Final Report of ESF-Programme

"Towards Atomistic Materials Design (Psi-k)"

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

1. Executive Summary

The Psi-k Programme concerns the rapidly developing field of computational material science. It focuses on the understanding of real materials and the design of new materials with improved properties and functionalities. The approach rests on the basic equation of quantum mechanics, the Schroedinger equation for the interacting electron system in a solid, without using any adjustable parameters, i.e. is "ab-initio", and 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. All these topics are covered by the 15 working groups of the Programme. Thus we are a rather diffuse community scattered across very different scientific fields, but we all use the same powerful but demanding methodology. It is the complexity of these methods, which keeps us together such that we can exchange information, learn from each other and bring the whole field forward.

Psi-k aspires to encompass the whole ab-initio community of Europe, which, as a rough estimate, consists of more than 2000 scientists, including PhD and master students. Thus the Psi-k Programme is an umbrella network for electronic structure calculations in Europe. It is funded a la carte by 17 (initially 20) European countries. The main objective of Psi-k is the promotion and coordination of collaboration within the European research community by, among others, the following measures which are open to all European researchers in the field: (i) to support workshops and small conferences on specific topics of active research, (ii) to support summer schools, tutorial courses and other training activities for young and new researchers in the field, (iii) to organize large "Psi-k conferences" every 5 years, (iv) to disseminate information about research progress, job opportunities, relevant workshops, conferences etc, via a Newsletter available freely to anyone in the world by electronic means.

To achieve this goal we have organised in 2003-2008 a total of **94 workshops**, hands-on computer courses and summer schools and in addition the large Psi-k 2005 Conference. About **6 000 participants** have attended these meetings. In detail 77 research workshops took place, the topics of which ranged across all fields of our Network: from Nanoelectronics and Spindependent Transport to ab-initio Many-Body Theory and Superconductivity to Excitations in Biological Systems and Hydrogen Bonding, to Simulations of Nanostructures and Mineral Systems, etc. To train the young researchers we have organised in total 19 training activities, i.e. 3 summer schools, 3 Graduate Schools (on a some what lower level) and 13 hands-on computer tutorials to learn about the many outstanding codes developed in our community. The large Psi-k 2005 Conference was extremely successful and attended by 560 participants.

Since the beginning in the 1970s our research field has been continuously growing and will be further growing in the foreseeable future. This growth is fuelled by the continuous progress of computer technology and to an even larger extent by the steady improvements of computer codes and the invention of new conceptional methods. A literature search shows that in the years 1991 to 2007 the number of publications using density functional and related methods increased from 2 000 to 13 000 per year, i.e. by about a factor 6. However many challenges remain: more accurate total energies, reliable excitation energies, application to larger and more complex systems and access to new material properties. More and more these calculations reach the goal of our Network: “Towards Atomistic Materials Design”.

Europe is the world leader in our field, both in terms of number and quality of publications as well as in code development. For instance, of the 13 000 publications published in 2007 about 5 400 are from European authors (as compared to 3 300 from the USA). Thus Europe is ahead and since its existence 15 years ago Psi-k has strongly contributed to this success.

2. Main Objectives and Progress achieved

The main objectives of the Psi-k Programme are: (i) to support the whole European community of researchers in our field by a series of first-class workshops, computer tutorials and summer schools, such that we stay worldwide at the international fore-front of research, (ii) to expand our field through training and collaborations with young researchers, with experimentalists and scientists in industry and to apply it in practically all natural sciences and relevant technological fields.

To achieve this goal, our members have organised in the 5 year period, i.e. 2003-2007, an unmatched series of 87 workshops, tutorials and summer schools in all relevant fields of our science. In addition in the last, unfunded, year 2008 another 7 workshop activities were organized from saved funds, thus in total 94 workshops. Moreover we organised in 2005 the big "Psi-k 2005" Conference, the only international conference on ab-initio calculations, which was attended by 562 participants. In particular this conference has shown, that the European research in our field is outstanding, both in quality and quantity, and that Europe is in fact world-wide leading. To a considerable extent, this great success has been achieved by the Psi-k Programme of the ESF.

