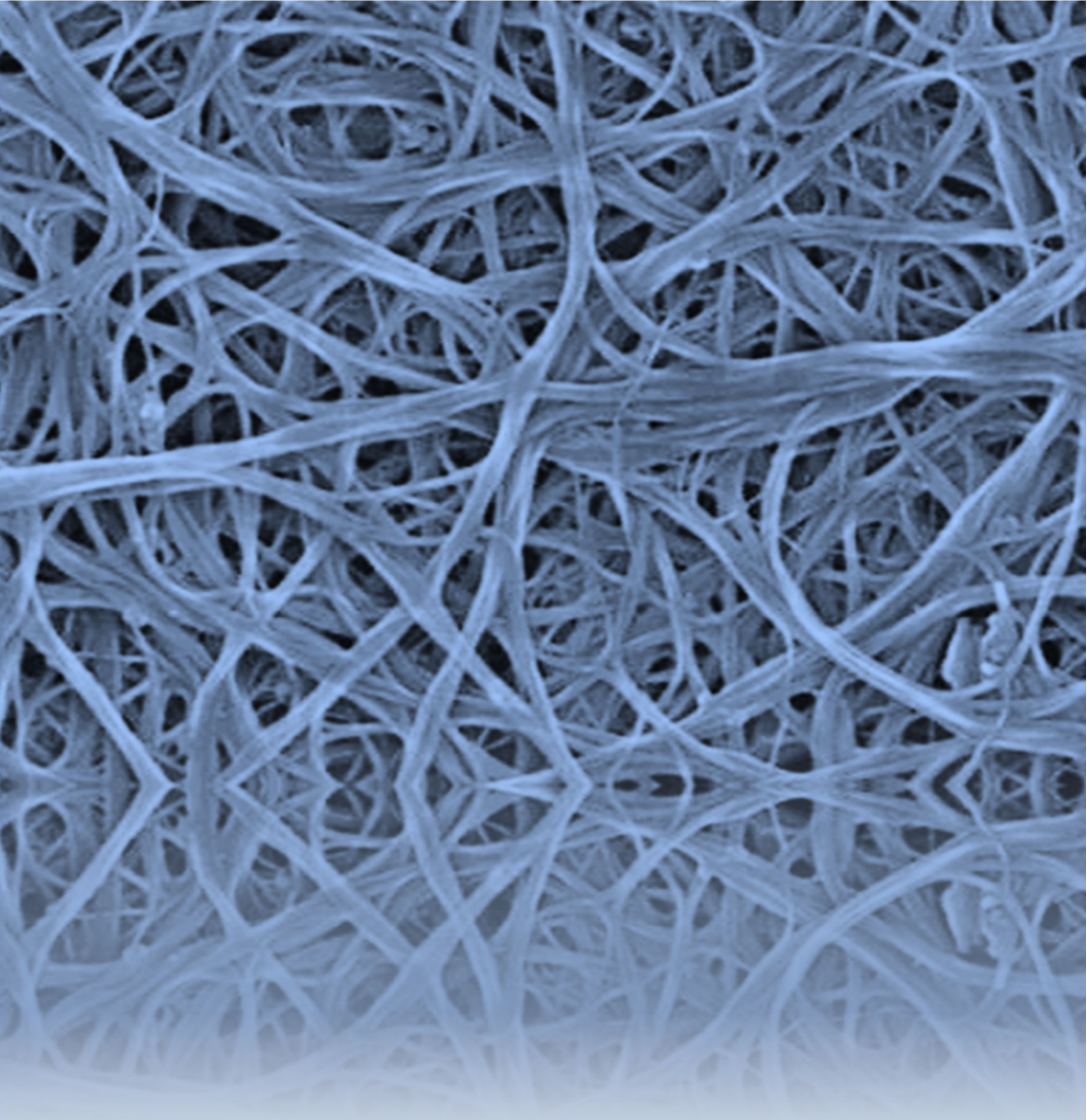
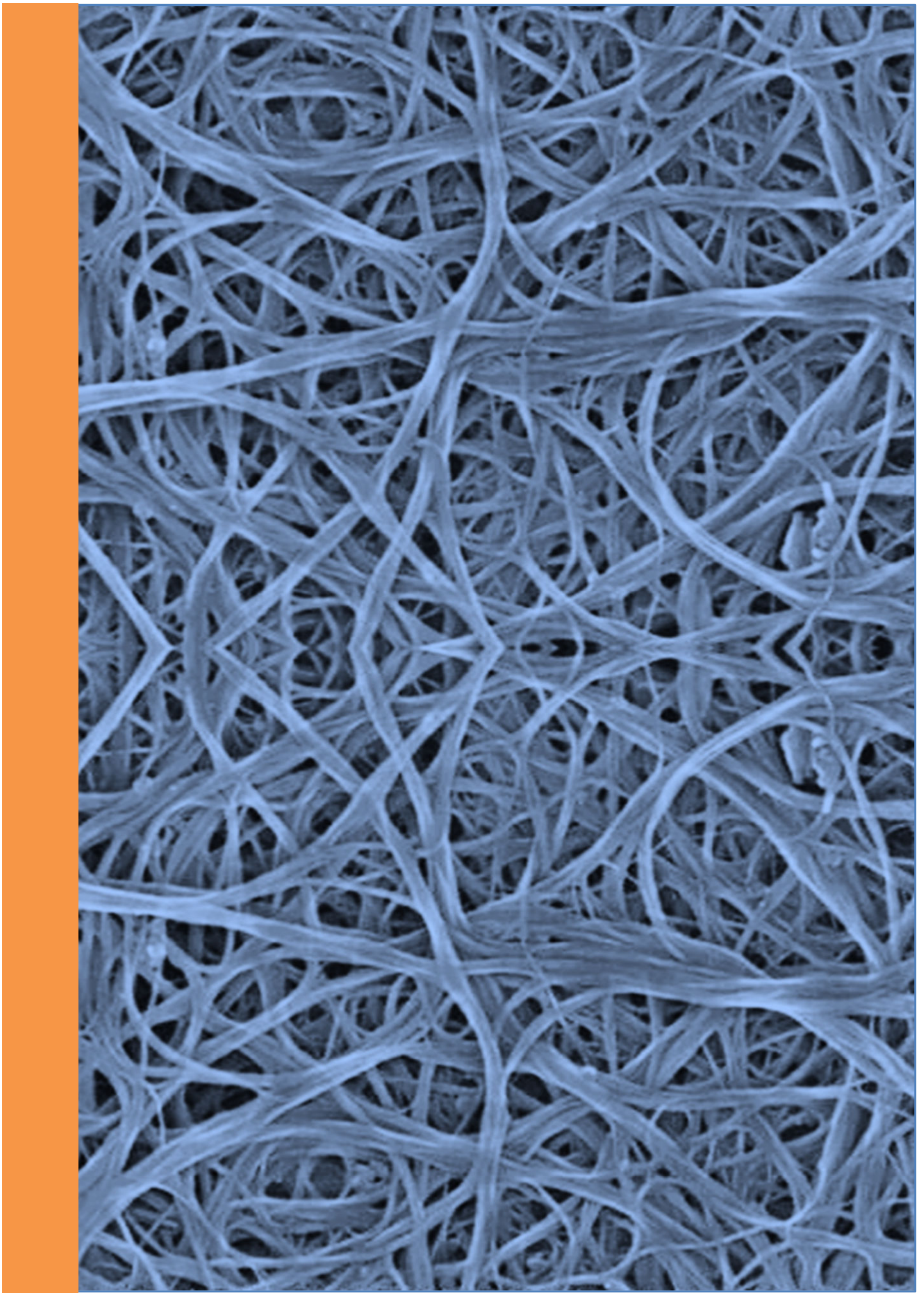


nanoICT
STRATEGIC RESEARCH AGENDA

nanoICT

Strategic Research Agenda

Version 2.0



Index

Foreword

Antonio Correia
Coordinator of the nanoICT CA
Phantoms Foundation (Madrid, Spain)

At this stage, it is impossible to predict the exact course the nanotechnology revolution will take and, therefore, its effect on our daily lives. We can, however, be reasonably sure that nanotechnology will have a profound impact on the future development of many commercial sectors. The impact will likely be greatest in the strategic nanoelectronics (ICT nanoscale devices - nanoICT) sector, currently one of the key enabling technologies for sustainable and competitive growth in Europe, where the demand for technologies permitting faster processing of data at lower costs will remain undiminished.

Considering the fast and continuous evolvements in the inter-disciplinary field of Nanotechnology and in particular of "ICT nanoscale devices", initiatives such as the nanoICT Coordination Action[1] should identify and monitor the new emerging fields research drivers of interest for this Community and put in place instruments/measures to address them.

One of the main challenges is the timely identification and substantiation of new directions for the physical realisation of ICT beyond CMOS that have a high potential for significant breakthrough and that may become the foundations of the information and communication technologies and innovations of tomorrow.

Therefore, the second version of the nanoICT Strategic Research Agenda (SRA) provides focus and accelerate progress in identified R&D directions and priorities for the "nanoscale ICT devices and systems" FET proactive program and guide public research institutions, keeping Europe at the forefront in research. In addition, it aims to be a valid source of guidance, not only for the nanoICT scientific community but also for the industry (roadmapping issues), providing the latest developments in the field of emerging nano-devices that appear promising for future take up by the industry.

