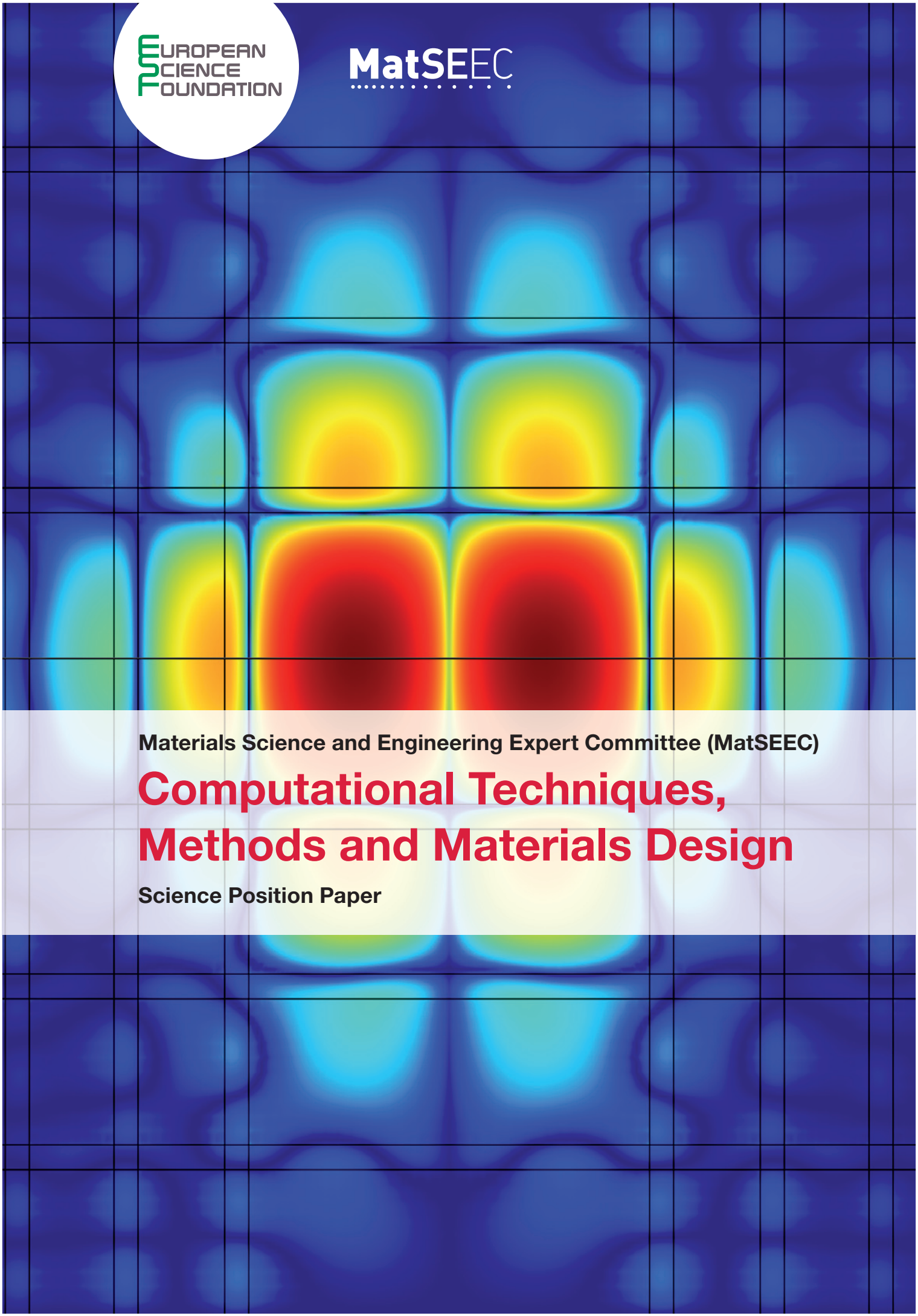

Materials Science and Engineering Expert Committee (MatSEEC)

Computational Techniques, Methods and Materials Design

Science Position Paper

European Science Foundation (ESF)

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Materials Science and Engineering Expert Committee (MatSEEC)

MatSEEC is an independent science-based committee of over 20 experts active in materials science and its applications, materials engineering and technologies and related fields of science and research management. Committee members are nominated by the member institutions of ESF and they maintain strong links with their nominating organisations and their respective scientific communities.
The aim of MatSEEC is to enhance the visibility and value of materials science and engineering in Europe, to help define new strategic goals, and evaluate options and perspectives covering all aspects of the field.

