HCM Newsletter

Ψ_k Network

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

Special Issue November 1996

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1 Editorial

This is a special issue of the *Newsletter* containing the *Network's* application to European Science Foundation (ESF), and the outline of the Training and Mobility of Researchers (TMR) application. Preceeding these two applications is an explanatory introduction by Professor Volker Heine, the chairman of the *Network*.

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

	function
psik-coord@daresbury.ac.uk	**messages to the coordinator & newsletter**
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2 Chairman's Message

The Future Beyond the Present Ψ_k-Network

First of all about the present Ψ_k-Network: as announced before, it has been extended (without any extra money) until 31 Dec 1997. To help budget for the rest of our time and money please inform Walter Temmerman as Co-ordinator immediately about any major application for financial support. As most people will know, this Network has been funded by the European Union (EU) from its Human Capital and Mobility (HCM) Programme.

Two applications are in the pipeline for the future. One is to the European Science Foundation (ESF), and I want to explain it carefully to you for two reasons. In ESF terminology it is called a 'Programme' but it really is an open-ended mega-network. If the application is successful, it will provide an infrastructure of workshops and of travel for small collaborations, open to all across the whole of Europe. And it would last for 5 years. Does that sound too good to be true? Of course there is a catch and this is the other reason for explaining it to everyone. The ESF has almost no money of its own and the Research Councils of all the European countries (**NOT** only the EU members) would have to 'buy into' such a 'Programme". This means everyone may need to press their national Research Council when the time comes to put up some money for it. Note that the ESF is quite separate from the EU, and it is really a co-ordinating body for all the Research Councils of all the European nations. I attach a copy of the application so that you are fully informed, because in submitting this to the ESF, we (the Management Board of the present Network) claim to be speaking for the whole 'family' of researchers working with *ab initio* electronic structure calculations for solids. Please read it, and decide whether you wish your National Research Council to support it. I shall inform everyone later when the time for decisions comes and who are the national representatives. It is not quite clear where this application (if successful) would leave the *Newsletter*, but we give the highest priority to its continuations.

The other application in the process of being written will be to the EU for a Network in its Training and Mobility of Researchers (TMR) Programme, which is the new version of HCM. Fortunately and unfortunately for us, the rules for the new Networks under TMR are quite different from those for the previous HCM Networks. The new Networks will consist of only a few groups in EU countries collaborating on one major project, but they will be well funded with one post-doc each for three years. The good aspect is that such a Network would really create active and deep collaboration. I also attach a brief description of what is planned for the EU TMR Network application. We are trying to make it as broad as possible by associating an international team with each of the eight major centres, but it would still only cover a small fraction of our whole community. That is why we have also launched the ESF application. You may be a bit surprised at the amount of emphasis in it on the application to industry. There are two reasons for this. Firstly this document has been written for use in approaching industrial people for some verbal support, so it naturally plays up that part. However we quite genuinely believe in the future role of electronic structure calculations in industrial research. Secondly

there is such a high pressure of applications for these networks that the chance of success is almost zero, and by invoking industrial applications we feel we might raise the probability a bit. We are clear that it does not adversely affect what people want to do.

Volker Heine

Cambridge
29 October 1996

Outline of an application for a Network on "Electronic Structure Calculation of Materials Properties and Processes for Industry and Basic Sciences" for funding by EU (European Union) programme on TMR (Training and Mobility of Researchers). Autumn 1996

In the face of increasing international competition, tighter environmental regulations, rising research and development costs, and high employment costs, the European chemical and materials related industries find themselves in a difficult and challenging situation. On the other hand, European researchers in the field of chemical and materials sciences continue to be world leaders and innovators, especially in the field of computational physics, chemistry, and materials science. In fact, computational science is becoming a strategic technology in the sense that the methods are starting to be applicable to industrial problems while the performance and economics of computer hardware continue to change at a dramatic rate. Therefore, it is mandatory to accelerate the transfer of computational methods from academic research to industrial exploitation in order to take full advantage of these opportunities, thus leading to increased industrial competitiveness. In this context, electronic structure theory is at the heart of computer-aided molecular and materials design.

It is the aim of the proposed Network to bring together leading European groups in the area of electronic structure calculations of materials properties and processes and to focus their efforts on the accelerated development of this technology and its transfer from the pre-competitive research stage to an industrial R&D tool which will help European chemical and materials related industries to maintain their competitive position.

This goal will be accomplished through the following actions:

- Dialog with leading industrial organizations to identify the industrial needs and requirements for atomistic computational tools. The Network would convene an initial workshop inviting the key industrial contacts to participate and to provide the network with their needs and requirements.
- Coordination among all network members to maximize complementarity and eliminate unnecessary duplication of efforts.
- Application of the newly developed tools to industrial problems to demonstrate their usefulness.
- Training and dissemination of the newly developed capabilities to all researchers in the network and to the industrial laboratories.

Specifically, this planned Network (if funded) would be concerned with understanding basic processes and properties at the atomic level in solid materials and at solid surfaces. The work is

based on large scale computation, solving the quantum mechanical Schroedinger equation to a high level of approximation for all the electrons in the solid. Since these electrons are responsible for the chemical bonding, the magnetism, superconductivity, optical and other effects, a good description of such processes and properties is obtained.

The field has made remarkable strides forward in the last ten years, driven by the exponential growth of computer power and matched by improvements in the numerical algorithms. The techniques are already in use in a few industrial laboratories worldwide for a few specific types of problem, e.g. identifying impurity centres in semiconductors, developing detailed chemical reaction models for chemical vapor deposition in microelectrons, calculating the magnetoresistance properties of materials for high-density magnetic recording devices, understanding the reactivity of heterogenetous catalysts, and understanding the adhesive properties at interfaces.

It is clear that we are at a threshold of a much wider application of these methods in industrial research and in several basic sciences.

