The story of Psi-k: From CCP9 to Psi-k

This is a brief, personal and unofficial account of the first 25 years of the Psi-k Network, put together by members of the Band Theory Group at Daresbury Laboratory. We felt with some sense of urgency that it was important to record our own recollections, particularly of events in the early days and of the subsequent evolution of the Network as our field itself evolved technically and intellectually. This is how we saw things; it is in no way an "authorised history" of Psi-k[1].

The idea of creating Psi-k Network in a way originated from ***CCP9***, the UK's Computational Collaborative Project No 9, on the "***Electronic Structure of Solids***", funded through the UK's Science Research Council (SRC) in 1981. Volker Heine (Cambridge) was instrumental in establishing CCP9, one of a number of computational collaborative projects (CCPs), funded at the time by SRC to support research at UK's universities. Balazs Gyorffy (Bristol) became the first, long term, CCP9 chairman, and Walter Temmerman (Bristol, Daresbury Laboratory), its scientific secretary. Walter did his PhD with Balazs Gyorffy on the realistic first-principles KKR-CPA description of the electronic structure of a disordered, substitutional random alloy. In the process of his research he became one of the first people in the UK whom one could call a practitioner of computational science, the emerging discipline, that some regarded with suspicion. He has done a great deal to establish its credibility in condensed matter research. As the CCP9 scientific secretary Walter joined the Theory Group at Daresbury Laboratory, then part of the Science Research Council. That was very exciting time for the Daresbury Laboratory, as the building of the Synchrotron Radiation Source (SRS) was being completed and the Cray 1s computer had just arrived. The key tasks of the Theory Group were to support the synchrotron radiation science programme and to establish the portfolios of various CCPs placed at the Laboratory. Walter worked on both tasks, but his focus was CCP9. Together with Balazs Gyorffy, G. Malcolm Stocks (Bristol, Daresbury, Oak Ridge), and others, they worked hard to get a national "band theory project" off the ground to provide collaborative theoretical and computational support to the condensed matter research done in UK and on SRS. Many scientists, often from abroad, converged on the Laboratory to use the SRS and computer facilities, and CCP9 quickly became involved in many collaborations not only with the UK's scientists but with also those from abroad. One of the first tasks of Walter was to import and adopt Ole Krogh Andersen's (MPI Stuttgart) LMTO computer code, as a "workhorse" for self-consistent band structure calculations. That was the beginning of a productive collaboration with Ole and his Stuttgart group. Over the years, CCP9 has become a key resource for the UK condensed matter research community, both theoretical and experimental. Volker Heine once referred to the CCPs as the "jewel in the crown" of the UK Research Councils. Of course, CCP9, although a UK initiative, always had many colleagues and collaborators from outside the UK (see the General News sect. of the Psi-k Newsletter No 102 at https://psi-k.net/download/newsletters). So, it had a European aspect from its inception. Many scientists associated with CCP9 came to feel that the collaborative approach embodied in CCP9 would work best on a European scale and, after discussions with many European colleagues, it was decided that the future of our field lay in European collaboration. Thus creating a CCP9-like, European-wide, network has become an important goal for the condensed matter research community and search for funding began. The greatest opportunity presented itself with the European Union's Human Capital and Mobility (HCM) Framework III Programme (FP3). A proposal application to FP3, prepared by Volker Heine, always a great champion of European science, and Walter

[1] Which, by the way, would be a good idea.

Temmerman, to create a network of European researchers in the field of "***Ab-initio (from first-principles) electronic structure calculations of complex processes in materials***", was successful and granted three year funding of in total 400k EUR, from 1994 to 1996. On the suggestion of Walter Temmerman (the Network's coordinator), this newly funded network was named "Psi-k Network", referring to the wave function Ψ of an electron in state k (at the early stages of its existence written as Ψ_k), which has become its unique characteristic, very quickly well-known all over the world.

The aim of Psi-k was to promote excellence in the subject of quantum mechanical calculations for electronic properties of solids through collaborations across Europe, including helping those in smaller, new or isolated research groups. At the beginning, in total about 200-300 European scientists were part of Psi-k, including both established scientists and their PhD students and postdoctoral fellows. They came from **40** funded nodes (Belgium – one node, Denmark – two nodes, Finland – one node, France – five nodes, Germany – 10 nodes, Great Britain – six nodes, Greece – three nodes, Ireland – one node, Italy – three nodes, Portugal – one node, Spain – one node, The Netherlands – two nodes, Austria – three nodes, Switzerland – one node). In line with the proposal application, the Network was organized around **12** Working Groups, **six *horizontal*** and **six *vertical*** ones, the former referring to methods and the latter to applications. Specifically, the horizontal Working Groups were: H(a) Density Functional Molecular-Dynamics Techniques [Spokesperson: J. Martins (Lisbon)]; H(b) Muffin-tin Techniques [Spokesperson: O. K. Andersen (Stuttgart)]; H(c) Improved Density Functionals [Spokesperson: A. Svane (Aarhus)]; H(d) Pseudopotential Techniques [Spokesperson: V. Heine (Cambridge)]; H(e) Algorithms for Parallel Computers [Spokesperson: W. M. Temmerman (Daresbury Laboratory)]; and H(f) Green's Function Techniques [Spokesperson: J. E. Inglesfield (Nijmegen)]. The vertical Working Groups were: V(a) The Electronic Structure in the Normal and Superconducting State [Spokeperson: B. L. Gyorffy (Bristol)]; V(b) Magnetism [Spokeperson: P.H. Dederichs (Juelich)]; V(c) Reduced (0-1-2) Dimensionality [Spokeperson: O. Bisi (Trente)]; V(d) Oxide Materials [Spokeperson: M. Gillan (Keele)]; V(e) Molecular and Organic Solids [Spokeperson: C. Koenig (Rennes)]; and L) Large systems [Spokeperson: M. Finnis (Stuttgart)].