This updated version of the research agenda is an open document to comments and/or suggestions and covers a very wide range of interdisciplinary areas of research and development, such as BioICT, NEMS, Graphene, Modelling, Nanophotonics, Nanophononics, etc. providing insights in these areas, currently very active worldwide.

Expected impact of initiatives such as this nanoICT strategic research agenda is to enhance visibility, communication and networking between specialists in several fields, facilitate rapid information flow, look for areas of common ground between different technologies and therefore shape and consolidate the European research community.

I hope you will enjoy reading this document. Please contact coordinators of the working groups if you are interested in providing a comment or would like to see your research featured in future editions.

---

[1] www.nanoICT.org

1. Introduction

Introduction

Robert Baptist
CEA (France)

The nanoICT Coordination Action (CA) ends with an extremely positive balance. This CA had for purposes, first to draw up, according to the current worldwide situation, the relative situation of the nanosciences & nanotechnologies towards Information and Communication Technologies (ICT) and secondly to give an insight of the European research in these domains. We shall give successively an outline of these two points during this introduction.

To start with, it is useful to specify that the world context in microelectronics escapes the academic world for the most part of the decisions which are taken. A decision such as passing from 300mm to 450mm wafers leads to major economic, strategic and political changes. On the financial plan, sums of the order of 5-6 billion dollars are put forward to estimate the price of the construction of such factories. It thus reduces to the leading players of the microelectronics the possibility of embarking on such operations. As the amount of planned investments should restrict the number of factories in the world to some units, it is probably desirable that besides US and Asia, it exists at least a manufacturing unit in Europe.

A lot of web sites and blogs echo rumours of meetings, discussions, forecasts, between industrial actors, institutional and the lobbies or organizations connected to the domain of microelectronics. In the same way, discussions just as much technical as strategic on the adoption of the FinFET or FD-SOI transistor, on the possibilities of using in short or middle term such or such type of lithography (EUV or e-beam) or of continuing with the double patterning at 193nm, or of adding to it the self-assembling of di-block copolymers hit the headlines of international conferences or the titles of reporting done by consulting firms. Nevertheless microelectronics laboratories will certainly continue to work on silicon chip scaling, more computing power, lower energy consumption during the next 15-20 years introducing new technologies, new materials and new fabrication techniques.

This relative tightness on the economic plan between big industrial actors of the microelectronics sector and the world of the nanosciences/nanotechnologies is, maybe, less marked in a domain in very fast emergence which is the Organic Electronics one (OE). To get an opinion on the growth of this sector, it is enough to quote some relative figures in one of the major conferences of this sector, the conference LOPE-C which is organized every year in Germany, (on 2011, Frankfurt, on 2012 in Munich). In 2011 this conference gathered, indeed, 1500 participants and attracted 88 exhibitors. Its major sectors of development are OLED screens, organic electronics for the photovoltaic, and lighting with organic diodes, three sectors of considerable economic importance. All the techniques of manufacturing, roll to roll printing, impression on substrates or foils, deposits under vacuum are neck and neck to the applications, the size and the nature of the substrates and the game thus remains relatively open. The academic and the laboratories of R&D play a major role and feed this infant industry with new manufacturing processes, with new molecules or new functional electronic layers (blocking layer for electrons or holes, adaptative layers for the work function, etc.). Furthermore they feed the perspectives by aligning performances which improve regularly as time goes by. Let us note that a lot of concepts or functional nano-objects developed in molecular electronics meet right now in the prototype lines. It is the case for numerous nanomaterials that we find under hybrid shape (nanowires, carbon nanotubes, graphene - organic material) or "simple" shapes, such as the sheets of grapheme or the conducting metallic nanowires both used for flexible transparent electrodes in place of ITO. We also find a lot of work on applications in connection with ICT and we shall quote in particular those on memories, on printed batteries, on RFID tags and CMOS organic devices. Naturally, the analogue devices which can be fabricated on flexible substrates (recently works on graphene transistors working in the GHz domain have been published), or thinned and then added to flexible substrates are indispensable for number of applications.

These two big electronics sectors have different strategies of development, but each "absorbs" more or less quickly the novelties stemming from developments at the nano scale, whether it is for the components of the More Moore option, the More than Moore one, those of the OE or for the manufacturing processes (for example, the above mentioed self-assembling with di-block copolymers). Moreover, a certain number of researches in nanosciences/nanotechnology will also meet in programs such as the new European projects (Flagships) "Guardian Angels", "Graphene", or "Human Brain Project"...

It is a tribute to nanoICT to have launched, in the course of project, the creation of working groups such as those on grapheme or bioICT. Both members of these groups and their conclusions played an essential role in the progress of the first phases of each of the corresponding Flagships. Besides, if we imagine that “critical” dimensions for “of today” CMOS devices will be reached in 10 or 15 years, we also see that new original fields of research can appear to study original tracks on calculation or on new manufacturing techniques. For the first, we may mention, of course, quantum computing, unconventional architectures (reversible computation, those combining logic and memory (memory embedded in logic, MLU), neuromorphic approaches, etc. For the second ones, will mention in the first place the difficulty in defining the future device itself and separating it from the physical link carrying the information delivered by the device; this will probably lead in the future (10 years-15 years) to radical changes in manufacturing processes like the one we observe today with 3D-assembling. The same holds with the inclusion of numerous new materials in CMOS since 5-10 years. It is foreseen that problems due to interferences, leakages and parasites will predominate across the entire ultra-dense systems, with dimensions of about 100nmx100nm and containing many devices in close proximity. Furthermore, these systems will not be allowed to dissipate more than allowed by the physics and they will therefore comply with the rules set by the energy management system. Solutions will have to be found for all these problems.

In view of this industrial landscape, what are still the major trends in nanoscience research related to ICT? The first observation is probably the fact that nanosciences in the 2000s were able to manufacture nano-objects, to characterize them and use them for some microelectronics applications. But above all these nanomaterials were used in applications such as new energy and health. Examples of application of carbon nanotubes or nanowires or quantum dots in electronics exist, but researches essentially remained at the level of R & D. These are, for example, transistors or vias with nanotubes, chemical or biochemical sensors, resistive type memories. On the other hand, many functional objects made by a bottom-up approach are now found in batteries' electrodes, in thermoelectric elements, LEDs and catalysts for fuel cells. ICT has likely benefited from researches on nanochemistry and functionalization of nano-objects for OE, more than for silicon electronics.

Many current instruments, sensors or actuators, already incorporate applications derived from nanotechnology. In particular those applications which are derived from the convergence between computers/consoles on the one hand and mobile phones on the other hand. It is also likely that the next ten years of academic research in nanoscience will be, to some extent, devoted to the development of hybrid nano functional materials. These materials, will feed areas of microelectronics such as logic (microprocessors) or conventional memories but also more probably communication. Providers for these applications are currently matrices of optical sensors, touch screens, MEMS (accelerometers, gyroscopes), digital microphones, and tomorrow chemical and biological sensors, producers, collectors and stokers of energy. All these applications include results of nanophotonics, plasmonics, spintronics and even phononics (engineering of phonons in nano and micron structures) (See position paper Annex 1, by Clivia Sotomayor and Jouni Ahopelto)

The transition from MEMS (micro scale) to NEMS (nano scale) is in turn at a pace slower than could be imagined. One can see at least two reasons. The first one is that the MEMS industry is still growing regarding special or custom applications, but mature for consumer applications. It is not even necessary to change the strategy. The second is that neither the specific applications of NEMS are fully defined, nor the transition from academic samples to 6'' or 8'' commonly undertaken. WG 2 was involved in describing all the significant potential of these nano-objects (NEMS for switches, NEMS for mass spectrometers, digital switches for nanoelectronics, NEMS for the study of quantum systems, networks of NEMS, etc.) which, we hope, will be developed by the European industrial players in the field (large ones such as Bosch, STM ...), and smaller ones like Tronics, Memscap, etc. We refer to the report by Jürgen Brugger et al. for a more precise insight into this field.

As regards health or medicine, many applications also exist, but the necessary clinical trials before introduction on the market make that only few functional objects (such as biocompatible electrodes made from carbon nanotubes, drugs based on intelligent "containers", nanoparticles for luminescent imaging...) are found on the shelves. Due to the merge of medicine with information technologies (imaging: X-IRM, IR terahertz, impedance..., new smart drugs, smart implantable medical devices., new devices connecting the body with environment, memories for storing terabytes of individual information, individual medicine) it is expected that this combination will have a significant impact in terms of diversification of electronics devices. This is already the case with, for example, blood pressure monitors, detectors of diseases, mobility issues, screening of biomolecules. This trend will certainly be extended to ambient/mobile applications and to the internet of objects.