The following titles illustrate the wide range of applications taken from papers presented at the first world conference specifically devoted to the subject of electronic structure calculation of materials. It was held recently in Germany (September 1996), attended by 332 scientists. Some titles of papers were as follows:

First-principles study of oxygen defects in GaN and GaAs
Elastic and thermal properties of refractory carbides
Band-gap engineering by III-IV infill in sodalite
Magnetism, structure and stability of ultrathin magnetic films
Towards an understanding of platinum-based drugs with the Car-Parrinello method
Giant magnetoresistance in magnetic multilayers
Chemical reactions in initial oxidation of Si(100) surfaces
Reactivity of methanol adsorbed on a zeolite catalyst
Influence of thermally induced surface roughening on hydrogen dissociative adsorption on Pt(111)
Theory of metal-ceramic interfaces
Strained tetragonal states and Bain paths in metals

We note applications to several aspects of materials science, surface chemistry and even biochemistry, all of which are relevant to various industries. Hence one can see a clear pathway to industrial applications, but in most cases this will first require further academic reseach, and often the next generation in computer power. The variety of applications is also growing in basic sciences, including now mineralogy.

Europe has been the world leader in this field in recent years, and the purpose of the proposed EU TMR Network would be to develop the techniques and the applications further in various directions. The collaborators all have first class reputations by world standards. The chairman will be Dr Erich Wimmer of Molecular Simulations Inc. (Paris); Professor V. Heine FRS of Cambridge University will be retiring shortly but will take an active interest as Honorary Co-chairman. The work will be divided among seven research groups (each international) concentrating on some selected leading-edge applications or the methodology adapted to particular types of material.

The groups and group leaders are as follows:

1. **Molecular processes at oxide surfaces** (Dr. E. Wimmer, MSI, Paris)

2. **Improved code for materials with rare earth and actinide elements** (Dr. A. Svane, Aarhus)

3. **Interfaces between oxides and metals** (Prof. M. Finnis, Belfast)

4. **Non-collinear magnetism** (Prof. J. Hafner, Vienna)

5. **Improved LAPW code for general applications** (Dr. S. Bluegel, Juelich)

6. **Excited states and optical properties of semiconductors** (Prof. R. Nieminen, Helsinki)

7. **Electronic structure of the superconducting state** (Prof. E. Gross, Wuerzburg)

8. **Coordinating dissemination and advanced training** (Prof. W. Temmerman, Daresbury)

Particular attention will be paid to disseminating the results and training young post-doctoral workers in the techniques. Industries are warmly invited to become involved or to keep a watching brief on any groups of interest to them, and to discuss how the techniques might be applied to their particular concerns now or in the future. The time is ripe for a dialogue with industry about how to bridge the gap to the adoption of the techniques, which the Network plans to initiate. Training and planning are very important because this type of research requires considerable expertise, expense in computing power and time, but not more so than most laboratory work.

4 ESF Application

Proposal for an ESF Programme on Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces.

Summary

This Programme application comes from a group who have promoted their scientific field and built links to about 300 researchers across Europe with an EU HCM Network and four ESF ERC Conferences. The main future needs of this community fit the objectives of an ESF Programme but not the new EU TMR concept. The science is to understand complex atomistic behaviour of solids and surfaces through computer simulation, with the extra new ingredient that all interatomic forces and atomic effects are calculated quantum mechanically from first principles because that is the only way to obtain them reliably. The field is expanding rapidly in mainstream physics, surface science and materials science, with new applications pushing into mineralogy, chemistry and even two calculations in biology. The scientists are mostly young because the field is new and computational. The need is for a wide open-ended network for sharing a broad range of techniques and new developments, and for forging links to experimentalists in the growing range of applications. There will be (a) an electronic Newsletter to disseminate information, (b) research workshops and collaborations, (c) short visits for in-depth consulations, (d) hands-on workshops for disseminating computer codes, and (e) secondment visits.

4.1 The type of science we do

Three steps are needed to explain the science we do. Firstly we are interested in all types of complex behaviour in solids and liquids which depends on processes at the atomic level. Examples are magnetically 'hard' and 'soft' materials for various applications, dissociation of methanol in a zeolite catalyst, embrittlement of aluminium by gallium impurities in the grain boundaries, the superconducting gap in the high temperature superconductors, defects in semiconductors, chemical processes at metal surfaces, adhesion of an oxide film on a metal: the list is endless and these are actual examples of recent or current calculations. The second point is that we use 'computer experiments' to supplement laboratory measurements because the latter cannot observe and manipulate individual atoms except in rare special circumstances. But that is easy in the computer, and we throw the atoms into a box (up to several hundred atoms into a superlattice cell repeated periodically in three dimensions) and solve the relevant equations for the whole lot.

The third point is the defining feature of our community: to determine the behaviour of the atoms, we solve the quantum mechanical Schrodinger equation for all the atoms with their bonding electrons. What is new in the last decade or so is the ability to solve these quantum mechanical equations for useful systems to useful accuracy (which has to be of the order of one part in a million often, or even better, in relative accuracy). The chemical bonding between

atoms is a quantum effect and attempts in the past to represent this by simple empirical interatomic force models have not been very successful. To be precise, the empirical models cannot do justice to the quantum effects in the types of non-standard atomic arrangements which one usually has in "a process in action", e.g. at the top of an activation barrier. Unfortunately the full quantum treatment is extremely expensive in terms of computer time so that the empirical potentials continue in wide use (but the quantum calculations can now test and improve their accuracy). Nevertheless our type of quantum mechanical 'first principles' calculations are so much superior to the empiricial interatomic potentials used previously that they represent the leading edge of research wherever they have been applied. They are opening up questions for research for the first time, e.g. what goes on inside a grain boundary during mechanical deformation of a metal, with or without impurities.