We summarize below and in the Appendices all the activities of the Psi-k Programme in the years 2003-2008. Final reports of all these activities are available in the corresponding issues of the Newsletter or on the website, as indicated after the title in the Appendix. If you use Word for Windows, you can follow in the Appendices the links by "clicking". All issues of the Psi-k Newsletter as well as the detailed information about the activities are available on the Psi-k website http://psi-k.dl.ac.uk. In short, we have organised in 2003-2008 a total of 94 workshops, hands-on computer courses and summer schools and in addition one large conference. About 6 000 participants have attended these meetings.

Research Workshops

The organisation of topical research workshops is the most important activity of the Psi-k Programme, since it represents the most efficient way of transferring information and know-how across the Network as well as getting collaborations started. As listed in the Appendices, the number of research workshops organised in the different years are: 2003: 10; 2004: 15; 2005: 8; 2006: 19; 2007: 17 and in 2008: 6. Note that the number of workshops in 2005 was kept low due to the organisation of the big Psi-k 2005 Conference (see below). The topics of the workshops range across all fields of our Network: from Nanoelectronics and Spindependent Transport to ab-initio Many-Body Theory and Superconductivity to Excitations in Biological Systems and Hydrogen Bonding, to Simulations of Nanostructures and Mineral Systems, etc.

Hands-on Computer Courses and Summer Schools

These activities are particular designed for educating and training of young researchers. The computer courses usually run for one week. The mornings are devoted to lectures on back ground theory to make intelligent use of the code, while the afternoon are reserved for practical sessions on using the particular code. In the evening the students can discuss their own research topic with the organisers, e.g. in poster sessions. The participants are mostly Ph.D. students, with some senior researchers, who want to enter a particular field, as well as some experimentalists, who want to perform ab-initio calculations in order to interpret their experimental data.
Summer Schools are intended to review the present state of the art and understanding of a certain field such as e.g. magnetism. An overview about theoretical and experimental methods is given and possible technological applications are discussed. These schools basically aim at last year PhD students and post-doctoral researchers. In addition to theory lectures, contributions from experimental and industrial lecturers play an important role.

Graduate Schools are special training schools for master and beginning PhD students and have a somewhat lower level than summer schools and hands-on tutorials. In 2006 and 2007 we have organized 3 such schools, partly by an EU contract.
As listed in detail in the Appendix the Network organised a total of 13 Hands-on Courses and 3 Summer Schools in the period 2003-2008.

Psi-k 2005 Conference

The third large Psi-k Conference of the Psi-k community took place in Schwäbisch-Gmünd, Germany, during Sept. 17-21, 2005. It is the only international conference on ab-initio calculations and was organised by Risto Nieminen and his group from the Helsinki University of Technology.

More than 560 scientists, representing 33 countries gathered to survey and discuss the latest developments in the field of electronic structure theory and calculations. The program covered a huge selection of topics in condensed-matter and materials research, ranging from new semiconductors to high-temperature superconductors, from magnetism to biomolecules, from surfaces and interfaces to geological and planetary sciences, etc. The programme of the event consisted of four plenary sessions, 34 scientific sessions (running three in parallel) with 93 invited and 124 contributed oral presentations, and two poster sessions with more than 260 contributions. The complete collection of abstracts is available at http://www.fyslab.hut.fi/psik2005/psikbook.pdf.

The number of participants at the big Psi-k Conferences has increased from 316 for the first Psi-k Conference in 1996 to 424 for the second Conference in 2000 to 562 for the third Psi-k Conference, where the last number was unfortunately limited by the hotel capacity in Schwäbisch-Gmünd and in the surrounding small cities. Thus the next conference Psi-k 2010 will take place in Berlin.
(www.fhi-**berlin**.mpg.de/th/Meetings/**psik_2010**/)

3. Assessment of the Results

3.1 Growth of Our Field

Since the beginning in the 1970s our research field has been continuously growing and will be further growing in the foreseeable future. Due to the development of density functional theory and related improved methods, parameter-free and very accurate calculations of material properties have become possible. This method is universal and can be applied to everything from biological molecules to magnetic nanostructures to catalytical reactions and even to transport and electronic excitations. This growth is fuelled by the continuous progress of computer technology and to an even larger extent by the steady improvements of computer codes and the invention of new conceptional methods.

To demonstrate the growth of our field, Fig. 1 shows the annual number of "ab-initio" publications in the years 1991-2007 (from ISI Web of Science). We have searched for publications, which in title, abstract or keywords contain one of the following topics: "ab-initio", "first principles" or "density functional". One observes a continuous increase, e.g. from 1991 to 2007 by more than a factor 6. The figure also demonstrates that this increase will not stop in the foreseeable future. Moreover in 2007 there exist breathtaking 13.000 publications in the field. Clearly nobody can read this. Thus, it is very important that a network like Psi-k exists, which covers practically all subfields and which with many training and workshop activities helps to catch up with the fast developments in the field.