Another observation concerns the famous synergy between technologies or between platforms. We have already mentioned the importance of these rapprochements, for example, with the chemical or biochemical functionalization of nano-objects. We can probably also mention the rapprochement between cognitive science, information and bio-interfaces. Innovation comes in part from these links. One can imagine for the near future, and there are a number of achievements that support it, that chemical or bio-inspired nanoconstructions will assist the conventional top-down manufacture. A well known example is the use of artificial DNA as a complementary way to lithography and patterning to achieve nanometer resolution via self-assembly. Or the use of DNA for manufacturing structures or plasmonic metamaterials (see report WG10 by Jen-Pierre Aime et al.). This kind of convergence or synergy has become widespread over the past ten years. All nanoICT reports show strong interactions between microelectronics, nanoscience, nanobiotechnology systems, energy management, which causes or brings new applications in health, defense, transportation, media and entertainment. However, the technical gap between technological laboratories, universities and companies in these sectors remains important and a major effort towards multidisciplinary education is still needed. This naturally refers to KET (Key Enabling Technologies in Nanoelectronics, Nanomaterial and process) for reducing or removing these gaps.

In the field of the modelling and digital simulation, in particular for nanosciences, which is the theme handled in detail by Massimo Maccuci et al. (WG5), we shall retain two strong trends that are the access to supercomputers and that of data mining at large-scale. This last one indeed allows, thanks to the exploration of the big data banks (crystallography, metal industry, thermodynamics, chemistry, genetics, etc.) to make "in silico" new materials with predefined or novel properties (electric, mechanic, optical, chemical,) which opens an almost infinite field of exploration, as far as many of these properties result from phenomena developing at different scales (for example electronic properties of gold aggregates dependent on the number of atoms in the aggregate, the properties of a massive material depend partially on defects in the material). The complexity and its processing are not absent, of course, and the multi-scale simulation will allow (perhaps) intending a description of devices from their constituent atoms. However data-mining, based on knowledge acquired since more than 50 years open really new routes for technologies based on nanomaterials.

About this document and the nanoICT project:

The nanoICT CA was initiated in January 2008. Group members of its community have done a continuous watch on key topics of nanosciences and micro and nanotechnologies in order to provide stakeholders from research and from EU with analysis supporting them to understand the evolution of these technologies. Reports have been published, describing the state of the art for many technologies. In two cases new groups have been formed which also provided information on weak signals leading to new developments or future ruptures.

Expected impact of initiatives such as this nanoICT research agenda is to enhance visibility, communication and networking between specialists in several fields, facilitate rapid information flow, look for areas of common ground between different technologies and therefore shape and consolidate the European research community.

This Research Agenda is aimed to be an open document to comments and/or suggestions. It covers a very wide range of interdisciplinary areas of research and development, such as Graphene, NEMS, bioICT, modelling, nanophotonics or nanophononics.

2. Strategic Research Agenda

graphene

Graphene is considered to be one of the most serious candidate materials for post-silicon electronics by the International Technology Roadmap for Semiconductors (ITRS), the strategic planning document for the semiconductor industry. Indeed, there are many potential uses of graphene because of its unique combination of properties, but those applications not only cover logic and radiofrequency applications. Graphene is a transparent like plastic , but it conducts heat and electricity better than metal, it is an elastic thin film, behaves as an impermeable membrane, and it is chemically inert and stable, thus offering a more functional “plastic-like” material with reinforced properties in terms of stability and mechanical strength, while providing enhanced electrical and thermal conductivities. Potential electronics applications of graphene include high-frequency devices and RF communications, touch screens, flexible and wearable electronics, as well as ultrasensitive sensors, NEMS, super-dense data storage, or photonic devices. In 2010, the first roll-to-roll production and wet-chemical doping of predominantly monolayer 30-inch graphene films grown by chemical vapour deposition (CVD) onto flexible copper substrates were reported. The produced films were found to exhibit low sheet resistances and 90% transmittance, competing with commercial transparent electrodes such as indium tin oxides (ITO). Graphene electrodes could therefore be incorporated into a fully functional touch-screen capable of withstanding high strain. In the energy field, potential applications include supercapacitors to store and transit electrical power and highly efficient solar cells. However, in the medium term, some of graphene’s most appealing potential lies in its ability to transmit light as well as electricity, offering improved performances of light emitting diodes (LEDs) and aid in the production of next-generation devices like flexible touch screens, photodetectors, and ultrafast lasers.

Strategic Research Agenda Graphene

nanoICT Working Group Graphene[1]

Stephan Roche
Catalan Institute of Nanotechnology and ICREA (Spain)

Graphene is considered to be one of the most serious candidate materials for post-silicon electronics by the International Technology Roadmap for Semiconductors (ITRS), the strategic planning document for the semiconductor industry. Indeed, there are many potential uses of graphene because of its unique combination of properties, but those applications not only cover logic and radiofrequency applications.

Graphene is a transparent like plastic , but it conducts heat and electricity better than metal, it is an elastic thin film, behaves as an impermeable membrane, and it is chemically inert and stable, thus offering a more functional "plastic-like" material with reinforced properties in terms of stability and mechanical strength, while providing enhanced electrical and thermal conductivities.

Potential electronics applications of graphene include high-frequency devices and RF communications, touch screens, flexible and wearable electronics, as well as ultrasensitive sensors, NEMS, super-dense data storage, or photonic devices. In 2010, the first roll-to-roll production and wet-chemical doping of predominantly monolayer 30-inch graphene films grown by chemical vapour deposition (CVD) onto flexible copper substrates were reported. The produced films were found to exhibit low sheet resistances and 90% transmittance, competing with commercial transparent electrodes such as indium tin oxides (ITO). Graphene electrodes could therefore be incorporated into a fully functional touch-screen capable of withstanding high strain.

In the energy field, potential applications include supercapacitors to store and transit electrical power, and highly efficient solar cells. However, in the medium term, some of graphene's most appealing potential lies in its ability to transmit light as well as electricity, offering improved performances of light emitting diodes (LEDs) and aid in the production of next-generation devices like flexible touch screens, photodetectors, and ultrafast lasers.

Graphene Production

The production of high quality graphene remains one of the greatest challenges, in particular when it comes to maintaining the material properties and performance upon up-scaling, which includes mass production for material/energy-oriented applications and wafer-scale integration for device/ICTs-oriented applications. The industrial

---

[1] Contributors: Francesco Bonaccorso, Johann Coraux, Chris Ewels, Andrea C. Ferrari, Gianluca Fiori, Jean-Christophe Gabriel, Mar Garcia-Hernandez, Jari Kinaret, Max Lemme, Daniel Neumaier, Vincenzo Palermo and Aziz Zenasni.

exploitation of graphene will require large scale and cost-effective production methods, while providing a balance between ease of fabrication and final material quality. One advantage of graphene is that, unlike other nano-materials, it can be produced on large and cost-effective scale by either bottom up (atom by atom growth) or top-down (exfoliation from bulk) techniques. Graphene layers can be epitaxially grown by carbon segregation from silicon carbide (SiC), or metal substrates following high temperature annealing. Large area growths of graphene-stacks on the C-face and monolayer graphene on Si-face of SiC have been demonstrated, but work is needed for large scale transfer of high quality material to more convenient substrates. Chemical vapour deposition (CVD) of graphene on Cu-foils remains the most competitive method, although the produced polycrystalline graphene needs to be better characterized, and intrinsic limits for high mobility identified. There are alternative schemes to produce wafer-scale graphene which still require important research efforts, which should yield fabrication of higher quality material, integrated onto a larger variety of substrates, including CVD of graphene on insulator, CVD/PECVD deposition and MBE-growth. Exfoliation of pristine or functionalized graphite (graphene oxide, GO) in liquid, followed by ultrasonication also stand as a very cost effective approach, of concern for different types of applications. It particularly offers advantages because of the ease of scalability and the absence of substrates, thus standing as a golden way to produce graphene inks, thin films and composites.

High frequency electronics

Graphene combines exceptional electronic properties with excellent mechanical properties. Its ambipolar transport properties, ultrathin and flexible, and electrostatic doping offer a new degree of freedom for the development of advanced electronic devices with many potential applications in communications and RF electronics. Graphene transistors with a 240nm gate operating at frequencies up to 100 GHz were demonstrated in 2010. This cut-off frequency is already higher than those achieved with the best silicon MOSFET having similar gate lengths. Simulation show that graphene-based FET can cross the THz-border in the mid-term, which will then allow the development of novel applications like spectroscopy or automotive RADAR in analog high frequency electronics. Significant impact in analog RF communication electronics in areas as diverse as low noise amplifiers, frequency multipliers, mixers and resonators could then follow. The demonstration of high-speed graphene circuits is also offering high-bandwidth suitable for the next generation of low-cost smart phone and television displays.

Concerning the domain of mainstream ICT, Silicon technology is getting close to fundamental downscaling limits, and graphene could offer several alternatives (especially in the CMOS back-end processing), despite the current lack of an efficient wafer-scale integration protocol compatible with CMOS technologies.

Flexible optoelectronics and transparent conductive coating

New low cost nanomaterials, including graphene and other 2d layered materials, could have a disruptive impact on current optoelectronics devices based on conventional materials, not only because of cost/performance advantages, but also because they can be manufactured in more flexible ways, suitable for a growing range of applications, stemming as clear competitors for current ITO devices. Graphene is also promising as addictive for composite materials, thin films and conducting inks. High quality graphene inks can now be produced via solution processing and ink-jet printed thin film transistors with mobility ~90cm^2/Vs have already been demonstrated, paving the way towards fully graphene-based printable electronics.