The actual examples above show that we are involved in many interdisciplinary collaborations with experimentalist and other types of computer simulators. The fields of application include surface science, materials science, chemistry, mineralogy and newly biochemistry, as well as physics where these techniques were developed, and they are extending rapidly every year.

The techniques are very broadly common: the computer in a sense does not know whether it is dealing with a defect in a semiconductor or some chemistry at a catalyst surface. However there cannot be two or three standard codes to cover everything. Magnetic systems require some special modifications, as do rare earth atoms in another direction; similarly, loosely bound systems like water, random systems such as alloys, minerals with triclinic unit cells, metals generally, dynamic systems, energy barriers, these and other features all require specific additional handling. Thus there is a broad range of ideas and techniques that get combined in a wide variety of ways, and it is this feature of our subject that makes networking among our community so important.

4.2 Characteristics of our community

Our research community comprises several hundred workers (including graduate students) in Europe. They are spread throughout most countries and many university and research institutes, engaged in a wide variety of main-line research in physics, chemistry, materials science and mineralogy.

Europe rather than USA or Japan is the leader in this field of research. To maintain and build on this success, good human contact in a broad network is required because the field is undergoing extremely rapid growth in algorithms and range of applications, driven by the growth in computer power. New developments are reported monthly. Our community has lacked cohesion for two reasons, making the sharing of expertise difficult and leaving small new groups rather isolated. For example there was no address list until the present EU HCM Network. Firstly we are not linked to some large facility which can act as a gathering centre. Secondly it is characteristic of our field that researchers have been closely linked to interpreting experiments,

so that they have identified with the field of science that they are applying their calculations to. This is excellent in its way, but it has resulted in fragmentation, people "re-inventing the wheel", general inefficiency and sometimes frankly second class work due to not being fully aware of the latest developments. This illustrates the need for a long-term broad networking infrastructure for our community, such as the present EU HCM Network has been building up. It has 40 nodes, and would have been extended to a further 25 in western Europe and 10 in the former communist countries if Brussels had allowed: we include them as much as we can through association with funded nodes. Thus it includes or has close links to practically all the significant research groups in the field in Europe.

The researchers are mostly young because of the rapid expansion of the field and its computational nature. Many are establishing this type of work newly in universities and institutes from the Atlantic Ocean to the Ural Mountains. Good networking to the more established centres is essential to remain up-to-date. Actually the major centres need the networking just as much, to incorporate advances made elsewhere and remain at the world's leading edge. Sometimes it is a matter of avoiding what has been shown not to work satisfactorily, which one usually only learns about through personal contact.

4.3 The need for an ESF Programme, based on a track-record of promoting collaboration

The remarks already made at the ends of Sections 4.1 and 4.2 indicate that the type of networking needed is a wide Programme serving the whole community. This type of work has been built up through the present EU HCM Network (1 Jan 94 - 31 Dec 97). However it does not fit at all into the new TMR programme of the EU. (The latter are to fund post-docs at about six collaborating centres only in EU countries for a tightly defined project.) Even in the EU HCM programme our Network is anomalous in its large size. Of course collaborations started in our large network may in due course lead to specific focused joint projects which can apply for national or EU funding. One such EU TMR project is just starting and another is being formulated, but they involve only six or seven centres each, and do not touch the wider needs discussed in the present application. Also quite a few bilateral and trilateral collaborations have grown up, as discussed below.

There are four background reasons why a broad ESF Programme is needed in our community. The first is that the logical structure of our subject is like a multidimensional web: there are no tidy divisions. For example there are four basic methods of calculating the electronic structure but the special tricks for dealing with metals or magnetism or inhomogeneous electron exchange/correlations cut across all four of them. Hence the need is to encompass the whole community. Secondly the right scale for the networking is European, not national, while of course maintaining links to American and Japanese workers with whom we have good contact. For example all UK workers doing pseudopotential calculations more or less share one basic computer code, but improvements to this may result from experience or ideas in the four major

groups in Germany, Austria and Switzerland using a similar approach. Thirdly the rapid development of the subject means that efficient sharing of information is very important to maintain excellence and Europe's leadership in the field: hence the need for good networking. Mostly one researcher does one calculation or writes a computer code: it is not usually a team effort (though there are exceptions). But he or she does need to draw on a very wide range of expertise on many difficult technical points. The calculations are extremely intensive in use of computer time on large workstations or supercomputers, and need to be highly optimised to be feasible at all. Fourthly there is a vacuum which an ESF Programme would fill: our community has lacked cohesion because of the newness of the field and because it is not connected to large central facilities as explained in Section 4.2. The activities and help of the Programme would be open in principle to all European workers in the field showing a serious intent of attaining high quality research.

We turn now to more specific objectives of an ESF Programme. First and foremost there is the maintenance and enhancement of research excellence across Europe in all groups, including the strongest, through sharing of ideas and expertise including computer code development. Although we talk of a loose network, the leadership behind this application is rigorous in pursuing high quality in research. It has been said that in basic research, second class work is almost worthless. An ESF Programme would enable all workers to plug into the latest developments throughout Europe when they want to. This will be achieved through advertising all activities in the electronically distributed ψ_k Newsletter every two months, which also includes the emails of all Board members who can be approached, and which has preprints of research articles so that one knows what others are doing. Secondly the Programme would try to support especially the young researchers establishing our subject for the first time at their universities and institutes across the whole of Europe which is a feature of a growing research field. They have a special need to be linked to the more established groups in order to keep up to date. Thirdly there is the need to support the large number of small collaborations and ad hoc consultations which is how the in–depth sharing of expertise and computer codes often occurs in our community. They are too small and transient for separate Research Grant applications: flexible and rapid support through a Programme is much more appropriate. Fourthly the Programme would enhance opportunities for graduate students and young post-docs to enter our expanding field of research, wherever they come from. They need information about what is going on where, and often informal links between individuals in a network help them to get there.