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Working Group members

This MatSEEC Science Position Paper has been complied with the valuable contributions of the following members of the Working Group:
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Simulation of electric energy density for Bragg reflector resonator. © Jonathan Breeze

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Foreword

The Materials Science and Engineering Expert Committee (MatSEEC), founded at the European Science Foundation in October 2009, presents hereby its first report *Computational Techniques, Methods and Materials Design*. Under the leadership of Professor Risto Nieminen, a working group consisting of Dr David John Jarvis, Professor Krzysztof Jan Kurzydlowski, Professor Roberto Lazzaroni, Professor Dierk Raabe and Professor Paul Van Houtte, developed this report.

Beyond any doubt Europe has a worldwide leading position in computational materials science. A significant number of codes which are used worldwide for material science and engineering both in academia and in industry were conceived and further developed by European researchers.

However, we can witness a change of focus from pure modelling to modern *predictive* materials science based on recent groundbreaking advances in the methodologies. In order to maintain the strong position of European scientists and engineers in this field, to strengthen their role even further and to consolidate often fragmented and dispersed efforts, this report provides a number of recommendations. These are based on the insight that measures have to be taken which go beyond the capabilities of individual countries. The report recognises in particular the need for a stable European organisation in computational materials science, with strong links to European industry. The central recommendation is to establish the already existing CECAM, based in Lausanne, as a focal European organisation with links to national organisations and well-defined goals as outlined in the document.

This report aims at convincing the European funding agencies to find avenues for implementing its recommendations.

Professor
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MatSEEC Chair

Professor
Marja Makarow
ESF Chief Executive

Executive summary

Computational materials science is an exciting field which holds much future potential. In the modern "bottom-up" and "multiscale" approaches to materials development, it plays a crucial role. However, its approaches have to be developed to be even more robust and systematic, seamlessly coupled, and connected to the rapidly growing materials databases. What is also needed are more systematic approaches to verification of the simulation results and the development of error estimates of the computationally predicted properties. If these issues are addressed, computational materials science will be totally indispensable for materials discovery and design during the next decade.

The research community in this area is very wide and dispersed, with the hundreds of research groups embedded in a variety of environments and organisational structures. Good networking of these groups is essential to achieve excellence by world standards.

The central recommendations of the MatSEEC Working Group are:

- European activity in computational materials science can be considerably strengthened and consolidated through establishing CECAM as the focal organisation with funding links to national organisations. This should be complemented by grass-roots research networks supporting topical working groups, workshops, researcher training, and cross-thematic conferences. A mechanism for the long-term funding of these activities needs to be worked out. Links to experimental efforts need to become stronger, and technology transfer to industry needs to be vigorously pursued.
- The presently dispersed arrangements for supporting computational materials science are vulnerable. The long-term viability of this critically important field requires greater investment in and strengthening of CECAM.
- Code and database development, maintenance, distribution and support should be put on a more professional basis, in the context of European infrastructure developments in scientific computing, such as those outlined in the LINCEI Initiative and the PRACE project.
- A high-level policy unit should be established at CECAM to discuss scientific priorities and advise funding agencies.

1.
General survey

Computational methods and techniques are at the heart of modern materials research and development. Materials science and engineering is becoming a typical example of "simulation-based science and engineering". Firstly, powerful, predictive theoretical and computational methods are used to facilitate the *discovery* and *design* of materials with new functionalities and desired properties. Secondly, computational methods have a major role in the design and optimisation of *routes* for materials synthesis, processing and preparation, ranging from chemical reactions for growth to long-term annealing and recovery routes of materials. The third role for computational research is in the *analysis* and *interpretation* of experimental characterisations, often based on sophisticated probes. Nanotechnology is a striking example of the integration of computational science with engineering to develop new materials and structures, for such application areas as information technologies, energy harvesting and conversion, as well as biomimetic and biocompatible devices. The crucial role of materials research, including computational approaches, to global energy challenges is amply described in a recent document [1].