The informal inauguration of Psi-k took place at a meeting of the spokepersons in the Max-Planck-Institute (MPI) in Stuttgart in September 1993, while the real operations of the Network started in January 1994, with the first Psi-k Newsletter published in February 1994. At the meeting of September 1993, a Network Management Board (NMB) was set up, the general and organizational matters were discussed, and details established regarding Network's budget for the duration of its existence and the coordination of specific activities. Volker Heine was established as the first chairman of the Psi-k Network, and Ole Krogh Andersen as the vice-chairman. They, together with the Network's coordinator, Walter Temmerman, and the remaining spokepersons of the 12 Working Groups, plus M. Scheffler (Berlin), V. Van Doren (Antwerp), J. Norskov (Lyngby), C. Patterson (Dublin), F. Flores (Madrid), N. Stefanou (Greece), and P. J. Durham (Daresbury Laboratory), formed the Network Management Board, overlooking spending/finances and also approving specific activities of the Network. At the 2nd NMB meeting in Paris, in March 3, 1994, which was the first meeting after Psi-k had started its official activity, Walter Temmerman, who had fully coordinated the EU HCM application, was thanked by Volker Heine *"... for the enormous amount of work he had put into making the Psi-k Network to work"*, asking to have this recorded in the minutes of the meeting (see the Psi-k Newsletter No 2 at https://psi-k.net/newsletters). In total, until December 1997, the NMB met **eight** times to discuss both

the organizational and scientific matters. This number resulted from the fact that at the end of the third year of Psi-k's activity, EU allowed Psi-k to run for a fourth year, namely until the end of December 1997, but with no additional funding. Also, in addition to the original 40 funded nodes, more than 20 unfunded nodes, also from the Central and Eastern European countries, joined Psi-k, to benefit from its services and activities.

The Network's mission of bringing together all the European scientists working in the field of electronic structure was often referred to as creating a European-wide "family" of all the ab-initio researchers. This "family" aspect was from the very beginning stressed by Ole Krogh Andersen and subsequently it became a principal objective for the whole Psi-k Network. This was facilitated through collaborative visits, workshops, and other 'mobility' activities, as dictated by the nature of the HCM Programme, throughout the period of Network's operations, until the 31st of December 1997. The organization of the first large international scientific conference, where all the important/recent scientific accomplishments in the Network's field could be presented, was the culminating point of the Network's activity. Also scientists from outside Europe were welcomed to participate. This ***First International Psi-k Conference (Psi-k1996) took place on the 17-21 September 1996 in Schwaebisch-Gmuend (Germany), and its organizers were Ole Andersen (chairman) and his MPI Stuttgart Group*** (see Fig. 1)**.**

The conference was very successful and set the standard for this field, becoming the envy of many scientists all over the world. It gave an incentive to the NMB to seek further funds for such conferences and Psi-k activities in future, for many more years to come, beyond the end of December 1997. This conference had **319** participants. Most PhD students and postdoctoral fellows were funded by the Network. In addition, extra European funds were obtained to support students from countries not belonging to the EU. The conference had **three** parallel sessions to cover **37** subject topics, **57** invited speakers, plus **235** oral and poster contributed presentations. More information on this Conference can be found in the Psi-k Newsletter No 17 at https://psi-k.net/newsletters.

Fig. 1 The Schwaebisch-Gmuend Congress Centre where the Psi-k1996, Psi-k2000, and Psi-k 2005 Conferences took place.

In addition to the conference, the other regular Psi-k activities/operations that started at the beginning of 1994 and ran until the end of December 1997, resulted in: **six** hands-on computer codes training courses (5days each), **18** organized or co-organized workshops (2-6 days each), **253** supported participants to workshops/meetings, **57** collaborative visits (of less than two weeks each), **14** collaborative visits (of more than two weeks, but less than a month each), **eight** secondments (of one month or more each), **133** common publications acknowledging the Psi-k Network support, as well as many more common papers published without asking for the Psi-k financial support. **Three** major computer codes were widely shared within the Psi-k Network, and many more, less widely used, codes were developed or disseminated in collaboration within the Network. In addition, **seven** visiting scientists or consultants from outside the Network to workshops/meetings were supported. Establishing a ***Psi-k mailing list*** and a ***bi-monthly Psi-k Newsletter*** of both informative and scientific nature were also very valued outcomes of the Psi-k Network, handled by Z. (Dzidka) Szotek (Daresbury Laboratory). From the very beginning of Psi-k, the Psi-k Newsletter was its main medium for information, each containing most important/relevant news from all the different Working Groups of Psi-k, reports on organized workshops and/or individual collaborative visits, job/meeting/workshop announcements, abstracts of newly-submitted research manuscripts and/or recently published scientific papers. Apart from presenting all the Psi-k activities, the Newsletter also reported on the relevant events and initiatives, including conferences, training courses and post-doctoral positions, outside of it. In total **24** Psi-k Newsletters had been published by the end of 1997. The '***Scientific Highlight of the Month***' section of the Psi-k Newsletter was established right from the beginning, containing comments on scientific papers, write-ups on recent scientific developments, review articles, usually volunteered by or solicited from various European research groups participating to the Network, but sometimes also from outside of it. The Psi-k Newsletters became rather popular fairly quickly and more and more scientists from further afield joined the Psi-k mailing list to receive the Newsletters as well as all the Network announcements. At the later stages Psi-k has also got its webpage set up, where all the Newsletters and announcements could be found, in addition to being also distributed by email or accessed via the ***anonymous ftp***. In the words of Volker Heine "… the Psi-k Newsletter perhaps more than anything else has created a cohesive European community of researchers in the '**A*b initio electronic structure field***' where previously there had been many rather isolated individuals and some largely national connections" (see the final report on the HCM Psi-k Network activity in the Psi-k Newsletter No 25, at https://psi-k.net/newsletters).