The leadership behind the present application has been successfully pursuing the above aims funded as an EU HCM Network. Our ψ_k Newsletter is published every two months and reaches a few hundred people. It includes announcement of all Network activities with reports afterwards, a scientific highlight article, preprints of papers to be published, and has become the main medium for job advertisements in our field. Research workshops have been held under the aegis of ten Working Groups. Some one week hands-on workshops have been held for disseminating computer codes and another is in the pipeline. Many short visits have been supported in relation to bilateral or trilateral collaborations. The first general international conference in our field will be held in September 1996 with many invited speakers and opportunities for all

researchers to present brief talks or poster presentations. The original 40 Network nodes have been expanded by 25 more in western Europe and 10 in the former communist countries which are partially funded (see Section 4.2). We want to build on that success. We have the existing connection with the ESF in the ERC conferences on Electronic Structure of Solids, and would like to extend that to an ESF Programme in the belief that the objectives described above are full in accord with those of the ESF.

Other groups of scientists have a large facility such as a synchrotron around which they are organised to maintain at least an address list, or they have a well established regular world-wide conference organisation such as the International Union of Crystallography. But our community has nothing like that. It is too new, and its scientific interests are too diverse. However the enormous amounts of computing resources used, the sophistication of the techniques and their rapid development make some kind of networking essential.

4.4 Specific Programme proposals

4.4.1 Information services via the ψ_k Newsletter.

We want to continue this Newsletter already described above. It is published purely electronically to about 200 email addresses listed in Appendix 4 some of which are for general display in substantial research groups. In addition to the email distribution, other readers take it from the World Wide Web. Since researchers have previously tended to identify with the experimental field of application of their calculations, this Newsletter has filled a real gap and rapidly become the main medium for information about conferences, workshops, training courses and post-doc positions available in our field. It includes all Network activities and relevant ones outside it. All researchers can attach to the Newsletter an abstract of a paper submitted for publication, to inform others of what they are doing. It also contains reports of workshops and other Network activities and short articles on recent highlights and ideas.

Although there are no printing and postage costs with electronic distribution, the editing occupies the half-time effort of an established scientist. This surprisingly large effort is needed partly because of technical problems such as incompatibilities between LATEX on different machines which can be very time consuming, and partly because people are not yet trained in the use of electronic templates from the WWW for submitting their contributions. The converting of figures to electronic form in the highlight articles is a particular problem. Achieving the correct electronic form requires educating the contributors and developing their cooperation, which needs an established scientist and is a substantial effort for a Newsletter of 70 to 90 pages per issue. Often announcements and short reports etc. have to be converted by the editor or the English corrected. Special editorial effort goes into achieving a high standard for the articles on Network highlights.

A partial contribution of 1.5 kECU per Newsletter issue is requested, which will be used to seek

matching funds from industrial and other sources.

4.4.2 Workshops and meetings of major research collaborations.

A series of workshops would be held. A list of 14 proposed topics is shown in appendix 1, with the names of organisers and collaborating groups, some topics needing two or three meetings over the 5 years. These topics are all at the leading edge of research and are described as we would have them if held now but of course the ESF Programme would run for the period 1998 - 2002 during which time there would be changes. The named participating groups are known to be interested, but of course the workshops would be advertised in the Newsletter and open to others.

The workshops cover a wide area and a range of different types. Some are for sharing different approaches and kinds of work in assessing where a field is at and where it is going, e.g. on adhesion of oxide-metal interfaces. At the other extreme are collaborations putting together different expertise to write a new computer code aimed at a specific set of research problems, e.g. incorporating Self Interaction Corrections better in calculations on rare earth and actinide elements. The participants need to meet to do the work and then run a different type of workshop to disseminate the use of the code to a wider group of interested researchers. Some are focused on new techniques, e.g. to calculate excited states, while others are pushing into new areas of application e.g. mechanical strength of materials or silicate minerals. In some cases the workshop would draw in experimentalists to help plan what calculations would be most relevant.

The matter of reports and dissemination or results is dealt with in Section 4.5.

Seven of the proposed workshops (c,e,f,g,h,j,k,m in Appendix 1) overlap with the planned EU TMR Network application, which would fund one post-doc per topic if successful. That would certainly not cover all the calculations that should be carried out (!); rather it would open up the field. The ESF Programme would then be used to broaden the work and bring in other interested groups to become associated with and benefit from the TMR-funded activity

4.4.3 Short visits for small collaborations and individual consulations.

These are very important in our field, because basically one computation is carried out by one researcher. But often the difference between a first-class and a second-class piece of work, or getting something to go at all, depends on the right expertise at the right time. These collaborations arise from workshops, the ERC conferences, information in our Newsletter and other contacts. Indeed what is the point of putting people in touch if one then does not make it possible for them to collaborate? These are not long-term collaborations focused on a specific problem which can be planned years ahead and for which one can apply for specific research funding. While email is widely used, there is an occasional need to sit down together for in-depth consultation for several hours or days. These are of diverse type as illustrated by the

following recent examples. Dr. K. (France) is calculating electron transfer between molecules in mixed crystals as a model for biological systems and needs to consult Dr. B. (Switzerland) about his new type of computer code which she is using. Prof. G. (Britain), computing extreme electrical anomalies in molten alloys, visited Prof. H. (Austria) to compare the speeds of two computer codes using somewhat different algorithms: also to learn of experience with Vanderbilt pseudopotentials. Prof. H. (Britain) visited a group of experimentalists in Germany to discuss their latest data on the way tiny amounts of gallium impurities in aluminium grain boundaries make the metal brittle, and the calculations of his graduate student relating to them. Twelve such visits per year at 1 kECU each are proposed.

