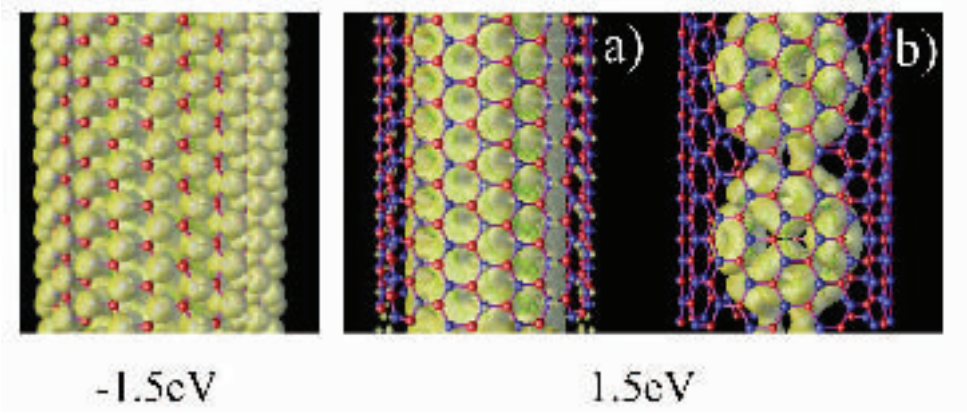


The constant current *spin-polarized scanning tunnelling microscopy* of an antiferromagnetic Mn monolayer on a W(110) surface. Using a magnetic tip one can measure a spin polarized STM image (see calculated height profile) showing one kind of Mn-atoms (red) as hills and the other one (green) as valleys, i.e. a direct image of the anti-ferromagnetic structure (Courtesy of Stefan Heinze and Stefan Blügel; Science 288, 1805 (2000)).

European dimension

The traditional fragmentation of Europe is one of the biggest problems for European research. As an umbrella network, the ESF Psi-k Programme tries to embody all European activities in electronic structure calculations. Because of the increasing importance of ab initio calculations we estimate that at present about 2 000 scientists, including PhD and master's students, work in Europe in this field.

Historically, the present activities started in the 1980s in Trieste with the workshop series entitled Total Energies and Forces. The year 1993 marked the start of an



Constant current mode STM image for an applied bias of +/- 1.5eV of a filled Boron-nitride nanotube: either with a C(5,5) tube or with a fullerene inside («peapod» BN(10,10)@C_{60}). Red, blue and green balls denote B, N and C atoms, respectively. It is seen that for negative bias (mapping of occupied states) the STM images show clear protrusions at the N sites with no clear signature of the filling material. Instead for positive bias we see states within the BN-band gap, those are specific signature of the filling of the tube (with either a carbon nanotube (a) or a fullerene (b)). (Courtesy of Angel Rubio, DIPC San Sebastian).

EU-HCM network on ab initio calculations, and with this the introduction of the Psi-k Newsletter. This was succeeded in 1998 by the ESF Programme on Electronic Structure Calculations (STRUC-Ψ_k) and from 2003 the current ESF Programme Towards Atomistic Materials Design (Psi-k). The underlying aim of all these activities was to unify Europe in our field and to make it the international leader. It is fair to say that to a large extent both objectives have been achieved. The two ESF Programmes have been vital in accomplishing this.

The primary objective of the present Programme is to maintain and enhance the lead that Europe still holds by promoting research excellence and encouraging collaborations and the sharing of ideas, expertise and computer codes. Our field is currently in a state of strong growth and there are no signs that this will change in the foreseeable future.

The Programme is structured around 15 topical working groups covering the whole field of ab initio calculations. The working groups as well as individual scientists make proposals for networking activities such as workshops and tutorials which have to be approved by the Steering Committee at its yearly meetings. Some of the working groups also participate in EU-funded research training networks or networks of excellence.