Summarizing the first four years of the Psi-k's activity, it should be stressed that this Network created an active and intensely cooperating electronic-structure community in Europe and that this community has achieved world-wide leadership by a common pursuit of excellence in this field. It is important to say that, citing Volker Heine, "… the Psi-k Network has sown very many seeds which we can see growing but whose 'fruits' lie in the future". Two of these seeds have been the new EU Training and Mobility of Researchers (TMR) Networks, funded by the EU Framework IV Programme (FP4). Since the EU rules for the TMR Networks were quite different from those of the HCM Networks, the new TMR Networks focused primarily on a number of research projects. The first of those new networks, the "***Interface Magnetism***" Network (TMR1) (see Fig. 2), operating from 01.09.1996 until 31.08.2001 (with no extra funding for the fifth year of operation), grew out of the ***"Magnetism" Working Group of the Psi-k Network*** (with Walter Temmerman its coordinator and Peter Dederichs its chairman), consisting of **six** research projects accompanied by seven to eight three year postdoctoral positions, placed in different EU countries than the post-docs' countries of origin, thus creating deep and active European collaborations. The specific topical

projects/nodes were: 1. Interlayer coupling [Node; Bristol, UK, post-doc: N. Lathiotakis (GR)]; 2. The magnetic anisotropy and surface structure [Node: Uppsala, Sweden, post-doc: J. Henk (DE); Node: Juelich, DE, post-doc: R. Abt (AT)]; 3. Giant Magneto Resistance (GMR) [Node: Philips, The Netherlands, post-doc: A. Brataas (NO)]; 4. Spin-polarised spectroscopies [Node: Vienna, Austria, post-doc: U. Pustogowa (DE); Node: Daresbury, UK, post-doc: A. Ernst (DE)]; 5. Tight-binding KKR-Green's Function Methods [Node: Juelich, DE, post-doc: N. Papanikolaou (GR)]; 6. Real space tight-binding LMTO method [Node: Strasbourg, France, PhD student: I. Galanakis (GR)]. In parallel to these focused projects, some funding was also secured to continue the usual Psi-k activities, namely the Psi-k Newsletter and other general information services, together with funding small meetings, workshops, and support of short collaborative visits. Owing to that, the Psi-k activities could run in parallel with the research projects of the TMR1 Network, further benefiting the whole Psi-k family, beyond the 31 December of 1997. During the five year period of its operation, the TMR1 Network had many scientific, training and networking successes, such as e.g. the year 2000 Agilent Technologies Europhysics Award won by the Network member, Gerrit van der Laan (Daresbury Laboratory), together with Paolo Carra (Grenoble) and Gisela Schuetz (Wuerzburg), for the "Pioneering work in establishing the field of magnetic X-ray dichroism" (This award is given for "work leading advances in the field of electronic, electrical and materials engineering which represents scientific excellence"). The final detailed report on the TMR1 Network activities and many accomplishments can be found in the Psi-k Newsletter No 48 at https://psi-k.net/newsletters, but the quick statistics are: **20** young researchers were employed and trained for **429.5** months in total, **24** researches went on secondments to another node of the Network for one month or more, **82** joint papers were published, **14** workshops and annual meetings were held, augmented by **5** mini-workshops.

The second TMR Network, on "***Electronic Structure Calculations of Materials Properties and Processes for Industry and Basic Sciences***" (acronym TMR "Psi-k", known also as TMR2), sown by the HCM-funded Psi-k Network (see Fig. 2), was meant as a direct continuation of the latter, involving most of the original Working Groups. It started its activity on the 1st of March 1998 to run originally for four years, but was finally prolonged until 28th February 2003 (without additional funding). The aim of the TMR "Psi-k" (TMR2) project proposal was to bring together leading European groups in the area of electronic structure calculations of materials properties and processes at the atomistic level in solid materials and at solid surfaces, and transfer this knowledge and developed tools to industry to increase its competitiveness. The Network was organized around **eight** international groups, employing during the whole period of its operation in total **10** postdoctoral fellows. It was focused primarily on research and developments, with an additional node (W. Temmerman, Daresbury Laboratory) fully dedicated to coordinating dissemination and advanced training, thus securing funding for the usual Psi-k-like networking activities. Axel Svane (Aarhus) was the TMR2 Network coordinator, and Erich Wimmer (Paris) and Volker Heine (Cambridge), respectively, became chairman and co-chairman. The eight research tasks and the scientists in charge of them were: 1. Molecular processes on oxide surfaces (E. Wimmer, Paris); 2. Self-interaction correction calculations on f-electron systems (A. Svane, Aarhus); 3. Oxide interfaces and surfaces (M. Finnis, Belfast); 4. Oxide interfaces and surfaces (M. Gillan, Keele); 5. Non-collinear magnetism (J. Hafner, Vienna); 6. Molecular dynamics with LAPW (S. Bluegel, Juelich); 7. Electron excitations and optical properties (R. Nieminen, Helsinki); 8. Superconductivity (E.K.U. Gross, Wuerzburg). Note that the hired post-docs could only come from the EU countries or countries associated with the EU, but were to be placed outside the countries of post-docs' origins. This network operated for **60** months, with **20** young researchers financed under the contract for a total of **371** postdoc man-months, which