4.4.4 Hands-on workshops for disseminating computer codes.

About one or two such workshops per year are envisaged, focused on a pseudopotential code, a linearised augmented plane wave code, a linearised muffin tin orbitals code, or perhaps the Korringa Kohn Rostoker method. The workshops include hands-on experience in using the code, advanced seminars on background theory, and discussion of how our type of computer simulation can best advance scientific understanding in the research areas of the participants. Those attending are new post-docs and graduate students in the research groups, established researchers wanting to receive and learn newly developed codes, and some researchers wanting to get into the field, e.g. from having previously used simulations with empirical interatomic potentials (see Section 4.1). One such workshop per year is planned, lasting one week, at 15 kECU.

4.4.5 Secondment visits.

Occasionally there is a need, not covered by various exchange and fellowships schemes, for extended in-depth visits of a few weeks. These are to learn the use of a specific computer code, and to plan and start on a collaborative research project with it. Six secondments per year at 2 kECU each are proposed.

4.5 Diffusion and dissemination

Clearly dissemination of the latest ideas, techniques and experience in this rapidly developing field is what the proposed Programme is all about. Moreover it is structured to make it easy for people to join in: anyone can add their email address to the distribution list of the ψ_k Newsletter. The names and addresses of the Board members will be published: almost every European country is represented so that there is someone local who can be approached. Even for someone taking no part in the Programme activities, there is a lot of information in the Newsletter about other conferences, job opportunities, preprints etc.

Turning to the workshops, some of these [Section 4.4.4] are specifically for disseminating widely

in the community some computer codes that have been developed, as are the Secondment Visits [Section 4.4.5]. These techniques are highly sophisticated, and experience has shown that a one week workshop with hands-on experience etc. is the effective mode for dissemination.

However disseminating the results of research workshops present two well-known difficulties, and we believe our electronic Newsletter could help with both of them, though not without some pain. Firstly almost no-one reads reports of conferences and workshops. One reason is that the written papers produced by the authors tend to be more formal scientific presentations than the oral style at the workshop which includes more of the wider framework, tentative ideas, work in progress and ideas that have failed: it is this wider perspective that one goes to a workshop for. If however it is a very focused workshop on some research problems then it tends to be of interest to those actively involved, who should be at the workshop: others can stand aside and wait for results while the technical problems are overcome.

We suggest that a better mode for disseminating the proceedings of a research workshop would be to commission an informal article that considers the issues under discussion, with a survey of the current state of the research and what still needs to be done, written for a wider audience in our community. This could be made a requirement on the workshop organiser. Sometimes such an article may be suitable for publication in a journal such as Comments on Condensed Matter Physics, but it would almost certainly be read more widely if it appears in our Newsletter because this has a wider circulation among the community interested in our workshops. In the Newsletter it would appear together with the workshop programme, list of participants, email addresses of contributors with abstracts of their talks. Anyone wanting more information on specific points can then obtain it easily.

The second problem about workshop reports is the cost and work of production and mailing paper copies. One non-trivial aspect is assembling a specific distribution list each time if one wants to avoid the cost of sending it out to a long list of probably two hundred or more addresses. Moreover we simply do not have the secretarial resources to contemplate this. We propose that the ψ_k Newsletter email distribution is in allways better, however short or long the report. However there is an editorial cost involved, as explained in Section 4.4.1: teaching authors to get equations, mathematics in the text and especially figures into the correct electronic form is a big task which also has to be financed. One day everyone will be trained in how to do this, as children now surf the Internet before they can write, but we are not there yet. In addition there are the severe technical problems of incompatibility of LATEX etc. between different machines.

However we believe firmly that the Newsletter is the right way to go and we should persevere with it. Clearly the question of how to pay for distribution of Reports will have to be looked at again. We understand the ESF is keen on dissemination but not keen on the costs involved. Perhaps a charge on each workshop would be appropriate and acceptable to ESF.

4.6 Relation to industry and wealth creation

Two members of the Management Board will come from industry, one of them being on the Coordinating Committee. These are not token appointments. Dr. Paul Kelly is part of a small group at Phillips Research in Eindhoven who have been doing electronic structure calculations for many years connected with research at Phillips on magnetism and on semiconductor surfaces. Dr. Erich Wimmer at MSI-Biosym has been involved with electronic structure calculations all his working life, particularly the application to industrial concerns. MSI-Biosym markets one of the computer codes developed by a group associated with the Programme. These comments suffice to show that our techniques are developing in power, with a few examples of use in industrial research already now and a growing number of applications envisaged in the future with the growth of computer power and development of techniques. This is also clear from the list of workshop topics in Appendix 1: e.g. one workshop focuses on extension to rare earth elements which are used in certain chemical catalysts for cleaning car exhausts. Workshop (n) in Appendix 1 will be focused specifically on furthering the interaction with industry.

4.7 Management: Programme Board and Coordination Committee

The following slightly unusual management structure is designed to meet three desiderata.

1. We wish to keep involved all those who have worked through the EU HCM Network to achieve the present level of activity. Their loyalty and continuing input will be important to the success of an ESF Programme.

2. It is necessary to add a few people who are leading major new collaborations, and several representatives of countries not in the EU at the time of the EU HCM Network application in 1993, including those in the former communist bloc.

3. However for efficiency it is necessary to have a smaller Coordinating Committee with executive powers.

We therefore propose a Programme Board of 32 members (listed in Appendix 2 with addresses in Appendix 3) with a wide scientific and geographical spread. They would only meet physically once, in the second year of the Programme to oversee its directions after the initial start-up. But they would be in continuous virtual session, i.e electronically by email, to advise on all matters. Final executive decisions would be made by a Coordinating Committee of 11 members drawn from the Board, whose names are also indicated in Appendix 2. This Committee would also be in continuous virtual session and have one real meeting per year. Committee members would have specific areas of responsibility.

Financial control for the workshops would be by giving each organiser a budget which he must not exceed. For the individual visits, each application would be considered automatically by at least two Board members, one in whose area of science it falls and one for the geographical area.