The Programme supports all the training and networking activities of its members. However, what is not provided is financial support for continuity in code development and maintenance, in particular cleaning up the code and making it user-friendly. Yet this is an extremely important activity if we want to disseminate the highly sophisticated codes to the community and in particular to experimental and industrial scientists. Unfortunately it is not sufficiently realised that this is of equal importance as hardware infrastructure.

From 1 April 2004, Peter Dederichs, Research Centre Jülich, became the new chair of the Psi-k Programme. The previous chair, Volker Heine from the University of Cambridge, will duly serve the Programme as vice-chair with special emphasis on funding.

Activities of the Psi-k Programme

Newsletter

Psi-k publishes bi-monthly the fully electronic 'Ψ_k-Newsletter' which is distributed to more than 1 300 e-mail addresses. The newsletter typically has more than 100 pages and has established itself as the primary medium for distributing information about conferences, workshops, training courses, summer schools as well as positions available in the field for postdocs and PhD students. In addition it contains the reports on all ESF (and of related EU Network) workshops in the field. Every issue contains a scientific highlight presenting recent outstanding results in our field.

Workshops

The most important activity of Psi-k is the organisation of topical workshops. This is clearly the most efficient way of transferring information across the network and getting collaborations started. In 2003 and 2004, network members organised in total 28 workshops covering a very broad spectrum of condensed matter physics.

Some of the workshop topics were:

- Nanoelectronics and Spindependent Transport
- Superconductivity and Bogoliubov-de Gennes Equations
- Ab initio Many-Body Theory for Correlated Electron Systems
- First Principles Simulations in Mineral Sciences
- Electronic Excitations in Nanoscience
- Electronic Structure of Light Actinides
- Transport in Molecular Systems
- Ab initio Excitation Theory for Biological Systems
- The Nature of Hydrogen Bonding and Density Functional Theory
- Electronic Structure Simulations of Nanostructures
- Ab initio Design of Structural Materials
- Dilute Magnetic Semiconductors
- Advances in Theory of Nanotubes
- Workshop and School on Time Dependent Density Functional Theory
- Three workshops on KKR, FLAPW and ABINIT methods

Hands-on computer courses and summer schools

As an important vehicle for transferring knowledge and the sophisticated computer codes in our network to young researchers inside and outside our community, Psi-k strongly encourages hands-on courses and summer schools on various topics in the field.

In 2003 and 2004 the following schools and courses were organised:

- Summer school on New Magnetics, Poznan, 15-19 September 2003
- XIII Workshop on Computational Materials Science, Sardinia, 13-18 September 2003
- XIV Workshop on Computational Materials Science, Sardinia, 18-23 September 2004
- Hands-on Course: Continuum Quantum Monte Carlo Method, Trieste, 12-23 January 2004
- Hands-on Workshop: Application of Density-Functional Theory in

Condensed Matter Physics, Surface Physics, Chemistry, Engineering and Biology, Berlin, 21-30 July 2003

- Psi-k-CECAM Tutorial on Linear Scaling of Density Functional Calculations with Local Orbitals, Lyon, 9-13 September 2003

Psi-k 2005 Conference

Following the success of Psi-k 1996 and Psi-k 2000, the network is organising its third international conference Psi-k 2005 in Schwaebisch-Gmuend, Germany, 17-21 September 2005. More than 500 participants have registered. Worldwide, this is the only international conference in the field of ab initio electronic structure calculations.

The newsletter and information on all networking activities is available at the Psi-k website (http://psi-k.dl.ac.uk). Reports of all workshops, tutorial courses, summer schools and scientific highlights are published in the newsletter.

Funding

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For the latest information on this programme consult the *Psi-k* home page:
www.esf.org/psik or
http://psi-k.dl.ac.uk

Cover picture:
Stability of helical confirmations. Under compressive or tensile strain the twist of the polyalanine a-helix is changed leading to thicker or thinner helices with different hydrogen bonding patterns (Courtesy of Joel Ireta, Martin Fuchs and Matthias Scheffler, FHI Berlin).

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