Materials modelling utilises several tools already widely used in engineering practice, such as finite-element and finite-difference methods for solving continuum equations in mechanics, fluid dynamics and diffusion, or free-energy minimisation programmes for phase equilibria. However, modern *predictive* materials modelling goes much further [2]. It is necessary to dig down to the atomic level and to understand and exploit atomistic structure and behaviour. Electronic structure calculations, atomistic and molecular dynamics, kinetic and statistical modelling, together with new and emerging techniques and increased computational power can provide answers to versatile and complex questions related to materials manufacture, properties, performance and technological applications.

The keys to the emergence of computational materials science have been the dramatic advances in the *methodologies* for *multi-scale* and *multi-physics/chemistry* simulations, spanning several temporal and spatial scales, and the increasing availability of powerful *computing resources* now routinely running at a performance level of teraflops and reaching petaflops in the near future.

The importance of modelling to *industry* and scaling-up of new processes and technologies is dramatically rising. In many areas of high-tech product development, such as semiconductor foundries and heterogeneous catalysis, the potential for cost and time savings as well as risk reduction is considerable. There is a clear industrial driving force for modelling as a way to enhance the global competitiveness of European industry.

Predictive modelling can and should also inspire new experimental concepts and techniques. The *two-way dialogue* between modellers and experimentalists will unlock the full potential of both areas.

1. *Science for Energy Technology: Strengthening the Link between Basic Research and Industry*, U.S. Department of Energy, Basic Energy Sciences Advisory Committee (BESAC) Report, USA 2010.
2. M. Stoneham: *Predictive Materials Modelling*, in European White Book on Fundamental Research in Materials Science, Max-Planck Institute, Germany 2002.

2. Landscape

The subject area of (computational) materials science is vast. On the physics side, it covers more than half of the PACS (Physics and Astronomy Classification System) titles. It includes solid-state and materials chemistry, physical and chemical metallurgy, granular materials, foams and flocks. *Biological, biomimetic* and *biocompatible* materials from DNA to replacement hips are in its domain. The field also continues to grow to encompass new areas. One example of materials with new properties is that of artificially engineered *metamaterials* with unique and unexplored responses to electromagnetic and elastic waves across a wide spectrum of frequencies.

Computational materials science has simultaneously developed in several research communities. Some observations are given below.

The *first-principles* community uses quantum-mechanical methods to solve for the electronic structures of condensed matter and then calculate properties of materials and devices based on these solved structures.

Any process that involves making or/and breaking of bonds between atoms requires such an approach, because bonding between atoms is fundamentally a quantum effect, and no generally useful method exists to represent it by classical interatomic force models.

This area has progressed tremendously during the past several decades and has reached a level where well-documented and tested software can be used to solve problems of wide variety and increasing complexity. For small system sizes at the molecular level, subtle quantum phenomena can be investigated by using sophisticated many-body quantum-mechanical methods. For larger systems, methods based on the density-functional theory and its extensions can now handle unit cells with thousands of atoms, especially for their structural and thermodynamic properties. Atomic and molecular dynamics can also be handled from first principles, with similar system sizes and time-spans in the nanosecond regime.

If the quantum-physical treatment is replaced with techniques based on less accurate semi-empirical force laws, system sizes can be extended to millions (or even billions) of atoms, also in the *molecular-dynamics* case.

One aspect of first-principles methods is the ability to attack interpretation problems arising from the rapid development of various spectroscopic techniques, probing electronic excitations and their decay. This has given the impetus for the **European Theoretical Spectroscopy Facility** (ETSF)[1], which now provides services for the experimental spectroscopy community using advanced methods for quantum-mechanical spectroscopy calculations.

For *mesoscopic* simulations in the micrometre regime, several techniques are available for more coarse-grained calculations that can also span much longer time scales. These include various kinetic Monte Carlo and cellular automata methods, as well as stochastic techniques based on the Master Equation and its derivatives.