This system has worked well in the EU HCM Network.

4.8 Quality control

In a large flexible Programme as proposed here, quality control is a necessary concern. It has been said that second rate science is almost worthless, as has already been remarked. In our field there are some who collect computer codes without using them properly. Several steps are proposed.

1. The stated purpose of the Programme would be to enhance research quality in our field across Europe and that must take priority over all nationalistic, bureaucratic, or other concerns in all decisions.

2. Members of the Management Board and Coordinating Committees have been chosen with a track record of excellence in research and other activities.

3. There is clear subdivision of responsibility, particularly regarding support for individual visits. When a request (with brief scientific case) comes across the email, the Committee and Board members covering the relevant scientific and geographical areas would automatically be expected to advise. Similarly each Committee member will have responsability to oversee particular workshops in collaboration with the organizers.

4. Applicants to workshops will be expected to indicate their existing or planned related research project, where these are not already known. Six months after the workshop there will be a follow–up questionnaire to learn what the participants have gained from it and whether this has been applied.

5. There must be a suitable report in the Newsletter of every visit and workshop covering the science and the cost.

4.9 Budget for 1 Jan 1998–31 Dec 2002

i) Information services through electronic ψ_k Newsletter including Reports of Workshops	
Partial contribution to costs @ 1.5 kECU per issue for 6 issues per year	45 kECU
ii) Research Workshops and Major Collaborations	
3 per year @ 10 kECU	150 kECU
iii) Small Collaborations and Individual Consulations	
12 per year @ 1 kECU	60 kECU
iv) Hands-on Code Sharing Workshops	
1 per year @ 15 kECU	75 kECU
v) Secondment Visits	
6 secondments per year @ 2 kECU	60 kECU
vi) Meetings of Coordinating Committee and Programme Board	
1 Board and Committee meeting 32 kECU	
4 Committee meetings @ 11 kECU = 44 kECU	76 kECU
Total over 5 years	466 kECU

Appendix 1: Proposed Workshops and Major Collaborations

Where specific groups are known to be interested, they are indicated in brackets: but of course workshops will not be limited to those groups.

(a) Contribution of ab initio electronic structure simulations to understanding the mechanical strength of materials.

Two workshops, one in 1997 and one 3 years later, would be a key initiative to broaden the application of Programme techniques in an interdisciplinary direction. The crucial issue for discussion is how to connect the role and scale of atomistic effects studied by ab initio methods to the mesoscopic scale of deformation processes. The latter are studied by materials scientists and in particular by the empirical potential modellers, and an important purpose would be to develop a dialogue with them, including some from USA. A few calculations in the area already exist which could serve as a basis for critical evaluation and future calculations. This is a case where proceedings might be worth publishing, with a review to sum up the conclusions of the workshop. Organiser Prof. M.W.Finnis, Belfast, Northern Ireland. Other participants: Prof. V.Heine and Dr. P.Bristowe, Cambridge, UK; Prof. J.Norskov, Lyngby, Denmark; Prof. B.Johansson, Uppsala, Sweden; Dr. P.Mohn, Vienna, Austria; Prof. D.G.Pettifor, Oxford, UK; Prof. M.Stoneham, London, UK; and materials scientists outside the Programme Prof. V.Vitek,Philadelphia, USA; Prof. A.Carlsson, St.Louis, USA; and others.

(b) Contribution of ab initio electronic structure simulations to understanding the properties of silicates and other minerals.

The workshop and hoped-for collaboration arising from it, would represent a key initiative to broaden the application of Programme techniques in an interdisciplinary direction. A few calculations have been done, which point to the need for a wider dialogue between the code developers, physicists and others trained to do the actual calculations, and the mineralogists whose wider research objectives the calculations should feed into. The most appropiate initial form of dissemination would be review articles of general interest in mineralogical magazines. Organiser Dr. B.Winkler, Kiel, Germany. Other participants: Prof. V.Heine, Cambridge, UK; Prof. R.Dovesi, Torino, Italy; Dr. J. Ortega, Madrid, Spain; Dr. E.Krasovski, Kiev, Ukraine; Dr. K. Refson, Oxford, UK; Dr. P.Balloni, Stuttgart, Germany; Dr. A. de Vita, Lausanne, Switzerland; Dr. P.Blaha, Vienna, Austria; Dr. J.Angyan, Vandeouvre, France; and experimental mineralogists outside the network Prof. J.D.C.McConnell, Oxford, UK; Prof. A.Putnis, Muenster, Germany; Dr. R.Angel, Bayreuth, Germany; Dr. M.Andrut, Potsdam, Germany; Dr.M.Wildner, Vienna, Austria.

(c) Self-interaction corrections for rare earth and actinide elements.

These elements test the usual density functional theory (DFT) to destruction, and require an explicit treatment of the so-called self-interaction correction (SIC).Two workshops are required (i) To develop a full-potential relativistic version of the existing SIC code. 5 people for 5 days. (ii) To compare the SIC approach with another orbital dependent density functional, the optimize effective potential, which is also self-interaction free. 15 people for 3 days. The results will be disseminated by published articles and through the Newsletter, and use of the code through a hands-on training workshop or/and ad hoc collaborations. Organiser Dr. A. Svane, Aarhus, Denmark. Other participants Dr. W.Temmerman and Dr. Z. Szotek, Daresbury. UK; Dr. H. Eschrig, Dresden Germany; Prof.B. Johansson, Uppsala, Sweden; Prof. E.K.U. Gross, Würzburg, Germany.

(d) Screened LMTO and KKR.