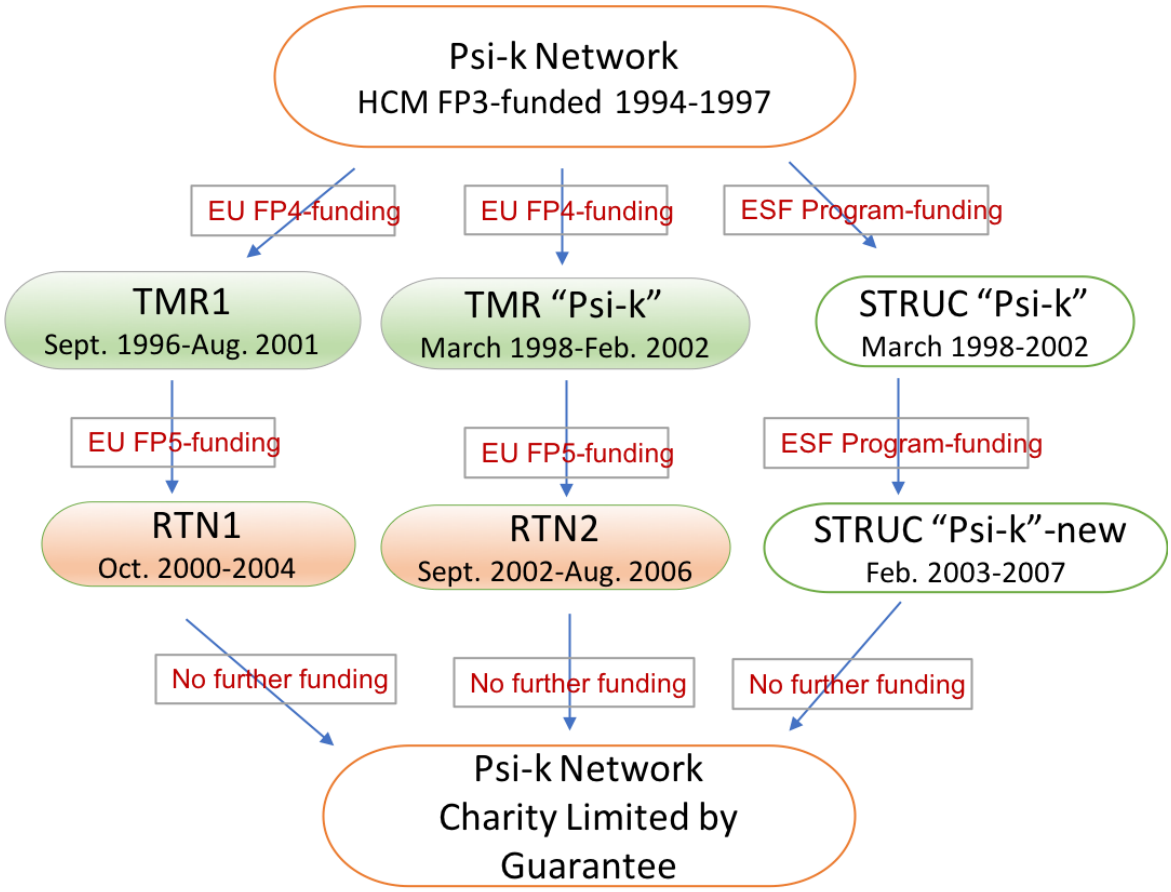

Fig. 2 A Schematic presenting how the Psi-k, its structure and funding, evolved throughout the years, from its inception in 1994 until 2007, after which the Psi-k Network Charity Limited by Guarantee (Psi-k.org) was established as the only means of funding.

has exceeded the contractual number of 264 by 40%. A total of **27** workshops, mini-workshops and other scientific/coordination meetings were organized and fully or partly supported by the Network grants. There were **61** joint publications and **71** publications involving the Network's postdoctoral fellows, with several more in the pipeline due to continuing collaborations. Moreover, all young researchers have continued after their Network's association with employments in academia or industry. The main effort of the Network was devoted to the advancement of the ab initio quantum mechanical modelling of solid state systems. The final report of this Network can be found in the Psi-k Newsletter No 57 at https://psi-k.net/download/newsletters.