Graphene Photonics, Optoelectronics and Plasmonics

Another potential field of application is photonics and optoelectronics, where the combination of its unique optical and electronic properties can be fully exploited, even in the absence of a band-gap, and the linear dispersion of the Dirac electrons enables ultrawideband tunability. The rise of graphene in photonics and optoelectronics is yet evidenced by several recent results, ranging from solar cells and light-emitting devices to touch screens, photodetectors and ultrafast lasers. Graphene could be employed as active optoelectronic material to achieve light-matter interaction, convert incident light energy into detectable electrical signals, and, vice versa, use electrical signals to modulate light and realize optical switches. To that end, graphene should however be integrated with established and mature technologies such as dielectric (silicon or plastic) waveguides, optical antennas, plasmonic structures (e.g. gratings or nanoparticles), metamaterials, quantum dots, etc. Graphene's constant optical absorption over a spectral range covering the THz to the UV allows light detection over a wavelength range superior to any other material. Combinations of 2D heterostructures with plasmonics would allow for creation of active optical elements. 2D heterostructures are ideally suited to be used with plasmonic structures, as they can be positioned exactly at the maximum of electric field from plasmonic nanostructures. Such elements are of great importance in different areas of science and technology: from ubiquitous displays, to high tech frequency modulators.

Graphene spintronics

Electronic devices that use the spin degree of freedom hold unique prospects for future ICT technologies, and graphene stands out as a very promising material for such a purpose. Predicted ultralong spin-coherence lengths in graphene, due to its weak spin-orbit and hyperfine interactions, offer true capability for efficient spin manipulation and for the creation of a full spectrum of spintronic nanodevices: from (re-)writable microchips to transistors to logic gates, including information storage and processing on a common circuit platform. Efficient spin injectors and spin detectors based on sputtered tunnel junctions have been yet demonstrated, establishing magnetoresistance signals that are strong enough to ascertain the true potential of lateral spin devices with large-scale production methods. These achievements open perspectives for engineering external ways to control (gate) the propagation of spin currents, achieving operational reliability, room temperature operation and architectural compatibility with CMOS. These research directions could form the basis for future ultralow-energy data processing using spin-only logic circuits.

Conclusion

Thanks to graphene versatile and multiple properties, one could envision integrating on the same chip advanced functionalities including chemical sensing, nano-electromechanical resonators, thermal management, and electronic functions. If successfully monitored, graphene spintronics will also offer a co-integration of memory and computation functions on the same substrate, a possibility with unprecedented impact for low power computing devices and circuits. All this optimistic future however requires a proper level of networking European excellence and bridging research to technology innovation for larger societal impact in the frame of horizon 2020.

Modeling

We are presently witnessing the final phase of the downscaling of MOS technology and, at the same time, the rise of a multiplicity of novel device concepts based on properties of matter at the nanoscale and even at the molecular scale. Ultra-scaled MOS devices and nanodevices relying on new physical principles share the reduced dimensionality and, as a result, many of the modelling challenges. In addition, new materials and process steps are being included into MOS technology at each new node, to be able to achieve the objectives of the Roadmap; these changes make traditional simulation approaches inadequate for reliable predictions. So far modelling at the nanoscale has been mainly aimed at supporting research and at explaining the origin of observed phenomena. In order to meet the needs of the MOS industry and to make practical exploitation of new device and solid-state or molecular material concepts possible, a new integrated approach to modelling at the nanoscale is needed, as we will detail in the following. A hierarchy of multi-scale tools must be set up, in analogy with what already exists for microelectronics, although with a more complex structure resulting from the more intricate physical nature of the devices and the intrinsically multi-physics nature of the problems to be solved. A dedicated effort in the field of modelling is apparent in the United States, where significant funding has been awarded to the Network for Computational Nanotechnology, which is coordinating efforts for the development of simulation tools for nanotechnology of interest both for the academia and for the industry. Although the required integrated platforms need to be developed, the efforts made in the last few years by the modelling community have yielded significant advances in terms of quantitatively reliable simulation and of ab-initio capability, which represent a solid basis on which a true multi-scale, multi-physics hierarchy can be built. The combination of

Strategic Research Agenda Modeling

nanoICT Theory and Modeling Working Group [1]

Maximo Macucci
Dipartimento di Ingegneria dell'informazione, Università di Pisa (Italy)

Introduction

Here we summarize the main conclusions reached during the meetings of the Working Group on Theory and Modeling during the 4 years of the NanoICT project.

Discussions have been lively and with the participation of researchers both from academia and from the industry (in particular ST Microelectronics and IBM). A large consensus was reached on a few issues, such as the need for a new hierarchy of multi-scale simulation tools capable of supporting the final downscaling of the CMOS technology, as well as the efforts to develop devices based on disruptive concepts and exploiting properties of matter at the nanoscale. It was recognized that the distinction between modeling of materials and modeling of devices is fading as we get further into the nanoscale, because the properties of the device cannot be distinguished from those of the device any longer. A similar process, although less evident and for the time being still mainly occurring only for some types of emerging devices, is taking place between modeling of devices and modeling of circuits, where SPICE-like approaches cannot be taken for granted any longer. Furthermore, it is apparent that a much larger number of degrees of freedom has to be included with respect to the past, even in the simulation of relatively simple systems, because heat transport, for example, as well as thermoelectric effects play important roles at the levels of power density that have been reached. This implies that simulators have to be not only multi-scale but also multi-physics, including different physical quantities and guaranteeing a smooth connection between their mathematical treatments. Computing platforms were also discussed, concluding that hybrid GPU-CPU systems represent the future of high-performance computation, and new simulation tools should be developed with them in mind. Finally, the main current needs of the industry were identified and it was noted that in Europe there is currently clear excellence in some fields of modeling, such as ab-initio methods, but there is still little coordination that leads to duplication of work in some cases, and in general to a less than optimal performance on the global scale.

Multi-scale modeling

Hierarchical approaches are not new in the field of device and circuit simulation: since a long time ago software tools have been devised to treat the single device with a great amount of physical detail, while for the analysis of circuits simpler, often analytical

---

[1] Contributors: S. Roche, A. Correia, J. Greer, X. Bouju, M. Brandbyge, J. J. Saenz, M. Bescond, D. Rideau, P. Blaise, D. Sanchez-Portal, J. Iñiguez, X. Oriols, G. Cuniberti and H. Sevincli.

compact models, have been used to represent the devices. Going upwards in the hierarchy, complex logical circuits are modeled on the basis of a simplified, two-level circuit response. In the case of nanoscale and quantum devices the different levels of the hierarchy are not so well defined any more, because, at the lowest level, materials cannot be treated simply with parameters obtained from experiments on bulk samples or from calculations dealing with periodic crystals, because the "material" properties themselves are a result of the device geometry and operating conditions. The same can be said for the distinction between device and circuit models, which becomes blurred, for example, in circuits that rely on single-electron effects, whenever the capacitances at the device terminals are not much larger than those of the internal tunnel junctions. This implies that the separation between different levels must be identified much more carefully and that passing of parameters is not as straightforward as it used to be. Several participants in the WG meetings have mentioned the need for a standardization of benchmarks to evaluate the reliability of parameter passing between the different levels. It was also remarked that example should be taken from the fields of biological molecules or crack propagation, where advanced, seamless multi-scale hierarchies have already been developed.

Multi-physics approaches

If we consider a structure as simple as a nanowire transistor, the electronic properties are dependent on the amount of strain, which, in turn, is influenced by the temperature and by the mechanical constraints. This implies the need for a simulation that takes into account a model for heat propagation and one for the mechanical degrees of freedom. The same is true, for example, for nanophotonic devices integrated with CMOS on the same chip, which require a simultaneous treatment of traditional semiconductor equations and of the electromagnetic problem. Lessons can be learned from the existing approaches to semiconductor laser simulation, which has always included the solution of semiconductor equations, together with that of Maxwell's equations and those for heat propagation.

Future software tools for nanodevices will have to be “multi-physics” in nature, and include electrical, mechanical, electromagnetic and thermal degrees of freedom, while retaining an acceptable computational efficiency.

High-Performance Computing

There have been a few paradigm changes in the extraordinary development of computational power that we have witnessed in the last three-four decades, fueled mainly by CMOS downscaling. Besides a very important leap forward that in the 1980's was represented by the introduction of large-scale vector computing by Seymour Cray, up to the beginning of the new millennium CMOS scaling has allowed a steady increase in CPU clock frequency until, as a result of the excessive power dissipation per unit area (due to non ideality factors in the scaling), this reached an abrupt end, and multi-core CPUs started appearing, in order to make up the lost momentum in clock speed acceleration with an increase in the number of processors. More recently another change of paradigm has been initiated with the exploitation of GPUs (Graphic Processor Units) for general-purpose computation. GPUs have a massively parallel architecture, are particularly suited for matrix operations, and, depending on the type of numerical problem, can yield speedups of more than one order of magnitude with respect to traditional CPUs. With the development of standardized software environments for GPU programming and for the almost automated conversion of legacy codes, GPUs have made high-performance computing more easily accessible, which is important for the diffusion of advanced simulation codes, that are extremely demanding from the point of view of the required computational power. Hybrid systems, based on a proper mix of CPUs and GPUs are becoming the de-facto standard for the new generation of supercomputers, such as the Cray XK6, which will be based on a combination of AMD multi-core CPUs and NVIDIA GPUs, scalable up to 500,000 cores. From the point of view of nanoscale device and circuit simulation, desktop computing equipment is most relevant (most of the actors in device and circuit design will not have easy access to a supercomputer in the foreseeable future), and therefore it will also be important to monitor the developments in low-cost hybrid CPU-GPU systems.