Approaching the *macroscopic* (continuum) limit, a wealth of computational techniques is available. These include the micromechanical and micromagnetism calculations, as two specific examples, based on classical theories of elasticity and electromagnetism, respectively. For fluid-mechanical problems, such techniques include lattice-Boltzmann methods and eventually Navier–Stokes equations of

1. www.etsf.org

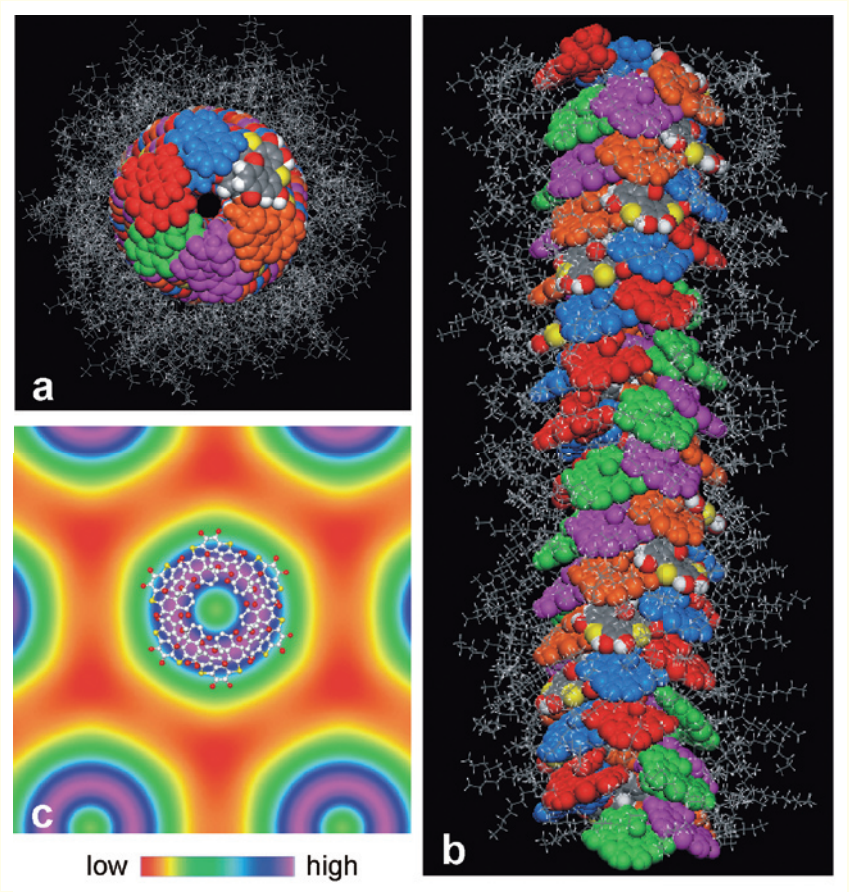

Figure 1.
Molecular organisation in the 6-stranded 132 helical column of a chiral helicene compound with four tethered alkyl chains. One repeat period of the helix (fig. b) contains two helical turns and 78 molecules, grouped in 13 units of six, hence six colours. (a,c) Views along column axis, (b) side view, showing the "pine-tree" structure. In (a) the aromatic cores and the alkyl tails are shown with space-filling and stick models, respectively, while in (c) only the aromatic cores of one 6-molecule unit are shown as ball-and-stick. In (c) a 6-molecule unit, without hydrogens, is superimposed on the electron density map, reconstructed from X-ray diffraction data. The high electron density ring (purple) is due to the high-density aromatic groups. The columns have a hollow core.

continuum flow. The fields of computational fluid dynamics and computational mechanics are mature, with high-quality software widely available. The research challenges are focused towards nonlinear and non-equilibrium behaviour and the complexity arising from multi-physics/chemistry application (*e.g.* reactive multiphase flow in external fields). Thermochemical modelling and simulation based on phase equilibria, often combined with chemical kinetics and fluid flow, are now systematically used in materials processing research.

As shown by these examples, the research mode in computational materials science is thus truly many-faceted. As well as there being the great diversity of techniques depending on different areas of basic science, the research is also highly dispersed among thousands of small groups across Europe. The situation is very different from that in some research fields cohering around just one or few large central facilities and organisations, such as CERN. For example, in Cambridge University (UK) alone, active computational materials science groups operate in the Departments of Physics, Materials Science, Earth Science, Physical and Theoretical Chemistry, Electrical Engineering, and Engineering Materials. Such diversity is typical, and in contrast to some other research fields that have just one or few large central facilities and organisations. Computational materials science also plays a very prominent role in PhD and post-doctoral research training, and the young scientists are in demand in both industry and academia.

