

Research Networking Programme

Advanced Concepts in ab-initio Simulations of Materials (Psi-k2)

Standing Committee for Physical and Engineering Sciences (PESC)



The research programme of Advanced Concepts in ab-initio Simulations of Materials (Psi-k2) concerns the fast developing method of ab-initio electronic structure calculations, which focuses on the understanding of real materials and the design of new materials with superior properties and functionalities. The approach rests on the basic equations of quantum mechanics, applied to the interacting electron system in a solid. The method does not use any adjustable parameters, and is therefore of 'ab-initio' or 'first principles' nature. Thus these calculations can be applied to all condensed matter systems, ranging from metals, semiconductors and insulators to complicated nanostructures, to materials in the Earth's core or to biological systems such as proteins. Common to them all is the same powerful, but demanding methodology. Due to the steady advance of computers and computational methods, such ab-initio calculations and atom-scale simulations are now an indispensable part of materials science.

The results of a literature search on ISI Web of Science show the importance and growth of this field. The search (keywords: 'ab-initio', 'first principles' and 'density functional') shows a more or less linear increase in the number of worldwide publications per year, with about 16,000 in 2009, an increase by a factor of 6 from 1991. The search also shows (see Figure 1) that Europe is leading globally, ahead of the USA, and with even larger growth than the USA. This growth occurs in practically all European countries, including the smaller and East European countries. Czech scientists, for instance, tripled their number of publications between 2000 and 2010 (see Figure 2).

The present ESF Research Networking Programme Advanced Concepts in ab-initio Simulations of Materials (Psi-k2) was initiated by leading scientists of the European Psi-k community (http://psi-k. dl.ac.uk), the umbrella Network for Electronic Structure Calculations in Europe. Psi-k has existed for 17 years and is largely responsible for the European lead in the field. For the last three years Psi-k has been a Company limited by Guarantee and a Charity according to UK law. It is funded by membership fees from the larger European ab-initio groups.

The running period of the ESF Research Networking Programme Psi-k2 is five years, from January 2011 to January 2016.



Figure 1.

Density functional publications in Europe, USA and East Asia (including Japan, Korea, Taiwan, Singapore and China).



Figure 2.

Comparison of density functional publications in 2000 and 2010 for the 20 European countries with the largest numbers of publications in 2010. In all countries the activities during the last ten years increased strongly.

Aims and Objectives

The tremendous progress achieved in the last 20 years in ab-initio calculations is largely due to the success of density functional theory (DFT). But materials science has now developed to a point where ground-state and excitation energies and other properties must be predicted with even greater accuracy for larger and ever more complex systems, beyond the limit of present methodology. Therefore the present project aims at new concepts and ideas to bring the field forward, with more accurate, powerful and efficient methods.

The future success of our field will very much depend on the availability of more accurate total energies, more accurate activation energies and reaction energies with chemical accuracy, as well as on reliable excitation energies for comparison with experiments and for understanding the response of the materials.

Moreover, there is a strong need to be able to calculate larger and more complex systems, to invent realistic algorithms, which scale only linearly with the number of particles, and last, but not least, to be able to perform multiscale calculations both in space and in time. Finally, different application fields exhibit their own challenging tasks, like the development of global structure optimisation, application of Keldysh Green Function formalism for transport, or understanding and predicting superconductivity in nanoscale systems. These are some of the most important challenges for future electronic structure calculations and represent the central tasks of this Programme.

Topic Areas

A) More accurate Total Energies

Most density functional calculations use the local density approximation (LDA), the work horse of density functional theory. Despite its successes, the deficiencies of this approximation are well known and have led to a long, but only partially successful search for improved exchange-correlation functionals 'beyond LDA'.

At present, there is a strong focus on investigating hybrid functionals, consisting of an admixture of exact exchange to a (semi) local functional. They lead to very good results for molecules and insulating materials, but improved hybrid functionals for metals are urgently needed. Good progress is expected by combining the 'exact exchange' or the optimised potential method with a compatible correlation energy, as, e.g., given by the random phase approximation. Very promising too is the connection with quantum chemistry methods, where the extension to solids represents the challenging problem. Quantum Monte Carlo methods give very good results for relatively small systems. The excellent scaling of this method gives hope for applications to much larger systems on highly parallel supercomputers.

B) Excitations

Excited state properties are very important for comparison with experiment, but also for learning more about the internal interactions and the response to external perturbations. While for many systems LDA single particle energies do a reasonable job for excited states, they fail for the semiconductor bandgaps and even more for medium or strongly correlated systems.