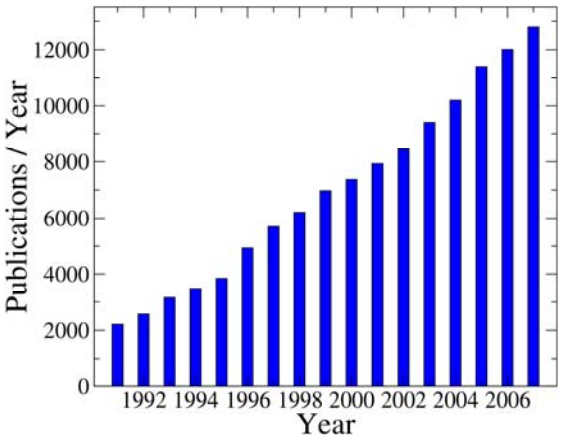

Fig. 1

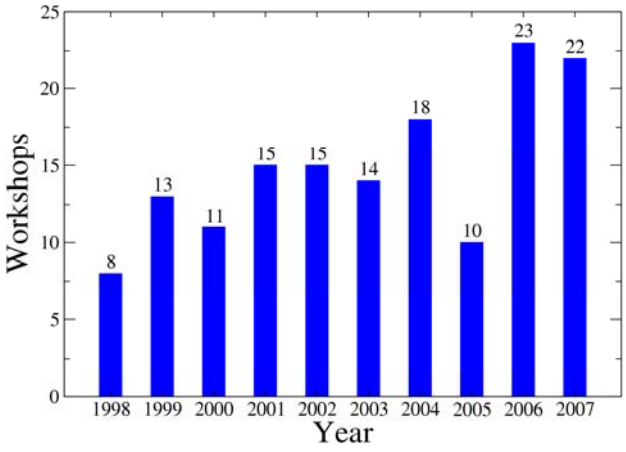

Fig. 2

This continuous growth is strongly reflected in our workshop activities. Fig.2 shows the annual number of Psi-k workshops (including tutorials and schools) organised during the years 1998 (the beginning of the ESF Psi-k (STRUC) Programme) to 2007. Thus we see a dramatic and continuous increase of our activities, from 8 workshops in 1998 to 22- 23 in 2006/07, i.e. by nearly a factor 3. (The year 2005 was an exception, since due to our large Psi-k 2005 Conference we only supported a small number of activities. In the years 2005 and 2006 there were several tutorials with MolSimu at CECAM and two Graduate Schools at Daresbury and Uppsala which were all funded by EU contracts and which are included in the figure). The figure shows clearly the growth of our field and at the same time the success of our network. We are particularly proud that we could achieve this factor of 3 increase with a budget, which has only been increased by about 20 %.

Of course, it is fair to say that all these workshops have in most cases been only partially funded by Psi-k; nevertheless the Psi-k Programme is the backbone of all these activities and without Psi-k most of these activities would not have taken place. This growth is also reflected in other numbers. For instance, the e-mail list for the Psi-k Newsletter (see Sect.6) increased from 500 in 1998 to nearly 2000 addresses in 2007 (At that time a Portal system was introduced). Another example is the number of participants of the large Psi-k Conference.

3.2 Collaboration with Industry

The relation to industry is part of our goal of applications of ab-initio calculations. More than a dozen of our members have long term collaborations or contracts with industry. Several of our members have set up small companies for collaborations with industries, i.e. partly doing code development and partly doing calculations for industry, in the same spirit as consulting companies do. A successful example of such a company has been established by our Steering Committee Member Dr. E. Wimmer.

Many of the successful codes developed by our members are actually used in industry. For instance, the VASP molecular dynamics code of our Programme applicant J. Hafner is licensed to about 75 companies, among them many from Japan and USA. Analogously the FLAPW code Wien 2k is licensed to about 50 groups in industry. Even higher numbers exist for the plane wave codes (CPMD and CASTEP). For instance the CASTEP code developed at Cambridge is licensed to several hundred companies. Thus industry is profiting enormously from the work of our members.