Such wide dispersion and diversity are also reflected in the spectrum of methodological and software tools used. There are hundreds of different methods and computer codes, as well as a large variety of computational platforms ranging from laptops to massive supercomputer resources. It is crucial that mechanisms for enabling *permanent European networking* are implemented in the near future. In this field, each calculation is ultimately done by one person at one computer, with researchers and computer hardware largely supported through national funding. However, the calculations also depend on a large amount of expertise originating elsewhere across Europe.

In response to the wide dispersion of researchers among many groups, even in one subfield or technique, some networks have grown up but almost all are informal and/or temporary. There appears to be no funding niche in Europe for long-term networking support unlinked to large experimental facilities.

3.
Objectives and prerequisites

The foremost objective is naturally scientific excellence by world standards. Paraphrasing **Sir Nevill Mott**: "In basic research, second-class work is almost not worth doing". In addition to ambitious exploration of underlying theoretical ideas and their computational implementation, scientific excellence requires close contact and collaboration with experimental efforts. Recognising the scientific value and European strength in computational materials science, the **European Science Foundation** has recently launched a new Research Networking Programme in **Advanced Concepts in ab-initio Simulations of Materials (Psi-k),** which continues the highly successful work of the previous Psi-k Programmes.

Among the obvious prerequisites for success is also access to computational resources, software tools and databases. These needs are shared with many other areas of computational science and engineering. They are elaborated upon in the **LINCEI Forward Look**[1] prepared by the European Science Foundation. Computational materials science, nanotechnology and quantum molecular science are important pillars of that initiative. Materials science and condensed-matter sciences are also underpinning the scientific case for PRACE, the **Partnership for Advanced Computing in Europe**[2] supported by the infrastructure funds of FP7 of the European Union.

To achieve and maintain global leadership, no European country is large enough to have the necessary wide and deep expertise in the underlying theoretical methods and their computational implementation. Thus European cooperation is crucial. This does not mean large sums of money pooled to a common European pot. Given the dispersed and diverse nature of the activities, normal national funding for research manpower and resources is adequate as the basic structure for research funding, augmented by European and international programmes .

However, **European networking** is the absolutely necessary element, the healthy state and sustained support of which need to be secured. The European computational materials science community has developed a common culture and a worldwide leading position. Through various temporary funding schemes and mechanisms it has flourished, but needs now a stable solution to enable extensive, high-class European networking that is easily accessible and unencumbered by excessive bureaucracy. The national Research Councils should strive without prejudice for a pan-European network in computational materials science, a multifaceted "CERN-like" organisation in a hugely important area, for a tiny fraction of the cost of the megascience projects such as CERN or ITER, or even compared with the sums spent on advanced computers. A possible organisational solution is presented later in this document.

1. *European Computational Science Forum: The LINCEI Initiative: From Computers to Scientific Excellence*, European Science Foundation 2009.
2. www.prace-project.eu

4.
Scientific outlook

With the exciting developments in many areas and with the advent of ever-increasing and pervasive computational resources, huge opportunities arise for computational materials research in Europe. While some projects do require the use of the largest available computers, most are in fact done on local clusters or modest regional supercomputers. We mention here just a few challenges and research opportunities. Many more examples are described in the cited LINCEI and PRACE documents [1,2].

4.1. Examples of research challenges

- The most pressing research challenge has to do with the integration of the various length and time scales relevant for materials science, briefly outlined above. *Multiscale materials simulation* is the holy grail of present research, where much effort must be focused towards more seamless integration of the length and time scales, from the electronic and atomic levels to the continuum. A typical example of a multiscale materials problem is chemical vapour deposition (CVD) or atomic layer deposition (ALD) growth of thin films and coatings, where the scales vary from the sub-nanometer surface region to the metre-scale reactor.
- The accurate description and robust modelling of *non-equilibrium* properties remains a challenge. At the atomic scale this poses major challenges for treating excitations and dynamics far from the ground state, with all the decay and dissipation channels properly included. Non-equilibrium thermodynamics and statistical physics are also highly relevant for the longer length and time scales and need to be robustly integrated into computational platforms.
- There are new and emerging classes of *strongly correlated* and *quantum materials*, where our understanding of the underlying physics and chemistry is still severely limited and is hampering technological applications. Examples of such materials are topological insulators, multiferroic materials and exotic superconductors. The complexity of the quantum properties of these materials requires both new theoretical ideas and large-scale computer simulations.
- Another exciting new topic is that of *programmable materials*, where bio-inspired building blocks such as DNA are used to grow pre-designed nanoscale objects and structures to a molecular- and atomic-scale precision. To exploit the opportunities presented by programmable materials requires new capabilities for predictive modelling of inter-molecular interactions and the self-assembly of nanoscale units in non-equilibrium conditions.