The GW approximation (Hedin, 1965) has been known for nearly 50 years, but we only recently learned how important it is to start from a good ground state functional or to include a very large basis set. Its application to optical spectra should



Figure 3. Energy bands of Sr_2RuO_4 . The quasiparticle bands calculated by DMFT are considerably narrowed and broadened due to lifetime effects as compared to the LDA bands given by dots [Liebsch, A. and Lichtenstein, A. (2000) *Phys. Rev. Lett.* 84, 1591].

include vertex corrections; for magnetic systems, a spin-dependent T-matrix approach is promising. For excitations in correlated materials from transition metal oxides to f-electron systems, the Dynamical Mean Field Theory (DMFT) in connection with the LDA (LDA+DMFT) is the method of choice. Here non-local corrections to the single-site DMFT can be included in cluster DMFT methods. Although the computing time is still very high, a major leap forward can be expected from new algorithmic and computational concepts. A hot topic is now time-dependent density functional theory (TD DFT), which allows the description of matter under the influence of timedependent field to be included. This leads to many new challenges like non-adiabatic molecular dynamics, time-dependent transport on the nanoscale, new exchangecorrelation functionals with memory, etc., so that progress is expected.



Figure 4. Spin-wave dispersion of ferromagnetic FeCo along high symmetry lines in the Brillouin zone. The low-energy branch close to gamma corresponds to the collective precession of the Fe and Co moments. The broadening of the dispersion is due to the coupling to spin-flip excitations (E. Sasioglu, C. Friedrich and S. Blügel, in preparation).

C) Larger and More Complex Systems

Usual density functional methods scale as N³, i.e., like the cube of the number N of atoms. However, if the 'nearsightedness' principle of Walter Kohn is applied, the computational cost should scale only linearly with the number of particles, which means that DFT calculations can be extended to much larger systems. N-scaling codes like ONETEP, SIESTA and CONQUEST have emerged and are very successful. However, more functionalities and more accurate functionals have to be implemented. Also, N-scaling methods for metals would be very desirable, for which new and fresh ideas are needed.

A vast range of materials properties and functions requires comprehensive modelling that extends up to macroscopic length. Even with N-scaling methods available, a multiscale strategy is required, since an increase of the number of particles by an order of magnitude changes the length-scale by only a factor of 2. Multiscale approaches will also be needed to extend the time-scales accessible to ab-initio simulations. Such multiscale techniques have to be adapted to the nature of the problem. For example, kinetic Monte Carlo (kMC) simulations can be used to model catalytic processes with many different competing chemical reactions. Similarly, ab-initio calculations can be linked to force-field molecular dynamics calculations. An analogous strategy can also be used to improve the accuracy of micromagnetic simulations by calculating the exchange coupling constants 'on the fly'.

D) Challenges for Specific Materials

While the previous topics are relevant for practically all materials, a large number of challenges exist which are relevant for specific application fields. For alloys and complex materials this is, for instance, the development of global structure optimisation tools. Moreover, not only the ground state properties are important but also the thermal properties at high temperatures, which for solids can be calculated by phonon theory and in other cases by ab-initio molecular dynamics. For molecular or spintronics transport, the application of Keldysh-Green function formalism is guite relevant. In superconductivity the iron pnictides are a hot problem; new challenges arise also for superconducting nanoscale materials like monolayers and nanowires. Most biologically and pharmacologically interesting processes in the cell occur on a ms time scale or even longer, which requires advanced statistical mechanics approaches. Thus practically every application field has its own methodology problems.

Psi-K WORKSHOPS 2011

In conjunction with ESF RNP "Advanced Concepts in ab-initio Simulations of Materials"

07 – 11 February, Jülich, Germany "Muffin-Tin Recipes - Hands-on Workshop on Electronic Structure Calculations with the FI-EUR Code"

http://www.fz-juelich.de/iff/fleur-ws2011/

09 – 13 February, Zurich, Switzerland "2nd CP2K Tutorial: Enabling the Power of Imagination in MD Simulations" http://www.cecam.org/workshop-529.html

13 – 18 March, Dresden, Germany "Symposium: Theory and Computation of Electronic Structure: New Frontiers" http://dresden11.dpg-tagungen.de/index.html

11 – 14 April, Han-sur-lesse, Belgium "5th International ABINIT Developer Workshop" http://www.abinit2011.be/

22 – 26 May, Magleås, Denmark "Psi-k Research Conference: Cat1P" http://www.cecam.org/workshop-569.html

7 – 10 June, Lausanne, Switzerland "Challenges and Solutions in GW Calculations for Complex Systems" http://www.cecam.org/workshop-562.html

8 – 10 July, Halle, Germany "Workshop on KKR and Related Greens Function Methods" http://www.physik.uni-halle.de/aktuelles/kkrws2011/

10 – 13 July, Zurich, Switzerland "X-ray Spectroscopy: Recent Advances in Modelling and New Challenges" http://www.cecam.org/workshop-537.html

10 – 15 July, Oxford, UK "Psi-k/CECAM/CCP9 Biennial Graduate School in Electronic-Structure Methods" http://www.psi-k.org/Psik-training/psi-k_training2011.shtml