Industry needs and outlook for the future of modeling

Representatives of the industry, which is mainly focused on the final downscaling of CMOS technology, pointed out that existing commercial simulation codes, although recently augmented with quantum tools, do not meet the requirements of the 22 nm node and beyond. In particular, existing commercial 3D Schroedinger solvers combined with nonequilibrium Green's functions do not include inelastic scattering, and, therefore, are not suitable for the current node and the next few ones, in which transport is not fully ballistic yet. Advanced codes that do include dissipation have been developed by universities and other research institutions, but they are in general difficult to use in an industrial environment, due to a lack of documentation, support and graphical user interface. It would be therefore important, in the near future, to have closer and more coordinated collaboration between industry and academic groups, with the objective to integrate advanced approaches into simulation suites with which people in the industry are familiar. Furthermore, what would really raise the interest of the industry and convince them to invest more heavily in these new tools is a capability to predict deviations in device behavior from what would be expected on the basis of intuition alone, rather than results that are extremely accurate from a quantitative point of view.

Overall Europe is very well positioned from the point of view of the development of state-of-the-art ab-initio simulation tools, both from the point of view of the electronic structure and of transport, and has made significant steps forward in multi-scale approaches, but the effort is still rather fragmented and duplications occur. There is a need for effective initiatives, such as those that are currently active in the US (e.g. the Network for Computational Nanotechnology), aimed at jump-starting a common effort towards the development a new generation of simulation tools for nanodevices and nanocircuits. This would be of essential importance for the competitiveness and sustainability of European ICT industry.

Nanophotonics
Nanophononics

Nanophotonics and Nanophononics are knowledge areas essential for the development of novel technology and products in ICT, energy, nanomanufacturing, environment, transport, health, security and several others. Photonics is recognised as a Key Enabling Technology and nanophotonics is likely to be at the base of the next wave of photonics innovation. Nanophononics is becoming more and more visible as the “energy issue” rears its head virtually in all research and development fields. In particular, heat transfer in the nanoscale is more than just thermal management since it underpins the science of fluctuations and noise, needed to develop knowledge at the system level all the way to quantum processes in biology and at the heart of information generation and transformation. Many discussions on the progress of the science and technology of both nanophotonics and nanophononics have taken and are taking place in a large number of conferences, workshops and schools. This is a first non-exhaustive attempt to condense what researchers think are priorities and hot topics in both nanophotonics and nanophononics. Among the commonly mentioned key issues in nanophotonics research is design for specific applications including a subset of generic architectures and device performance in the nanoscale. Power efficiency, both as in power management and wall plug efficiency, are also shared key issues and both are followed closely by the need of technologies and standards suitable for very large scale manufacturing. An increasing number of groups are working in various fields of nanophononics, covering modelling of phononic crystals and heat transport at macro and atomic scale. It is important to intensify the collaboration and create a more unified value chain ranging from design and modelling to heat transport calculations to experimental verification of the models. The latter requires ad

Strategic Research Agenda Nanophotonics and Nanophononics

nanoICT Working Group Nanophotonics and Working Group Nanophononics[1]

Clivia M Sotomayor Torres
ICREA, Catalan Institute of Nanotechnology and Universitat Autonoma de Barcelona (Spain)
Jouni Ahopelto
VTT Technical Research Centre of Finland (Finland)

Nanophotonics and Nanophononics are knowledge areas essential for the development of novel technology and products in ICT, energy, nanomanufacturing, environment, transport, health, security and several others. Photonics is recognised as a Key Enabling Technology and nanophotonics is likely to be at the base of the next wave of photonics innovation. Nanophononics is becoming more and more visible as the "energy issue" rears its head virtually in all research and development fields. In particular, heat transfer in the nanoscale is more than just thermal management since it underpins the science of fluctuations and noise, needed to develop knowledge at the system level all the way to quantum processes in biology and at the heart of information generation and transformation. Many discussions on the progress of the science and technology of both nanophotonics and nanophononics have taken and are taking place in a large number of conferences, workshops and schools. This is a first non-exhaustive attempt to condense what researchers think are priorities and hot topics in both nanophotonics and nanophononics.

Among the commonly mentioned key issues in **nanophotonics** research is design for specific applications including a subset of generic architectures and device performance in the nanoscale. Power efficiency, both as in power management and wall plug efficiency, are also shared key issues and both are followed closely by the need of technologies and standards suitable for very large scale manufacturing.

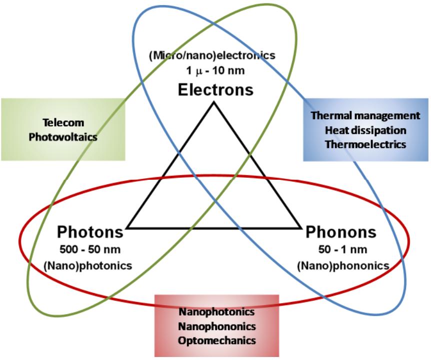


Figure 1. State variables for information processing. The length scales in the diagram also reflect the dimensions needed to manipulate the particles/waves.

---

[1] Contributors: J. Ahopelto, F. Alsina, P.-O. Chapuis, B. Djafari-Rouhani, J. Goicochea, J. Gomis-Bresco, N. Kehagias, T. F. Kraus, S. Landis, V. Laude, R. Li Voti, S. Lourdudoss, T. Mäkelä, A. Martinez, A. Melloni, N. Mingo, L. Pavesi, J. Pekola, M. Prunnila, V. Reboud, F. Riboli, C. Sibilia, C. M. Sotomayor Torres, S. Tretyakov, S. Volz, D. Wiersma and H. Wolf.

An increasing number of groups are working in various fields of **nanophononics**, covering modelling of phononic crystals and heat transport at macro and atomic scale. It is important to intensify the collaboration and create a more unified value chain ranging from design and modelling to heat transport calculations to experimental verification of the models. The latter requires advanced nanofabrication techniques sometimes well beyond the current state of the art. An extensive effort is being put into solving thermal management related issues in ICT at package level. It has become clear that the next step should be to go inside the transistors and find ways to control heat dissipation at micrometre and nanometre level. Here, new models for heat transport are needed to close the gap between continuum models and molecular dynamics modelling, and extensive experimental work is needed to support and qualify the new approaches.

Nanophotonics and nanophononics underpin basic science to develop know-how and methods to overcome scientific and engineering challenges in nanoscience and nanotechnology, impacting ICT. This is supported by the numerous applications mentioned throughout this position paper spanning not only communications but also energy, health, transport and the environment.

Nevertheless, the increasing complexity in the light-matter and phonon-(electron, spin) interactions in the nanoscale is resisting a reductionist approach. There are several sub-communities using highly specialised terminology and approaches which need to become more accessible to each other to enable qualitative progress in nanophotonics and nanophononics in their quest to become relevant ICTs.

Sustainable progress requires a strong synergy with new materials, instrumentation, modelling methods and nanofabrication. However, a much stronger interaction with components, nanomanufacture, design and architecture consortia is needed to make serious inroads into completing the value chain.

Recommendations

1) Targeted European-level support for *fundamental research in application-relevant nanophotonics and nanophononics focusing first on common issues*, for example, heat dissipation at component level, using noise in ICT and ways to cope with the fluctuations in key parameters. The latter bound to be a more serious issue in the nanoscale than in the current micrometre scale but crucial for heterogeneous integration.
2) Bring together the experimental and theoretical communities of phonon physics, heat transfer (mechanical) engineering, statistical physics, biology (fluctuations), nanoelectronics, and (solid-state) quantum communications to start with a *focused research programme on heat control in the nanoscale* in the first instance and on, e.g., *harvesting fluctuations* as a follow-on or parallel focus.
3) A research infrastructure for *emerging cost-efficient nanofabrication methods* jointly with a multi-level simulation hub and a comprehensive nanometrology associated laboratory targeting nanophotonics and nanophononics applications, complementing the Si and the III-V photonic foundries. This infrastructure could then evolve into a potential foundry, with industrial participation, covering combinatory lithography, cost-analysis, packaging and training.
4) Targeted European-level support for research on *material sciences* to develop techniques able to achieve material control at the sub-nanometre and, in particular, in 3-dimensions. This includes, e.g., control of multilayer thickness of silicon-rich silicon oxide and of the barrier dielectric at the wafer scale level.