4.2. Examples of computational challenges

- The *mathematical methods* required for multiscale modelling are rapidly developing. These include such topics as multiresolution analysis, high-dimensional computation, domain decomposition, turbulence, level sets, and discrete mathematics. These topics need to be explored

1. *European Computational Science Forum: The LINCEI Initiative: From Computers to Scientific Excellence*, European Science Foundation 2009.
2. www.prace-project.eu

from the point of view of application to various materials-science problems, ranging from differential equations to stochastic simulation.

- To be able to describe materials, processes and devices with increasing complexity, ever larger system sizes and ever longer simulation sequences are necessary. The computational cost often increases as power law with a large exponent as a function of system size. It is thus obvious that only *highly parallel computing platforms*, with tens of thousands of cores will be useful in the future. This requires critical investigation of the algorithms and their computational implementation to enable such platforms to be utilised. Truly massively parallel computing is a major challenge for the future.
- *Special-purpose processors*, such as powerful graphics cards, offer low-cost and scalable solutions for high-performance computing. Their usability depends critically on the problem type and its computational solution (molecular-dynamics, finite-element simulation, etc.). The utility of special architectures for computational materials science must be systematically examined.
- A rapidly emerging trend in computational materials science is the growth of *databases* of information relating to material properties, derived both from experiments and large-scale computational screening. The *curating and mining* of these databases is crucial. Standards have to be developed to structure the databases, and new methods are needed for their systematic mining. The databases must also be integrated with the other simulation platforms to allow seamless transfer of information between databases and simulation results. Advanced methods such as those based on neural networks can be used for combinatorial screening and optimisation of materials design for desired properties.

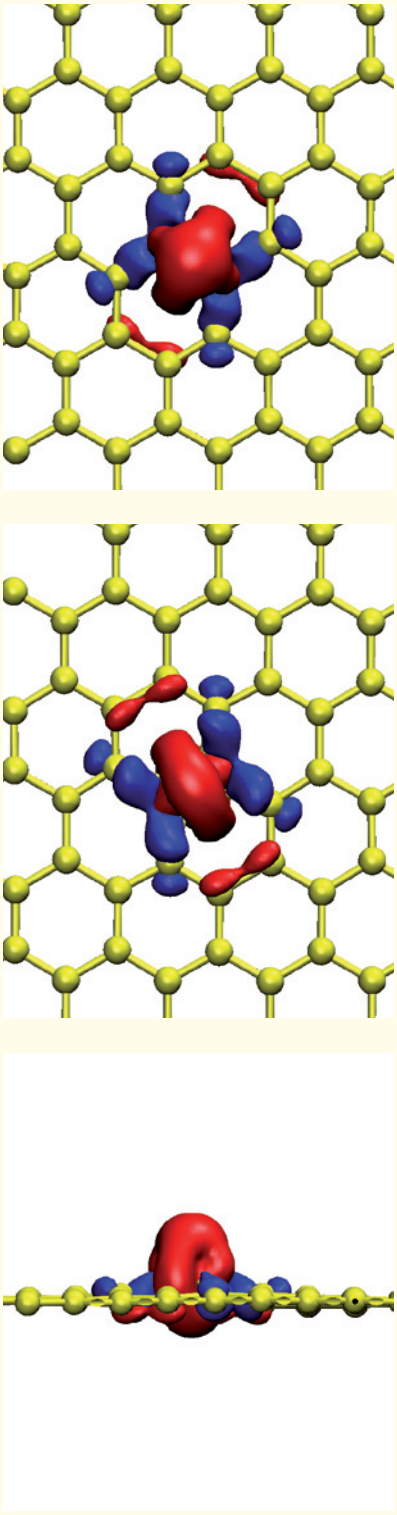

Figure 2.
Energy-resolved spin densities (red - majority, blue - minority) for Mn impurities in a divacancy in a graphene sheet. Two top views and one side view.