As mentioned above, the two TMR Networks and their funding had to be dedicated more to research projects than to other, Psi-k-like, activities. Therefore a dedicated proposal application on "***Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces***" was also submitted by the original Psi-k NMB to the European Science Foundation (**ESF**) Programme for a five year funding for networking and collaboration activities across the whole Europe, in the spirit of the original HCM Psi-k Network, thus creating a sort of a "mega-network". This application was successful, giving the network funding for five years (1998-2002), allowing it to continue publishing the Psi-k Newsletters, which, however, had a more general structure, accommodating news of all the Networks that derived from the original HCM Psi-k Network, and presenting all the

informative and scientific services to which all the European scientists active in the electronic structure field could have access. This ESF Programme Network (with the acronym STRUC Psi-k) (see Fig. 2) aimed primarily at organizing the next Psi-k international conference Psi-k2000 (in cooperation with TMR1 and TMR2), workshops and meetings of major collaborations, short visits for small collaborations and individual consultations. The other important mission of the STRUC Psi-k Network was funding hands-on workshops for disseminating computer codes and secondment visits. Also a relation to industry and wealth creation was given some importance. It should be noted here that only scientists from the European countries that contributed to the ESF Psi-k Programme (STRUC Psi-k) (in total 17 countries) could benefit from the available activities/funds. The whole operation of the Network was overlooked by a Programme Board consisting of **32** members with a wide scientific and geographical spread, however, the final executive decisions have been made by a Coordinating Committee of **11** members, who had specific areas of responsibility. The members of the Committee were: Volker Heine (chair), Juergen Hafner (co-chair), Walter Temmerman (secretary), plus Stefan Bluegel, Hugues Dreysse, Mike Finnis, Eberhard Gross, Jose-Luis Martins, Risto Nieminen, Rafaele Resta, and Erich Wimmer. The ESF Network started its full activity in early1998, at a common meeting with the TMR2 Network.

One of the outcomes of the ESF STRUC Psi-k Network was *the* ***Second International Psi-k Conference (Psi-k2000) which took place on the 22-26 August 2000 in the Congress Centre in Schwaebisch Gmuend, Germany*** (see Fig. 1). It was organized by the Daresbury Laboratory Group with Paul Durham as its chair, and co-funded by the ESF-, TMR1-, and TMR2-Networks. The Conference was run in **three** parallel sessions over four days. There were **four** plenary talks, **101** invited talks, **112** contributed talks and about **160** poster presentations. For the latter there were **two** dedicated four-hour long evening sessions, where free food and drinks were also available to keep participants relaxed and motivated till late hours! The conference was attended by **424** participants, with the largest representation from Germany (**137**), followed by the United Kingdom (**53**), then France (**29**), Austria (**22**), Italy (**20**), Finland (**19**), Sweden (**19**), Spain (**13**), The Netherlands (**10**), Denmark (**9**), Czech Republic (**8**), Poland (**5**), Switzerland (**5**), Ireland (**4**), Belgium (**3**), Russia (**3**), Greece (**2**), Hungary (**2**), Portugal (**2**), Norway (**1**), Slovakia (**1**), Slovenia (**1**), and Ukraine (**1**). From outside Europe there were **31** participants from the USA, **15** from Japan, **3** from Brazil, **2** from Argentina, and **1** from New Zealand. A full report on the Conference can be found in the Psi-k Newsletter No 41 at https://psi-k.net/newsletters.[2]

Since the funding of the TMR1 Network on "Interface Magnetism" was due to come to its end at the end of August 2001 (having run for five years, but with no extra funding for the fifth year), its Management Board submitted to EU Framework V Programme (FP5) a proposal for a ***Research Training Network (RTN) on "Computational Magnetoelectronics" (RTN1)***, meant in a way as a continuation of TMR1 (see Fig. 2). It was successful in receiving funding for four years, and able to start its activity from 1st of October 2000. Magnetoelectronics means, in the broadest possible terms, the manipulation of the electronic charge transport by the spin-degrees of freedom, and in the more narrow technical sense it refers to a new electronics which uses magnetoresistive properties in device applications. The research objectives of this Network were to use the power of Density Functional Theory (DFT) to model, understand and predict the transport properties of materials and material systems relevant to magnetoelectronics. This was a broad effort, ranging from the solution of

[2] The reaction of American participants at the conference was intriguing. Paul Durham recalls that a senior member of the American research community was reported by a reliable source as having said "We've got to do something. These people [the members of the European Psi-k family] are beating the pants off us!".

the basic quantum mechanical equations for the ground state of these systems to realistic calculations of the spin-dependent transport properties of industrial prototypes. Fundamental to this was the use of the Green's function language, allowing a transparent formulation of spin-dependent transport and guaranteeing high consistency of the calculated results. The proposed new RTN Network was based on three inherently connected themes, namely ground state properties of magnetoelectronics materials, probing the electronic structure of magnetoelectronics materials, and spin-transport. These themes were organized into **10** collaborative, scientific tasks of Ferromagnet/Semiconductor Interfaces, Ferromagnet/Oxide Interfaces, Ferromagnet/Superconductor Interfaces, Magnetic Nanostructures, Magnetic X-ray scattering, Giant Magnetoresistance, Spin Mesoscopics, Experimental Data and Assessement of Applicability. After a year or so of the Network's activity **one more** scientific flagship project was introduced on the "Novel Magnetoelectronics Materials", due to the fact that the field of Magnetoelectronics had progressed enormously since the RTN Network was established. In this new project more emphasis was put on methods which allowed correlated electron systems to be described, such as LDA+U and SIC-LSD, and also more demanding approaches as GW and DMFT were actively developed. In addition to these scientific tasks, the Network had **three** dissemination tasks of **six** Topical Workshops, four Annual Meetings and **24** issues of the Psi-k Newsletters published during the period of the Networks operation. The Network's composition of **10** nodes had as distinguishing features nodes that comprised all relevant national theoretical activities: in Daresbury Laboratory (Walter M. Temmerman), Juelich (Peter H. Dederichs), Halle (Patrick Bruno), Paris (Albert Fert), Vienna (Peter Weinberger), Twente (Paul Kelly), Uppsala (Borje Johansson); the participation of two Central European nodes from Hungary (Janos Kollar) and the Czech Republic (Ilja Turek); an experimental/industrial team member (Thomson; later renamed as Thales) in the French node, and a US node (Peter Levy), which substantially added to the interest of the community. Altogether **12** young research positions were available.