3. Annex 1
nanoICT working groups position papers

Graphene is considered to be one of the most serious candidate materials for post-silicon electronics by the International Technology Roadmap for Semiconductors (ITRS), the strategic planning document for the semiconductor industry. Indeed, there are many potential uses of graphene because of its unique combination of properties, but those applications not only cover logic and radiofrequency applications. Graphene is a transparent like plastic , but it conducts heat and electricity better than metal, it is an elastic thin film, behaves as an impermeable membrane, and it is chemically inert and stable, thus offering a more functional “plastic-like” material with reinforced properties in terms of stability and mechanical strength, while providing enhanced electrical and thermal conductivities. Potential electronics applications of graphene include high-frequency devices and RF communications, touch screens, flexible and wearable electronics, as well as ultrasensitive sensors, NEMS, super-dense data storage, or photonic devices. In 2010, the first roll-to-roll production and wet-chemical doping of predominantly monolayer 30-inch graphene films grown by chemical vapour deposition (CVD) onto flexible copper substrates were reported. The produced films were found to exhibit low sheet resistances and 90% transmittance, competing with commercial transparent electrodes such as indium tin oxides (ITO). Graphene electrodes could therefore be incorporated into a fully functional touch-screen capable of withstanding high strain. In the energy field, potential applications include supercapacitors to store and transit electrical power and highly efficient solar cells. However, in the medium term, some of graphene’s most appealing potential lies in its ability to transmit light as well as electricity, offering improved performances of light emitting diodes (LEDs) and aid in the production of next-generation devices like flexible touch screens, photodetectors, and ultrafast lasers.

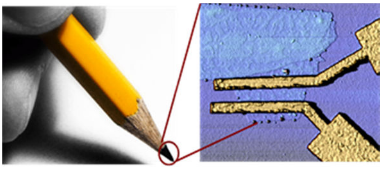
graphene

Position Paper on Graphene

Francesco Bonaccorso; University of Cambridge, UK
Johann Coraux; Néel Institute, France
Chris Ewels; IMN Nantes, France
Andrea C. Ferrari; University of Cambridge, UK
Gianluca Fiori; University of Pisa, Italy
Jean-Christophe Gabriel; CEA, INAC, France
Mar Garcia-Hernandez; ICMM CSIC, Spain
Jari Kinaret; Chalmers University of Technology, Sweden
Max Lemme; KITH, Sweden
Daniel Neumaier; AMO, Germany
Vincenzo Palermo; CNR Bologna, Italy
Stephan Roche; Catalan Institute of Nanotechnology and ICREA, Spain
Aziz Zenasni; CEA, LETI, France

Key Words

Growth: *CVD growth, epitaxial growth, modelling.*
Post-growth modification: *Doping, & functionalization, dispersion and separation, purification, annealing.*
Properties/characterization: *Defects, electron transport, phonons, thermal properties/conductivity, wetting, friction, mechanical, chemical properties, optical, structural properties, contacts.*
Electronic Applications: *RF devices, transistors, sensors, touch screens, flat displays, flexible electronics.*
Optical applications: *OLED, Absorbers, photodetectors, photovoltaics...*
Electromechanical applications: *NEMS (resonators), sensors, bio-medical.*
Energy applications: *Fuel cells, supercapacitors, batteries, solar cells.*
Blue sky: *Spintronics, quantum computing, plasmonics.*



1. Introduction

In this paper, we aim to position the current state and perspectives of graphene-based technologies and applications. This is not meant to be a comprehensive review of the field, but rather an overview with particular focus on European strengths and potential. Non-European researchers clearly give a huge contribution to the field, and set the benchmark against which the European work is measured.

7 years ago, the ground-breaking experiments on graphene in Manchester initiated a field of research moving at an ever faster rate, and gained the 2010 Physics Nobel prize to Andre Geim and Kostya Novoselov.

Even though, graphene science and technology has been pioneered in Europe, international competition is and will remain fierce, given the extensive applications domain. Graphene and related two-dimensional materials offer a completely new *"flatland playground"* for physicists, chemists and engineers. After the discovery of fullerene and carbon nanotubes, graphene

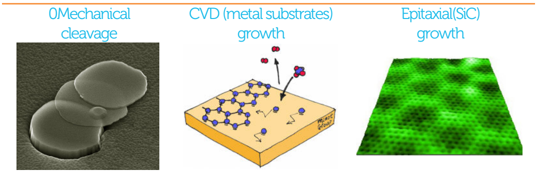


Figure 1. *Illustration of various techniques to either separate out a graphene monolayer by mechanical/chemical exfoliation of layers from graphite, CVD grow graphene on a metallic substrate, or epitaxial growth of graphene layers at the surface of Silicon Carbide.*

has complemented the sp^2 carbon family, being at the same time more suitable for (co)-integration and connection to CMOS technologies, benefiting from conventional techniques of lithography and material engineering. Graphene also appears as a unique platform bridging conventional technologies with the nanoscale Pandora´s box, enabling chemistry to enrich material and device properties.

Graphene-based materials as thus "*enabling materials for ubiquitous electronics applications*" in the fields of information and communication technology (ICT), energy or medicine/biology. Beyond Graphene and the (two-dimensional) flatland, engineering novel materials using the third dimension is also matter of excitement and future innovation. During his Plenary talk at IMAGINENANO 2011 (Bilbao April 2011, www.imaginenano.com), Kostya Novoselov called the scientific community to explore the "spaceland" which could complement graphene through its combination with other two-dimensional exfoliated materials (such as Boron-Nitride) [1]. This opens unprecedented horizons for the design of materials on demand, supplying the suitable structure for a given properties portfolio. Europe could take an international leadership in "novel material innovation", provided a strategic scientific and industrial roadmapping, implementation plan, team networking and relevant funding are smartly merged.

We report here a summary of recent developments in graphene science and technology, pinpointing future directions for innovation and discovery, with a particular emphasis on positioning the prospects for European research. This first version of the Nano-ICT position paper is thus to be considered a mixture between a short review of recent achievements and ingredients for the elaboration of a more specific and detailed roadmap, and not a comprehensive and final review and roadmapping exercise.

In that direction, a particular mention deserves the initiative named GRAPHENE FLAGSHIP pilot (see www.graphene-flagship.eu) which is currently establishing a large database of European groups and research activities focused on Graphene Science and Applications. To date more than 500 groups have registered, gathering several thousands of researchers and engineers and more than thirty companies. This initiative will issue a more exhaustive graphene roadmap in 2012.

2. Vision for the future

A. K. Geim and K. Novoselov, were awarded the 2010 Nobel Prize in physics for "*groundbreaking experiments regarding the two-dimensional material graphene*". Graphene is a one-atom-thick sheet of carbon whose strength, flexibility, and electrical conductivity have opened new horizons for fundamental physics, together with technological innovations in electronic, optical, and energy sectors.

The production of high quality graphene remains one of the greatest challenges, in particular when it comes to maintaining the material properties and performance upon up-scaling, which includes mass production for material/energy-oriented applications and wafer-scale integration for device/ICTs-oriented applications (see Fig.1 for illustration).

Potential electronics applications of graphene include high-frequency devices and RF communications, touch screens, flexible and wearable electronics, as well as ultrasensitive sensors, NEMS, super-dense data storage, or photonic devices (see Fig.2). In the energy field, potential applications include supercapacitors to store and transit electrical power, and highly efficient solar cells. However, in the medium term, some of graphene's most appealing potential lies in its ability to transmit light as well as electricity, offering improved performances of light emitting diodes (LEDs) and aid in the production of next-generation devices like flexible touch screens, photodetectors, and ultrafast lasers.

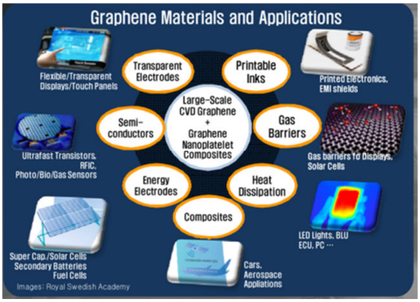


Figure 2. *Overview of Applications of Graphene. After Royal Swedish academy [2]. (by courtesy of ByungHee Hong Seoul National).*

There are many other potential uses of graphene because of its unique combination of properties. Graphene is transparent like plastic but conducts heat and electricity better than metal, it is an elastic thin film, behaves as an impermeable membrane, and it is chemically inert and stable. In 2010 Ref [3] reported the first roll-to-roll production and wet-chemical doping of predominantly monolayer 30-inch graphene films grown by chemical vapour deposition (CVD) onto flexible copper substrates. The produced films were characterized by low sheet resistances (Rs) and 90% transmittance (T), competing with commercial transparent electrodes such as indium tin oxides (ITO). This work demonstrated that graphene electrodes can be efficiently incorporated into a fully functional touch-screen capable of withstanding high strain. Such results allow us to envision the development of a revolutionary flexible, portable and reconfigurable electronics, as pioneered by NOKIA through the MORPH concept (See Fig.3).

Figure 3. *Graphene in NOKIA Morph concept: the future mobile device, Morph, will act as a gateway. It will connect users to the local environment as well as the global internet. It is an attentive device that shapes according to the context. The device can change its form from rigid to flexible and stretchable. For more information see [4].*

New horizons have also been opened from the demonstration of high-speed graphene circuits [5] offering high-bandwidth suitable for the next generation of low-cost smart phone and television displays.