The LMTO and KKR bandstructure methods have been revolutionized by making the structure constants short ranged through screening. A flurry of activities is taking place in further technical development and understanding and optimization of the screening concepts. At the same time, this methodology is being applied to systems for which the old methods were inadequate, such as disordered systems, multilayers to name but a few. Finally, coupled with order(N) methods, screening could take both the LMTO and KKR methods into the realm of ab initio molecular dynamics simulation of strong scattering electron systems. One workshop would be needed to cover these major new developments. Organiser Dr. O. Jepsen, Stuttgart. Other participants: Prof. O.K. Andersen ; Prof. P. Dederichs and Dr. R. Zeller, Juelich; Dr. W.M. Temmerman and Dr. Z. Szotek, Daresbury; Prof. B.L. Gyorffy, Bristol; Prof. P. Weinberger and Dr. L. Szunyogh, Vienna; Dr. B. Ujfalussy, Budapest; Prof. H. Dreysse, Strasbourg; Prof. B. Johansson, Uppsala; Dr. H. Skriver, Copenhagen

(e) Electronic structure of the superconducting state

It is proposed to hold a workshop on "The Exchange-Correlation Functional for Superconductors". The density functional theory of superconductors is a microscopic first-principles approach to describe the superconducting phase of matter. It leads to a set of Bogoliubov-de Gennes-type equations which, in addition to the usual mean-field (BCS) terms, contain exchange-correlation contributions that depend on the superconducting order parameter. An LDA-type functional for these exchange-correlation terms has recently been constructed. It is proposed to solve numerically the microscopic Bogoliubov-de Gennes equations for the high temperature superconductors with this first-principles functional. The solution is expected to shed some light on the pairing mechanism in these materials. Organiser Prof. B.L. Gyorffy (Bristol). Collaborators Dr. Z.Szotek & Dr. W.M. Temmerman (Daresbury), Prof. E.K.U. Gross (Wuerzburg), Prof. O.K. Andersen and Dr. O. Jepsen (Stuttgart)

(f) Magnetic materials with non-collinear magnetic order

Non-collinear magnetic order occurs when the magnetic moments are not parallel or antiparallel to a well defined axis of magnetization. This can arise due to competing ferro- and antiferromagnetic exchange interactions, due to fluctuating local anisotropies, and due to relativistic effects. Non-collinear magnetism has been found in many different materials: disordered systems, magnetic intermetallic compounds, magnetic insulators, thin films and multilayers. Ab-initio calculations of non-collinear magnetic structures are of considerable complexity. Therefore a workshop is needed to share the experiences of the various groups concerning techniques to implement the calculations. Organiser Prof. J. Kuebler (Darmstadt). Other collaborating groups: Prof. J. Hafner (Wien), Prof. H. Dreysse (Strasbourg), Dr. J. Staunton (Warwick), Dr. S. Bluegel (Juelich), Dr. L. Nordstrom (Uppsala)

(g) Molecular processes on oxide surfaces

This project would kick-start the application of the Programme ab initio density functional calculations to an area of wide-spread interest in chemistry and materials science. Applications include catalysis, environmental sensors, and interaction of atmospheric gases with paint. The Programme would bring together those capable of doing the calculations with other scientists in the field, both experimentalists and theoreticians using older less satisfactory methods. It is suggested that the research should start with TiO_2 following recent calculations on the bulk material and low index surfaces. The study of several important simple gases (O_2, CO, CO_2, H_2O, SO_2) with both perfect and defective surfaces would be desirable. A major aim would be to interpret the wealth of already existing experimental data. Organiser Dr. E.Wimmer, Biosym/MSI Paris,France. Other participants Prof. M.Gillan, Keele, UK and others from the network, and experimentalists outside the network.

(h) Development of an improved LAPW code.

The LAPW method is an ab-initio method which within density functional theory is universally applicable to all atoms of the periodic table and to systems with compact as well as open structures. It is generally considered to be the most precise electronic structure method in solid state physics. Due to the all-electron nature of the method, magnetism is included rigorously and nuclear quantities e.g. isomer shift, hyperfine field, electric field gradient, and core level shift are calculated routinely. Also open systems such as surfaces, clusters or inorganic molecules represent no problem of principle. The capability of calculating the forces exerted on the atoms within the LAPW method opens the gate to structure optimization and molecular dynamics and puts this method up on the same category as the widespread pseudopotential method, but able of treating systems painful or unattainable by the pseudopotential method (at substantial extra computing cost).

It is our aim to pool the experience and focus the effort of developing LAPW codes capable to do molecular statics and molecular dynamics simulations on (parallel) computer facilities (e.g. T3E). The codes will be applicable to nonmagnetic and magnetic systems allowing for collinear

and non-collinear magnetism as well as spin-orbit interaction. One particular focus is to explore the possibilities to extend the method to larger systems. These codes should become available by hands-on-program type workshops and its power should by demonstrated by applications to some challenging problems. Organiser Dr. S. Bluegel and coworkers, Forschungszentrum, Juelich, Germany . Other major groups are: TU-Vienna, Wien, Austria (Ass.Prof. P. Blaha and coworkers). University of Uppsala, Uppsala, Sweden (Dr. L. Nordstrom and coworkers). University of Vienna, Wien, Austria (Ass.Prof. R. Podloucky and coworkers), Fritz–Haber Institut der MPG Berlin, Germany (Prof. M. Scheffler and coworkers).

(i) Advances in techniques of Car-Parrinello calculations

Suggested improvements in the numerical algorithms continue to appear in this very important methodology. Two workshops two years apart are needed to share experience and evaluate these developments in various contexts. Currently being explored in Europe and USA are ultrasoft pseudopotentials, adaptive grid coordinates, multigrid methods, wavelets and real space kinetic energy. The CECAM workshops and bi–annual Trieste meetings may also be concerned with these issues, or may not. Either way, the issues are important for quite a lot of Programme members, and it must be possible for them to participate in the discussions. Organiser Prof. D.Bird, Bath, UK. Other prospective participants, at least 20 groups across Europe.