Following in the footsteps of the TMR1 Network, to secure a continuation of funding, the NMB of the TMR "Psi-k" (TMR2) Network also submitted a proposal to the EU FP5 Programme for a new ***RTN*** network on ***"Ab-initio Computation of Electronic Properties of f-Electron Materials"*** (known also by the acronym ***"psi-k f-electron"*** or ***RTN2***) (see Fig. 2), with Axel Svane its coordinator. The proposal was funded and the Network started its operation in 2002. The research project of RTN2 was *to provide a substantially improved theoretical understanding of the physical properties of materials containing atoms with incompletely filled f-shells*. There were two threads to this project. First, the application of existing methodology to specific problems of high current priority, and second, the development of new methodology for a more accurate description of f-electron systems. The expected outcome of the latter was to generate a computer code implementing DMFT for describing fluctuating f-electrons into state-of-the art ab-initio electronic structure methodology and then applied to calculate Ce and Pu phase diagrams, as well as several rare earth and actinide elements and compounds. The Network had in total **seven** post-docs and the institutions involved were: University of Aarhus (Axel Svane), Daresbury Laboratory (Walter Temmerman), Rutgers University (Gabriel Kotliar), IFW Dresden (Manuel Richter), Katholieke Universiteit Nijmegen (Alexander Lichtenstein), Ecole Normale Superieure Paris (Antoine Georges), Uppsala University (Olle Eriksson), and Materials Design sarl, Le Mans (Erich Wimmer). The final report of this Network, concentrating on the scientific outcome and number of publications, can be found in the Psi-k Newsletter No 78 at https://psi-k.net/download/newsletters.

In addition to the RTN1 and RTN2 Networks, another EU RTN was funded by the FP5 Programme that had originated from the Psi-k family, with the title "*Ab initio methods for calculation of optical properties of matter*" (**RTN3**) with an acronym **EXCITING**. Although it has not been contributing directly to funding the Psi-k networking and Newsletter initiatives, some of its meetings have been opened to the Psi-k community not directly associated with EXCITING. Also, all the activities of that Network have been presented in the Psi-k Newsletters, so that the broad scientific community world-wide could have access to it.

Such was the success of the first five years of the ESF "STRUC Psi-k" Network, that a follow-up application with the official title "Towards Atomistic Materials Design" was submitted for a further five year funding to continue as a new "mega-network" (with the acronym STRUC Psi-k new) (see Fig. 2), organized around **15** Working Groups; the idea was resurrected from the original very successful EU HCM Psi-k Network, to focus networking on a few particularly promising areas of work and serving the whole European community. The proposed ab initio computer simulations were to cover many areas of science from nano-technology to catalysis, from magnetism to minerals and even to biological macromolecules. A new dimension of this research proposal was computational many-body theory on real materials with strongly correlated electrons. This proposal application was successful and a broad Psi-k networking program could go ahead, starting in February 2003, until the end of 2007. Volker Heine continued as the chair of this follow-up ESF Psi-k Network, with the following three leaders of our research community: Juergen Hafner (Vienna), Matthias Scheffler (Berlin) and Börje Johansson (Stockholm & Uppsala). In addition to the latter, the main investigators of the ESF proposal were 15 spokespersons of the 15 Working Groups (for details see Psi-k Newsletter No 50 at https://psi-k.net/download/newsletters).
In the **10** year period of the stable ESF funding, namely for the 'STRUC Psi-k' and 'STRUC Psi-k new' "mega-networks", Psi-k grew very strongly, with its activities covering nearly all areas of computational materials- and nano-sciences. During those years Psi-k organized a total of **150** workshops, computer tutorials and summer schools. In the last years there were more than **20** activities per year, with more than **1000** participants. There were **two** very successful Psi-k Conferences, namely the **Psi-k2000** conference (see above) and the **Psi-k2005** conference. The latter one, the ***Third International Psi-k Conference (Psi-k2005)***, with the title ***"Towards ab initio materials design"*** (chaired by Risto Nieminen [Helsinki]) was, similarly to the two previous ones, organized in Schwaebisch-Gmuend, Germany (see Fig. 1), on 17-21 September 2005. It was attended by more than **560** scientist, representing **33** countries, from physics, chemistry, materials science, geophysics and biology, who gathered to survey and discuss the latest developments in the field of electronic structure theory and calculations, in the wide sense of the concept. The topics covered a huge selection of themes in condensed matter and materials physics, ranging from new semiconductors to high-temperature superconductors, from magnetism to biomolecules, from surfaces to interfaces to geological and planetary sciences, etc. The programme of the Conference 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. One could see the spectacular progress the Psi-k community had made from the roots in "band structure calculations" to tackle "complex many-electrons problems beyond mean field theories", and to apply the methods to an astounding array of real-world problems with demonstrated industrial relevance. A scientific report on the Psi-k2005 Conference can be found in the Psi-k Newsletter No 72 at https://psi-k.net/download/newsletters.