Concerning the domain of ICT, CMOS technology, as currently used in integrated circuits, is rapidly approaching the limits of downsizing transistors, and graphene is seen as an alternative. However, the technology to produce graphene circuits is still in its infancy, and probably at least a decade of additional effort will be necessary, for example to avoid costly transfer from metal substrates. The device yield rate also needs to be improved. The use of graphene in electrodes is probably the closest to commercialization.

In 2011 Ref. [5] reported the first wafer-scale graphene circuit (broadband frequency mixer) in which all circuit components, including graphene field-effect transistors (FETs) and inductors, were monolithically integrated on a single carbide wafer. The integrated circuit operated as a broadband radio-frequency mixer at frequencies up to 10GHz, with outstanding thermal stability and little reduction in performance (less than one decibel) between 300 and 400K.
These results pave the way to achieving practical graphene technology with more complex functionality and performance.

Another potential field of application is photonics and optoelectronics, where the combination of its unique optical and electronic properties can be fully exploited, even in the absence of a band-gap, and the linear dispersion of the Dirac electrons enables ultrawideband tunability. The rise of graphene in photonics and optoelectronics is shown by several recent results, ranging from solar cells and light-emitting devices to touch screens, photodetectors and ultrafast lasers.

Graphene is promising as addictive for composite materials, thin films and conducting inks. High quality graphene inks [6] can now be produced via solution processing [7] and ink-jet printed thin film transistors with mobility ~ 90cm^2/Vs have already been demonstrated, paving the way towards fully graphene-based printable electronics [6].

3. Scientific output

Europe is competitively placed in terms of scientific output, with total graphene publications[1] from North America and Europe closely matching (see Fig. 4).

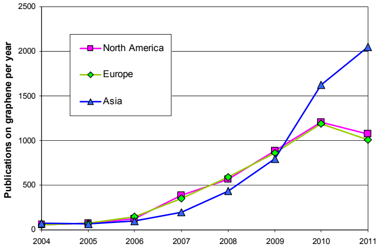


Figure 4. Total scientific publications on graphene by region (2011 January-September).

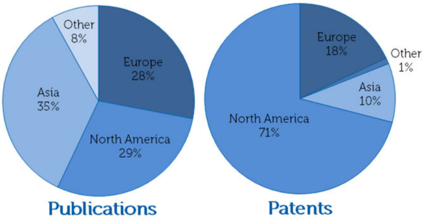


Figure 5. (Left) Total scientific publications and (Right) total patents on graphene by region. Source: Publications from Thomson ISI Web of Science 'graphene' topic search, Patents from WIPO PATENTSCOPE international patent applications.

---

[1] Topic search on 'graphene' from Thomson ISI Web of Science database. Note that this does not take into account any additional criteria such as impact factor of the publishing journals.

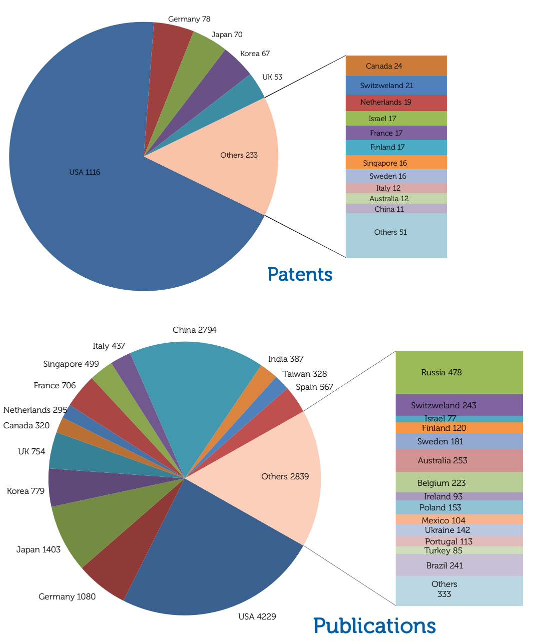


Figure 6. *Breakdown of total patents and publications on graphene by country. Source: Publications from Thomson ISI Web of Science 'graphene' topic search; Patents from WIPO PATENTSCOPE international patent applications.*

The rise in output from Asia since 2009 is clear, largely due to a rapid increase from China, in 2011 overtaking the US as the largest producer of graphene publications. While the division in academic graphene publications between Europe, North America and Asia is roughly equal (Fig.5(a)), the US produced so far over three times as many patents as the others (Fig.5(b)), with the ten highest applicants for patents[2] divided between US academia (Rice University, MIT, University of California and Harvard) and US industry (Sandisk 3D, Graftech, Hyperion Catalysis International, General Electric and BASF) [8]. This, to some extent, reflects the different patent regimes in the regions, and Europe is once again well placed with nearly twice as many patent applications as Asia. The importance placed on graphene research by Korea, Japan and Singapore is clearly represented in their patent and publication output. Within Europe the majority of scientific publications comes from Germany, the UK and France (followed closely by Spain and Italy), while European patent activity is concentrated in Germany and the UK (see Fig.6).

4. The sp^2 two-dimensional lattice: essentials

Graphene consists of carbon atoms arranged in a 2-dimensional honeycomb crystal lattice with a bond length of 1.42 Å [9,10]. A schematic of a single layer graphene (SLG) is shown in Fig. 7a, including "armchair" and "zig-zag" edges, named after their characteristic appearance on the atomic scale. The carbon atoms are sp^2 hybridized and three of the four valence electrons participate in the bonds to their next neighbours (σ–bonds). The schematic in Fig. 7b shows these in green (colour online). The fourth π electron orbital is oriented perpendicular to the sheet, forming with the neighbouring ones a highly delocalized network of π bonds (Fig. 7b, red).

The graphene lattice consists of two sub-lattices A and B, which lead to crystal symmetry [11,12]. As a consequence, the charge carriers (n) can be described by the Dirac equation [12], *i.e.* the band structure of graphene exhibits a linear dispersion relation for n, with momentum k proportional to

---

[2] Patent search on 'graphene' from the WIPO Patentscope international patent application database.

energy E [12]. The energy bands associated with the sublattices intersect at zero energy. For this configuration graphene has been “commonly” called a zero bang gap semiconductor. However, the conductivity of graphene is independent of the Fermi energy (E_F) and n as long as the dependence of scattering strength on E_F and n is neglected [13]. Thus graphene should be considered a metal rather than a semiconductor [13].

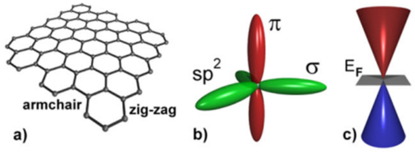


Figure 7. *a) Schematic of a graphene crystallite with characteristic armchair and zig-zag edges. b) Schematic of electron σ–bonds and π-electron orbital of one carbon atom in graphene. c) Band diagram of graphene at k = 0; From [14].*

Charge carriers in graphene have a very small effective mass [15], hence graphene shows extremely attractive properties relevant to electronic devices. These include carrier mobilities of up to 15000 cm^2/Vs for graphene on SiO_2 [15], 27000 cm^2/Vs for epitaxial graphene [16] and hundreds of thousands of cm^2/Vs for suspended graphene [17,18,19] (Fig.8), for typical charge density (n) ~ 10^{12} cm^{-2}. Very recently, mobilities up to 10^6 cm^2/Vs with n of $10^{11} cm^{-2}$ were reported for suspended graphene at helium liquid temperature [20]. These mobility values are at least 40 times higher than typical Si mobility. In addition, high current carrying capability exceeding $1x10^8$ A/cm^2 [21], high thermal conductivity [22,23], high transparency [24] and mechanical stability [25,26] have been reported. While similar promising properties have been reported for carbon nanotubes (CNTs) [27], the fact that graphene processing is compatible with conventional CMOS-technology is potentially a huge advantage.

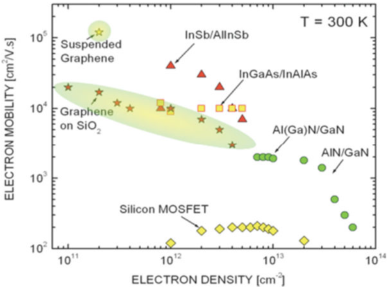


Figure 8. *Electron mobility versus density for an ensemble of materials, positioning graphene performances. Extracted from [17,18,19].*

5. Graphene chemistry: not a molecule, not a polymer, not a substrate

Graphene chemical properties have raised great interest and stimulated excellent research. The main reason of interest is that graphene cannot be easily classified from a chemical point of view, having a size which is atomic in one dimension, and mesoscopic in the other two, resulting particular and somehow contrasting properties.

Graphene can be patterned, etched and coated as a substrate. It can also be processed in solution and chemically functionalized, as a molecule. It could be considered a polymer, obtained by bottom-up assembly of smaller molecules [28], but it can also be obtained from top-down exfoliation of graphite (a mineral). It is not a nano-object similar to fullerenes or CNTs, because it does not have a well-defined shape; conversely, it is a large, highly anisotropic, very flexible ultra-thin material, which can have different shapes and be folded, rolled or bent.