12 – 21 July, Berlin, Germany "Hands-On Tutorial: Toward a First-Principles Understanding of Materials Properties and Functions"

http://www.fhi-berlin.mpg.de/th/Meetings/DFT-workshop-Berlin2011/index.php

17 – 22 July, Obergurgl, Austria "Charge Transfer in Biosystems" http://www.esf.org/index.php?id=7284

30 August – 02 September, Kloster Seeon, Oberbayern, Germany "Strong Correlation from First Principles" http://www.fhi-berlin.mpg.de/th/Meetings/sc1p/

05 – 09 September, Barcelona, Spain "CPMD2011: Extending the Limits of ab-initio Molecular Dynamics Simulations for Materials Science and Biophysics" http://www.pcb.ub.es/cpmd2011/ 15–18 September, Alghero, Sardinia, Italy "Superconductivity 100 Years Later: A Computational Approach" http://www.fkf.mpg.de/~conf/sc100

18 – 21 September, Chester, UK "Self-Interaction Correction: State of the Art and New Directions" http://www.cse.scitech.ac.uk/cecam_at_daresbury/self-interaction_correction.shtml

19 – 23 September, Bremen, Germany Perspectives and Challenges of Many-Particle Methods: Efficient Strategies and Tools For Describing Complex Systems"

http://www.bccms.uni-bremen.de/en/events/cecam_mpm_workshop/overview/ 27 – 30 September, Turin, Italy

"16th ETSF Workshop on Electronic Excitations: Bridging Theory and Experiment" http://workshop.etsf.eu

04 – 07 October, Bremen, Germany "Photo-Meets Electrocatalysis: United We Split (...Water)" http://www.bccms.uni-bremen.de/en/events/cecam_pme_workshop/overview/

10 – 14 October, Bremen, Germany "Prespectives and Challenges of Simulations at Bio-Materials Interfaces" http://www.bccms.uni-bremen.de/en/events/cecam_biomat_workshop/overview/

10 – 14 October, Lausanne, Switzerland "Dynamical Properties of Earth and Planetary Materials" http://www.cecam.org/workshop-551.html

4 – 18 January 2012, Benasque, Spain "Sth School & Workshop on "Time-Dependent Density-Functional Theory: Prospects and Applications" http://benasque.org/2012tddft/

9 – 11 January 2012, Lausanne, Switzerland "Topological Insulators and Non-Perturbative Spin-Orbit Coupling" http://www.cecam.org/workshop-564.html

12 – 14 January 2012, Barcelona, Spain "Computational Condensed Matter Physics and Materials Science from First Principles" http://www.imab.es/FSS012

20 – 22 February 2012, Levi, Finland "Towards Reality in Nanoscale Materials: Interfaces" http://trnm.aalto.fi/



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Programme Activities

Workshops and Training Courses

Within the ESF Research Networking Programme Advanced Concepts in Ab-initio Simulations of Materials, Psi-k will each year organise about 20-30 workshop activities. Most of them will be co-organised and co-funded by Psi-k Charity, some of them also by CECAM. Most of these activities, about 20. will be research workshops and small conferences. This also includes annually one joint Psi-k/CECAM Research Conference on a special high profile topic. Moreover, we will also organise training activities, like computer tutorials (2-3 per year), graduate schools (1 per year) and summer schools (1-2 per year).

As an example, in 2011, the first year of the Programme, in total 24 activities are being organised (see list of **Psi-k Workshops 2011** poster, left page): 19 workshops and small conferences, 3 Hands-on Tutorials, 1 Graduate School and 1 Psi-k/CECAM Research Conference, all co-funded by Psi-k Charity.

Psi-k 2015 Conference

In addition, in 2015, the last year of the Programme, a large Psi-k 2015 Conference for all fields of ab-initio calculations will be organised. The previous conference in the series, Psi-k 2010 in Berlin, was attended by 1000 scientists.

Short Visit Grants

To promote young researchers, collaborative visits of one to two weeks' duration at European partner institutions will be funded.

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- Fonds zur Förderung der wissenschaftlichen Forschung in Österreich (FWF) Austrian Science Fund, Austria
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- Hrvatska zaklada za znanost (HRZZ) Croatian Science Foundation, Croatia
- Suomen Akatemia/Finlands Akademi Academy of Finland, Finland
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- Norges Forskningsråd Research Council of Norway, Norway
- Consiliul National al Cercetarii Stiintifice (CNCS)

National Council for Scientific Research, Romania

- Vetenskapsrådet (VR)
 Swedish Research Council, Sweden
- Schweizerischer Nationalfonds (SNF) Swiss National Science Foundation, Switzerland
- Science and Technology Facilities Council (STFC), United Kingdom

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For the latest information on this Research Networking Programme consult the Psi-k2 website: www.esf.org/psi-k2 and also www.psi-k.org

Cover picture: Charge density oscillations induced in vacuum by an impurity buried below the Cu(111) surface. The anisotropy of the oscillations is a signature of the non-sphericity of the Cu Fermi surface [Weismann, A. et al. (2009) *Science* **323**, 1190]. Figure by S. Lounis

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