As can be seen in Fig. 2, the EU funding of the two RTN Networks, RTN1 and RTN2, came to their respective ends in 2004 and 2006. In addition, unfortunately, no further renewal of the ESF Psi-k Programme (STRUC-Psi-k new), "Towards Atomistic Materials Design", could be possible beyond 2007, for several reasons. First, because this would have been a third funding period, representing a problem for ESF, and in fact for any funding organization. Second, over the years, the Psi-k family had become extremely large and scientifically much diversified, differing from the usual definition of a network. For the latter reason, the Psi-k could no longer fit into the EU funding schemes within the Framework VI Programme (FP6), e.g. the I3 initiative (Integrated Infrastructure Initiative), although it has been well recognized that Psi-k had the role of an infrastructure for our community, with a well-developed pattern of research workshops, summer schools and training sessions, often with hands-on experience of codes, etc. Nevertheless, the Psi-k Steering Committee, with its chairman Peter Dederichs, were considering submitting a proposal to the EU FP6 I3 Programme, with a tentative title "*A Software Infrastructure for Atomic-Scale Computer Simulations of Materials for Many Sciences*", with the acronym SIASS. It was to cover both, ab initio simulation and the work of the colleagues in the SIMU community, based more on the statistical mechanics. Although a subgroup of nodes originating from Psi-k has been successfully funded from the EU FP6 Programme for a period 2004-2011 (for the first five years as a NANOQUANTA Network of Excellence (see Sect. 9 of the Psi-k Newsletter No 63 at https://psi-k.net/download/newsletters) and for the next three years continuing as its initiative ETSF (European Theoretical Spectroscopy Facility) I3, partnered with the Barcelona Supercomputing Centre), the idea of getting funding for the SIASS infrastructure had to be abandoned, and other concepts for funding the whole Psi-k family and its operations had to be considered.

A new chapter for Psi-k had to be opened. After many discussions, and owing to a tireless work of Peter Dederichs and Walter Temmerman, a legally independent, non-profit company "Psi-k", namely the Psi-k Charity Limited by Guarantee (see Fig. 2), was established and registered in England and Wales, with Company No 06440198, its office at the Daresbury Laboratory, UK (see Fig. 3), and a Board of Trustees selected from several European countries. Although the structure of the Charity has been very similar to the last ESF Programme Network, the Steering Committee has been replaced by a Scientific Advisory Committee. The management of the finances and the travel expenses, etc., as before, was entrusted to the members of the Daresbury Laboratory. The problem of basic funding of this non-profit company was partially solved by "financial contributions" ("Membership Fees") from the largest and financially strongest European Groups belonging to Psi-k, each donating annually between 2,000 and 10,000 EUR (from smaller groups even between 1,000 and 2,000 EUR), over a five year period, giving the Psi-k Charity a similar budget to the five year budget of the last ESF "STRUC Psi-k-new" Programme. That, however, has not always been sufficient to fund all the planned events. The bottom-up funding of the Psi-k Network (family), from the budgets of its members, has been a novelty in Europe. It shows how successful Psi-k has become that its members have been willing to continue all the activities at their own expense, and Peter Dederichs has worked very hard to get as many contributions as possible. It also shows a strong cohesion within Psi-k which has always been typical of a "family", starting with the EU HCM Psi-k Network and continuing strongly to these days. Following the establishment of Psi-k as a Charity, the original Psi-k webpage was changed to www.psi-k.org to reflect its different status and ways of funding. At the same time changes to the distribution and submission of various announcements were made by creating a 'Psi-k Portal'. This has also allowed for setting up discussion forums, etc. Although in principle more versatile, it has been more complicated in use than the original Psi-k mailing

Fig. 3. Daresbury Lab, Science and Technology Facilities Council, Sci-Tech Daresbury.

list. In any case, soon after establishing the Psi-k Charity, the Psi-k webpage was redesigned and accessible as https://psi-k.net. In a sense, it now acts as the Psi-k archive of all the past and present, relevant materials/files/documents.

All the activities of and the events organized by the Charity were opened to all European scientists. The goals and tasks of the Psi-k Charity were and remain very much the same as those of the last well-proven ESF "STRUC Psi-k new" Programme, with a rich portfolio of workshops (often co-organized with ***CECAM***), hands-on computer code training courses, summer schools, and especially the **two** large Psi-k International Conferences, **Psi-k2010** in Berlin, and **Psi-k2015** in San Sebastian. As in the case of the **three** previous Psi-k Conferences (1996, 2000, and 2005), the Psi-k2010 and Psi-k2015 covered theoretical and computational research of electronic structure and properties of matter, ranging from basic novel concepts and methods to applications for condensed matter and real functional materials to biological systems.
Since a detailed report on the Psi-k2010 Conference (chaired by Matthias Scheffler) can be found both on the Psi-k webpage and in the Psi-k Newsletter No 101 at https://psi-k.net/download/newsletters, here we only give the most important facts. The conference took place in the Henry Ford Building in Berlin. It had over **1000** participants, **five** parallel sessions, with the same number of plenary talks, **120** invited talks, **22** symposia, and about **700** poster presentations. The latter were distributed over **two** sessions, one per day, each covering **350** posters per day, with even and odd poster numbers receiving 1.5 hours slots in succession. Regarding the distribution of participants over their countries and continents of origin, they were as follows: Europe was leading with the highest number of **299** participants from Germany, **96** from the UK, **55** from France, **54** from Italy, **48** from Spain, **46** from Austria, etc. There were just under **80** participants form the USA, but **80** from Japan. In fact, Asia plus Oceania had **118** participants in total, but only **two** participants from Africa.
A new event of this Psi-k2010 Conference was a Young Investigator Award (YIA), set up in the name of Volker Heine, the "grandfather" of the Psi-k family. There was a very well attended dedicated session for this award, where **five** finalists gave 30 minutes oral presentations, and the winner was Christoph Freysoldt (MPI Iron Institute, Duesseldorf).