(j) Lengthening the time scale for calculations with thermal agitation and other dynamic processes

Unfortunately almost all ab initio simulations are still done in static form, effectively at zero Kelvin, because of the limitations of computing power. This workshop followed by a collaboration would firstly develop efficient adaptations of existing pseudopotential codes for computers with parallel architecture such as a 200 processor Cray T3E. Secondly it would develop much faster but somewhat approximate methods based on a tight binding formalism, but anchored to ab initio benchmarks. In each case there are several options to be explored in a workshop. Intended initial applications include deposition, growth and diffusion on semiconductor surfaces; and STM manipulation of surface structures. Dissemination of both codes would be through articles in the Newsletter and through a hands-on workshop or ad hoc collaborations. Organiser Prof. R. Nieminen, Helsinki, Finland. Other participants Prof. M. Scheffler, FHI Berlin, Germany; Prof. J.L. Martins, Lissabon, Portugal; Prof. J. Norskov, Lyngby, Denmark; Prof. J. Hafner, Vienna, Austria; Prof. M. Gillan, Keele, UK; Dr. S. Bluegel, IFF Julich, Germany.

(k) Adhesion of oxide-metal interfaces

This subject of immense and ubiquitous importance in materials science and chemistry (corrosion, microelectronics, catalysis, implants, protective coatings) is ripe for the application of the techniques of the Programme. The nature of the bonding is complicated and does not fit neatly into the usual catogories of ionic, covalent, metallic or Van der Waals, so that ab initio

calculations with the Programme techniques are essential. Two successful calculations in this field have been reported and point to several interconnected issues for discussion and collaborative investigation. (i) The nature of the bonding at interfaces with transition metals and non-transition metals. (ii) How and why is the adhesive energy affected by sulphur which weakens interfaces such as Nb-Al_2O_3. (iii) Can the generalised Harris-Foulkes functional be applied usefully in this area. (iv) The development of a simplified tight binding approach and testing it by fully selfconsistent calculations. (v) The development of the Discrete Classical Model as a faster semi-empirical scheme for larger areas of interfaces, and testing it against ab initio calculations. Experimental electron microscopists would generate data to test the theoretical modelling of structures. The workshop would involve those capable of doing the calculations from physics and experimentalists with interest in the applications. Organiser Prof. M.W.Finnis, Belfast, Northern Ireland. Other participants: Dr. H.Polatoglu, Thessaloniki, Greece; Dr. F.Ernst, Stuttgart, Germany; Prof. M.Gillan, Keele, UK; Dr. C. Noguerra, Paris, France; Dr. E. Kotomin, Riga, Latvia; Dr. T. Deutsch, Grenoble, France. Participating experimentalists: Prof. M.Ruehle, Stuttgart, Germany and Prof. A. Bourret, Grenoble, France.

(l) Molecular compounds

Charge transfer salts exhibit a dazzling variety of different structural and electronic phase transition. Members of this class are superconductors, ferroelectrics, antiferro- and ferrimagnets, and exhibit Peierls and neutral to ionic transitions. Close to the transition spin and charge solitons have been observed. The transitions can be driven by pressure, temperature, photoirradiation etc. Charge transfer salts are molecular crystals with typicaly two types of large organic molecules assembled in low dimensional structures. Thus they exhibit features ranging from zero to three dimensions. These structures are an ideal ground for fundamental studies, which may help in the understanding of other low dimensional and correlated materials.

Despite active research over several decades, a detailed microscopic understanding of these materials is still elusive. The structural complexity has prohibited accurate first-principles calculations in the past. Only recently this situation changed owing to new simulation techniques such as the Projector Augmented Wave method developed at the IBM Zuerich Research Laboratory, which will be useful to understand materials of technological interest such as organic magnets, superconductors, and dyes, conducting polymers and materials for light emmitting diodes. Organiser Prof. C. Koenig (Rennes). Other participants: Dr. P.E. Bloechl (Zurich), Dr.M. Springborg (Konstanz), Prof. K. Schwarz (Vienna)

(m) Application of recent advances in density functional theory to develop practical codes and functionals for excited electronic states

Traditional density functional theory in principle applies to ground state structures and properties only, so that electronic excitations are not given sufficiently accurately. A workshop would discuss recent theoretical ideas intended to overcome this problem and how to develop

them into practical computational tools, to be implimented by a subsequent collaboration. Dissemination would be through the Newsletter, plus a hands-on training course or/and ad hoc collaborations. Initial intended applications include light emission spectra from wide-gap semiconductors, and photoluminescence of defect complexes in doped nitrides. Organiser Prof. R.Nieminen, Helsinki, Finland. Other participants Prof. B.I.Lundqvist, Chalmers, Sweden; Prof. E.K.U.Gross, Würzburg, Germany.

(n) Application of ab initio electronic structure calculations to industry

The scope covered by the other listed workshops clearly implies the applicability of ab initio electronic structure calculations to industrial research. Indeed some of the methodology used in the research community was developed at AT & T Bell Labs in connection with identifying various types of impurity centres in semiconductors. A few ab initio electronic structure calculations are carried out in industrial research laboratories, and many more can be envisaged in the future with the growth in computer power and further improvement and development of algorithms. Some time during the next 5 years the time will be ripe to bring our community closer together with researchers from industry. The industry people would educate the academic community about the type of projects they would like to see tackled, and the computational community would inform industry about what has been done and is technically feasible in the near future. There will probably be a need to set up channels of communication for specific areas of application. Organiser Dr. E. Wimmer, MSI-Biosym, Paris.

Appendix 2 Programme Board and Coordinating Committee

Note: The Board would be in continuous virtual consulatation by e-mail with one real meeting in 5 years. The Coordinating Committee (denoted by **cc**) would be responsible for decisions by e-mail and one real meeting per year.

		e-mail
cc	Prof. V. Heine,FRS (Chairman)	vh200@phy.cam.ac.uk
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