To enhance the collaboration with industry, our member Juergen Hafner has organized a Workshop “Theory Meets Industry” in Vienna, 12-14 June 2007. 35 invited speakers, half of them from industry, presented results of ab-initio calculations in key areas of technology, concentrating on catalysis and chemical processing, information technology, automotive engineering and energy. The proceedings of the workshop are published in J.Phys:CM **20** (2008) 060310ff.

3.3 Training and Support of Young Researchers

For all Psi-k activities, we offer special support for young researchers. As example we pick out the support for the big Psi-k 2005 Conference. The standard support for junior researchers was 430 Euro, including 180 Euro registration fee and 250 Euro for partial travel support. In total 120 young researchers were funded, amounting to a sum of around 52.000 Euro.

In order to close the gap between university education and the considerable higher level at Psi-k workshops, we are regularly organizing within the "Psi-k Training" activity (see Sect.4.3) Graduate Schools and Summer Schools, specially aiming at master and PhD students. The strong emphasis on training is also part of our new “Psi-k limited”: e.g. in 2009 we will organize 10 summer schools, graduate schools and hands-on tutorials.

Several of our young researchers have won EU-Grants: Angelos Michaelides (FHI Berlin) and Dario Alfe (Univ. College, London) have won the prestigious 2005 European Young Investigator Award (EURYI), with an award sum of about 1 Mill. Euro each. Silvia Picozzi has won in 2008 a very well funded ERC Grant. Other junior members have received similar high national start-up grants.

4. European "Added Value" and Visibility

4.1 Visibility of Psi-k Network

Psi-k is the European Network for ab-initio calculations. With the about 20 workshops and the about 1000 participants per year and moreover the big Psi-k Conferences every 5 years, Psi-k has an extremely high visibility, not only in Europe, but worldwide. By taking Psi-k as the outstanding example, similar networks have been organised in USA, Japan, Brazil and Argentina, but none of these is of comparable importance as Psi-k.

Characteristic for Psi-k is a strong internal cohesion and the joint vision about the importance of ab-initio calculations for all fields of natural sciences. Since its existence 15 years ago Psi-k has strongly contributed to the world wide European lead in our field. This lead can also be quantified by publication statistics from ISI Web of Science: of the 12 700 publications world wide on ab-initio calculations in the year 2007 about 5 400 were published by European authors as compared to 3 400 each by authors from USA and from the Far East (incl. Japan and China). Thus Europe is far ahead.

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4.2 Collaboration with CECAM and MolSimu Network

Since several years we have strong collaborations with the Centre European de Calcul Atomique et Moleculaire (CECAM) and the Molecular Simulation Community (i.e. the MolSimu Network). While the methods used by the two communities, i.e. molecular simulations versus ab-initio calculations, were traditionally distinctly different, there is now a growing overlap in the methods used by both groups. Together both Networks represent the whole field of Computational Materials and Nanosciences on an atomistic basis in Europe and thus about 4000 scientists in all European countries. The first results of these collaborations are: (i) the Psi-k Network organises every year about 5-8 workshops at CECAM, jointly funded by Psi-k and CECAM, (ii) co-ordinated by CECAM, both Networks have successfully cooperated on the ESF-Forward-Look "European Computational Science Forum: The ‘Lincei Initiative’: from computers to scientific excellence", which aims at establishing code development as an infrastructure project, and will apply in the near future for a “Computational Sciences Expert Committee (CSEC)” at the ESF.

4.3 EU-Contract "Psi-k Training"

Psi-k and CECAM have jointly applied to the EU for a "Series of Events" within the Marie Curie Programme, including 8 Graduate Schools, 12 Hands-on Tutorials and 4 large Summer Schools. Despite the very unsatisfactory funding by the EU most of these activities are being organized, partly with the help of CECAM and the MolSimu Network (through their (very well funded) EU contract within the Series of Events).

4.4 Research Centres Daresbury and Jülich

Since a long time the Psi-k Network has very good relations to the Research Center Daresbury (UK) and to the Research Center Jülich (Germany). Daresbury edits the Newsletter, hosts the website and provides the major domo e-mail service. On the suggestion of Psi-k both centres recently joint CECAM. Both centres will also play an active role in the expansion of CECAM into a multi node structure.