Similarly to the Psi-k2010 Conference, a report on the Psi-k2015 Conference [co-chaired by Angel Rubio (San Sebastian & Hamburg) and Risto Nieminen (Aalto)] is available on the

Psi-k webpage as a highlight article of October 2015 (see https://psi-k.net/download/highlights/Highlight_128.pdf). Here we only summarize the most important statistics of this conference. The Conference took place in the Kursaal Congress Centre in Donostia-San Sebastian, Spain. It was the largest Psi-k Conference to date, with the total number of participants slightly under **1200**. There were **six** parallel sessions and **five** plenary talks, **160** invited and **180** contributed talks, distributed over **30** symposia. In addition, there were over **700** poster presentations, many of which were displayed during two dedicated sessions, with a buffet dinner served in the same location. The symposia that received the most abstract submissions were: Materials Design (**108**), Novel 2D Materials and Heterostructures (**72**), and Theoretical Spectroscopy (**58**). As at the previous Psi-k Conference, the dedicated YIA session was also present, and the winner was Marco Bernardi for his work/presentation on *"Ultrafast Hot Carrier Dynamics in Materials from Ab Initio Calculations"*. As to the countries and continents of the origin of the participants, the largest number of **986** came from Europe, then **152** from Asia, followed by the USA, Latin America, Africa and Australia (further details can be found on the Psi-k webpage).

Summarizing this 'brief' story of Psi-k, one has to add that the last issue of the Psi-k Newsletter, No 118, was published in August 2013. From then on only the scientific highlights have been continued and handled by Leon Petit (Daresbury Laboratory), with a great support of Peter Dederichs (Juelich). In total **149** highlight articles were published to date and are available on the current Psi-k webpage (https://psi-k.net), as are also all those **118** issues of the Psi-k Newsletters. All the reports, various announcements, etc., which used to be published in the Psi-k Newsletters have also been placed directly on the Psi-k webpage, which presently has about **5000** subscribers from all over the world. The aim of this short story is mostly to give the younger scientists some background and understanding of the effort of many scientist, undertaken **over 25** years ago, to establish a cohesive and intensely collaborating community of ***Ab initio Electronic Structure Research***, bringing all to a very high standard across Europe. Owing to that, Europe has become a leader in this field to the benefit of many. Over the past years, many of those scientists have worked tirelessly to bring Psi-k to what it is now, with various chairmen, starting from Volker Heine (always a "father/grandfather" figure of Psi-k), eventually succeeded by Peter Dederichs, then Risto Nieminen (Aalto), and presently Nicola Marzari (Lausanne). Clearly, many people have greatly contributed to this success story and Peter Dederichs in particular should be thanked for keeping the Psi-k Charity financially capable to continue the usual Psi-k activities. Even after leaving his chairmanship position, he continued providing enormous support to his successor, Risto Neminen. But as Volker Heine himself has remarked "… it has always been Walter Temmerman who has been the true driving force behind Psi-k" (the General News sect. of the Psi-k Newsletter No 102 at https://psi-k.net/download/newsletters). It was an achievement of which he could have been truly proud and the rest of the community truly grateful. Unfortunately, Walter died prematurely in May 2014, after seven years' debilitating illness. We also should mention two other remarkable scientist and prominent figures of Psi-k from its beginning, namely Balazs L. Gyorffy (Bristol), who died in October 2012 (see the General News section of the Psi-k Newsletter No 114 and the 'Scientific Highlight of the Month' section of the Psi-k Newsletter No 115 at https://psi-k.net/download/newsletters), and Axel Svane (Aarhus), the coordinator of TMR2 (TMR "Psi-k") and RTN2 networks, who died in August 2016. To them and all those scientists who have done so much for Psi-k, we want to say a big "thank you".

Before ending this story, it seems appropriate to explicitly enumerate the most important accomplishments of Psi-k:

- Creating an immensely cooperating European “family” of scientists in the field of ab initio computational research covering many important areas of science – this included many real, long-term projects and collaborations between members of the family from ***all*** over Europe;
- Expanding the field of study from basic band theory towards calculating many observables also for complex materials and industrial applications;
- Development of new methods and computer codes, shared and disseminated within the Network, allowing to study not only simple solids but complex materials, also of technological relevance, through e. g. proper treatment of correlations;
- Five international Psi-k conferences were organized in 1996, 2000, 2005, 2010, and 2015, with the respective numbers of participants being 319, 424, over 560, ~1000, and just under 1200;
- Training young research scientists through the research project-dedicated EU Networks TMR1, TMR2, RTN1, and RTN2, in total ~60 post-docs and/or PhD students;
- 149 scientific highlights were published;
- Hundreds of workshops, hands-on computer codes training courses, summer schools, and meetings were organized;
- 5000 subscribers mailing list and a dedicated webpage set up, having also a role of an archive of all the information;
- Well over a thousand common papers published.

Finally, we would like to add that on the 19th of September 2020, Volker Heine will be 90 years old, and Peter Dederichs will become 82 years old on the 23rd of October 2020. Since, due to the coronavirus pandemic, the Psi-k2020 Conference has been postponed until next year or so, here we wish both of them “Happy Birthdays”, once again thanking them for all their efforts and contributions to Psi-k, hoping that Psi-k will grow further and stronger to the benefit of many.

Daresbury Laboratory, May 2020