5.
European organisation of computational materials science: recommendations

As already noted, the funding of researchers and computer hardware in materials science is dealt with through national agencies, but the provision of systems to promote networking to bring together all the required expertise has been badly neglected.

The need for a *stable European organisation in computational materials science* is obvious and acute. Such an organisation should engage all European countries where there are active research efforts in the area. The permanent organisation would provide the platform for various types of activities, ranging from topical research networks and software-support services for the computational community, to interfaces and services to experimental communities and industrial research.

As the central hub, we suggest the strengthening and broadening of CECAM (**Centre Européen de Calcul Atomique et Moléculaire**)[1] to become a true pan-European organisation.

CECAM is a solid, permanent organisation, an arm of several national Research Councils and organisations. Its headquarters are in Lausanne, Switzerland. CECAM has undergone a transition where it is developing a distributed structure with 'nodes' in several European countries, such as Germany, the Netherlands, Spain and Ireland. More countries, such as Austria, Finland and Sweden are now considering joining CECAM. We strongly support such initiatives, and encourage all countries to join. CECAM is an efficiently run, lean organisation, which can provide the necessary, stable and official platform for sustained activities in computational materials science.

There are and have been several successful research networks around specific aspects and traditions of computational materials science, such as the **Psi-k, MolSimu, SimBioMa**, and other networks and programmes, also sponsored by the **European Science Foundation**. These grass-roots, bottom-up networks are a necessary complement to the permanent organisation (CECAM), in that they embrace the whole research community. The activities of those networks range from individual research visits and small topical workshops to large conferences.

The European organisation for computational materials science would thus evolve to address the following key issues.

- To provide a strong, permanent central research organisation (CECAM) with active nodes in several European countries. This would provide stability and foresight and would develop to include all the multifaceted aspects of materials research.
- The central organisation should have a policy unit to follow the overall development of the field, to establish priorities for future developments, and to convey the opinion and needs of the research community to European and national funding agencies and research-policy bodies. The policy unit could act as an interface between the European Science Foundation and the computational materials science community.
- A selection of topical bottom-up networks with activities in specific topics, such as method and code development, research training, and hands-on workshops.
- The funding instruments for networking activities should be jointly developed by the national Research Councils. The added value and return on investment are exceedingly good, as the low-cost networks have developed efficient working mechanisms and traditions.

1. www.cecam.org

6. Other specific measures

There are presently several strong research communities in Europe, working with different aspects of computational materials science. A typical example is the electronic-structure community, based on physics/chemistry/materials-science departments of European universities and research establishments. This community is world-leading and has produced most of the software now globally used in atomic-scale materials research. There are other similar success stories, such as several networks in molecular modelling, computational chemistry, and related areas.

However, the integration of these various aspects into a more monolithic, materials-based approach is lacking. What are needed are *platforms for exchanging information and expertise between the communities*. This could enable the formulation of overarching efforts under which true multiscale capabilities would thrive. In addition to the overarching organisational solution outlined above, cohesion of the fragmented activities should be increased.

- One vehicle towards better integration would be *European-level research programmes* in computational materials science, where a prerequisite would be the multiscale approach, better linking the now somewhat disparate communities.
- Another vehicle, which would be relatively easy to implement, is to improve the possibilities for cross-breeding and exchange of ideas, for example in the form of *targeted symposia for computational materials science* in the meetings of the **European Materials Research Society** (E-MRS). While there are national programmes of a similar nature in place (for example in the Max-Planck-Society in Germany), such targeted activities would enhance interactions at the European level.
- *Code development and maintenance* should be organised in conjunction with European infrastructure efforts in scientific computing. Computer codes used in materials science have become very complex, with hundreds of thousands of lines, sophisticated libraries and versatile functionalities. As a resource they are a software equivalent of other major scientific infrastructures such as synchrotron beamlines, and need to be given appropriate attention and support by funding agencies. Modern methods of applied computer science and software engineering should be adopted to raise the level of professionalism in code development, maintenance, distribution and support.
- With the emergence of data-intensive research methods in materials sciences, action is needed to enable permanent access to the scientific record by promoting standards in archiving and preservation, for example through APA (Alliance for Permanent Access).

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