4.5 EU-Networks

The Psi-k community has a strong track record in applying for specialised Networks, partly within the EU Framework Programmes. During the period 2003-2008 six networks were active (the first three ones have expired):

Network of Excellence "Nanoquanta"
Research Training Network "Exciting"
Research Training Network "f-electrons"
European Theoretical Synchrotron Facility(ETSF)
Cost Action P19 Multiscale Modelling of Materials

4.6 Awards of Our Members

Many of our members have won important international and national awards and honours. A detailed list containing **80 awards** received by our members during the period of this Network, i.e. in the years 2003-2008, is given in the appendix. The impressive list clearly shows the outstanding excellence of our Network and the extremely high visibility of our members. This excellence is distributed over many countries and thus a truly European success.
The most prestigious prize, the **2006 EPS Europhysics Prize**, was awarded to Antoine Georges (Polytechnique Paris), together with Dieter Vollhardt (University Augsburg), Walter Metzner (MPI Stuttgart) and Gabriel Kotliar (Rutgers,USA) “For the Development and Application of Dynamical Mean Field Theory”.

5. Programme Finances and Managements

The annual expenditures are about 160.000 Euro. The summary accounts for the years 2003-2007 will be provided by Catherine Werner (ESF), together with the spending of the remaining funds in 2008.

The Programme is overseen by a Steering Committee of the National Representatives, to which we have attached the leaders of the 15 Working Groups. The list of the Steering Committee members is given in the appendix. The Steering Committee meets once per year, with the exception of 2004, when we had a second meeting to set up the program for the big Psi-k 2005 Conference. Urgent problems and decisions are discussed in a small Core Group of seven members of the Steering Committee. Chairman, Core Group and Steering Committee are in frequent e-mail contacts.

6. Publicity: Psi-k Newsletter, Web Site and Highlights

The electronic Psi-k Newsletter has been a great success and important in creating our community. The Newsletter itself and its e-mail list of about 2000 have now become the main vehicle for advertising jobs and for announcing Psi-k workshops and other conferences of interest to our community. Such items are inserted in the Newsletter but also circulated separately, especially in the time gap between successive issues. The Newsletter appears every two months, posted on the website with an announcement to the email list that it has appeared. Each issue now has regularly over 100 pages, and includes the activities of related EU-networks in our community. A report appears from every workshop or other activity funded by the Programme. Any researcher can submit an abstract of any new paper submitted for publication.

Every newsletter contains a "**Highlight**" article of some particular successful and important piece of work. These reviews have become very popular. Since the Newsletter exists already for 15 years, a total of **90** such highlights have been published already. All issues of the Newsletter, all Highlights and the information on all networking activities are available at the Psi-k website (http://psi-k.dl.ac.uk).

7. Future: The new Psi-k Company limited by Guarantee, a Charity

The Psi-k Network has been enormously successful. We have grown strongly and our activities cover now nearly all fields in computational materials- and nano-sciences. In fact we have been the most successful of all ESF Network Programmes, as we believe. Unfortunately for the same reason we were discouraged to reapply to the European Science Foundation: we are considered as "too big and too diversified" for a Network Progamme.

Therefore the Psi-k Steering Committee has decided that we have to help ourselves and form a legally independent, not-for-profit, science organisation. Since a year ago we have established Psi-k as a **"Company limited by Guarantee"** according to English law and have obtained recently also the status of a "Charity", meaning that we are exempt from taxes.

The problem of a basic funding is solved by financial contributions ("Membership Fees") of the largest and financially strongest Psi-k groups in Europe. Since last year in total about 30 groups from the major European countries are donating contributions between 3 000 – 10 000 Euro each, leading to an annual budget of about 160 000 – 170 000 Euro. In 2008 we have been able to organize 18 workshop activities, of which 7 were co-funded by remaining ESF funds. Of the 33 proposals for 2009, a total of 24 were selected for funding by the new Psi-k limited. The goals and tasks of the new Psi-k Network are very much the same as the well proven Psi-k Programme funded by the ESF. In particular, also the new Network is open for all European scientists, who e.g. can participate at Psi-k Workshops or make applications for Psi-k activities. Also the organisation is as lean as in the past; no staff positions are involved. The management of the finances and the travel expenses is handled by the Daresbury Laboratory.

The buttom-up funding of a Network from the budgets of its members is a novelty in Europe. It dramatically illustrates the success of our Network and that our members want to continue the Psi-k activities in the future. This success is closely connected with the stable funding by the ESF over two periods, for which we are very grateful.