The simplest and most studied chemical functionalization of graphite is oxidation [29,30,31]. This leads to the production of graphene oxide (GO), [29,30,31], with the formation of defects such as C-OH, COOH and C-O-C bridges on its surface and at edges. The functionalization with these hydrophilic groups greatly favours GO exfoliation, allowing to produce on large scale highly concentrated solutions of GO in water [32], containing high percentage of monolayers [33].

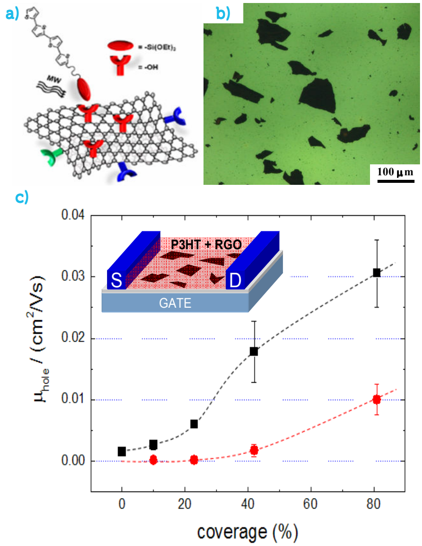


Figure 9. a) Schematic representation of covalent functionalization of GO. From [36] b) Fluorescence quenching image of graphene oxide sheets on a thin molecular layer of quater-thiophene. From [34] c) Evolution of measured charge mobility in transistor devices based on polythiophene (P3HT) and reduced graphene oxide (RGO) at increasing RGO coverage. In the inset, a schematic representation of the transistor device. From [36].

The chemical polar groups created by oxidation can also be used for further functionalization, allowing to exploit the full power of carbon-based organic synthesis to achieve different graphene-based materials (Fig.9a) [35,36]. By taking advantage of the extensive know-how already available for CNTs, either covalent [37, 38] or supramolecular [39,40] functionalization of graphene with different molecules can be achieved. This includes selective organic functionalization of graphene edges, taking advantage of the higher concentration of carboxyilic groups at the edges of exfoliated GO sheets [35].

Chemical functionalization from one hand makes graphene more processable, but from the other hand destroys its peculiar electronic properties, transforming it into an insulator [41]. The GO chemical structure can be highly variable, depending on the details of its production, but can be described as a mosaic of different domains, of nanometer size, featuring highly conjugated, graphene-like areas, alternated to completely oxidized, insulating sp^3 domains, as well as to void areas where the oxidation process has completely destroyed the carbon backbone, leaving a hole in the GO sheet [42,43]. Overall, the surviving graphene conjugated domains in GO can be seen as an ensemble of polycyclic aromatic domains of different size, all linked on the same sheet by a network of insulating sp^3 bonds, which hinder charge transport [43].

The conductivity can be increased by producing Reduced Graphene Oxide (RGO). Reduction can be achieved by thermal [41,55, 44] chemical [41, 45, 46] or electrochemical [47, 48] methods. Though this process never re-establishes the "perfect" lattice of graphene, being unable to heal some more stable defects, such as the voids in the sheets and some particular oxidized forms (carbonyl and ether groups) [49]. Nonetheless, RGO is

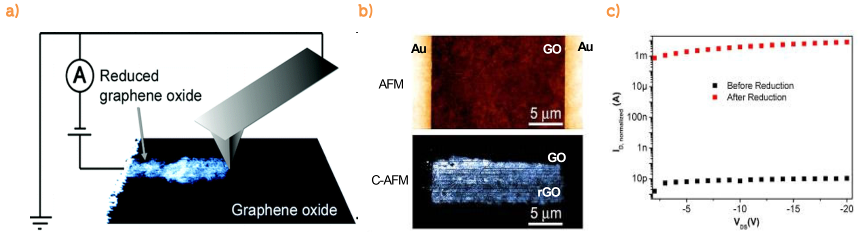


Figure 10. a) Schematic representation of the creation of conducting RGO patterns on an insulating GO layer using a scanning probe. b) AFM and conductive AFM image of a source-drain electrode pair bridged by an electrically conducting tip-reduced GO region. c) Drain current (I_D) vs. drain-source voltage (V_{DS}) measured on graphite oxide films before (black squares) and after (red squares) reduction by a scanning probe. An increase of about 10^8 in the normalized source-drain current is shown. From [57].

conductive, with a charge mobility larger than typical organic semiconductors, and can have promising applications as electrode [50] and charge transporter [33,51] in organic electronics, as interface layer in photovoltaic blends [52], to replace or improve indium tin oxide (ITO) electrodes, in dye sensitized solar cells, to improve charge collection and transport [53] and as material with high surface area and good conductivity for energy storage [54].

An approach for selective GO reduction is to use a scanning probe by locally applying high temperature [55], or to perform electrochemical reduction on microscopic scale [56], allowing to fabricate electronic devices where the active layer is formed by a sheet of conductive RGO “drawn” on an otherwise insulating GO layer (Fig. 10a) [57]. Once functionalized, either by covalent or supramolecular chemistry, graphene interacts strongly with the surrounding molecules (either small molecules or polymers), gaining new electronic, chemical and optical properties. Graphene-organic interactions are studied for a wide range of applications, form surface science [40], to electronics [33,54,56] to composites, to biological and sensing applications [58,59,60].

Organic molecules can be absorbed on graphene substrates forming 2D layers which tend to have a weak interaction with the underlying graphene [40], with small but significant differences with respect to the packing of the same molecules on bulk graphite [40]. The graphene-molecule interaction can be strong, resulting in a complex interplay of π-π stacking, electrostatic interactions, and molecule-molecule lateral interactions [40,61,62].

Graphene-organic interactions can lead to strong doping [63,64,65,66], and to charge [67] or energy [68] transfer, making graphene a strong quencher of fluorescence of several organic molecules (Fig. 10b,c) such as pyrene [67,68] oligo- and poly-thiophene [33,69,70], poly-phenylenevinylene [70]. Even one SLG, GO or RGO can effectively quench the fluorescence of an organic thin layer [69], allowing to visualize single sheets with high optical contrast (~0.8) [69], or to quench fluorescent molecules at tens of nm away [71]. For more detailed reviews on graphene interactions with organic materials, see Refs. [72,73].

6. Graphene fabrication

The industrial exploitation of graphene will require large scale and cost-effective production methods, while providing a balance between ease of fabrication and final material quality. There are currently five main approaches: 1) mechanical exfoliation, 2) carbon segregation from carbon containing metal substrates and silicon carbide (SiC) 3) chemical vapour deposition (CVD) of hydrocarbons on reactive nickel or transition-metal-carbide surfaces, 4) chemical synthesis and 5) liquid phase exfoliation (LPE).

Exfoliation; Novoselov *et al.* introduced a manual cleaving process of graphite, frequently called "mechanical exfoliation", to obtain SLG and few layer graphene (FLG) [12,74]. This process makes use of adhesive tape to pull graphene films off a graphite crystal. When observed through an optical microscope, SLG and FLG add to the optical path compared to the bare substrate. If a proper SiO_2 thickness is chosen, the resultant visible contrast is sufficient to identify the number of layers [75,76,77,78]. Fig. 11b shows the result of a contrast simulation of SLG on SiO_2, where the contrast is plotted for a range of wavelengths and SiO_2 thicknesses [75]. In the visible range, SiO_2 films of ~90 nm and ~300 nm maximise contrast, hence are widely used as substrates. This pragmatic, low-cost method has enabled researchers to conduct a wide variety of fundamental physics and engineering experiments, even though it cannot be considered a process suitable for industrial exploitation (even though approaches for large scale mechanical exfoliation have been proposed). An example of typical exfoliated flake, with a varying number of layers, on an oxidized silicon wafer is shown in Fig. 11c. These layers have a slightly different colour in the optical microscope (Figure 11c). While a trained person can distinguish single- from few layer graphene by "naked eye" with high fidelity, Raman spectroscopy has become the method of choice when it comes to scientific proof of SLG [79,80]. Indeed, the graphene electronic structure is captured in its Raman spectrum that evolves with the number of layers [79]. The 2D peak changes in shape, width, and position for an increasing number of layers, reflecting the change in the electron bands via a double resonant Raman process. The 2D peak is a single band in SLG, whereas it splits in four bands in bi-layer graphene (BLG) [79]. This is demonstrated in Fig. 11d, where Raman spectra for SLG and FLG are plotted. Since the 2D peak shape reflects the electronic structure, twisted multi-layers can have 2D peaks resembling SLG, if the layers are decoupled.

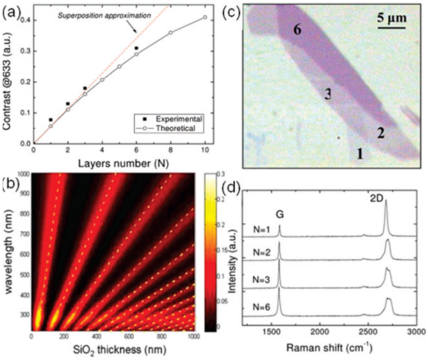


Figure 11. (a) Maximum contrast at 633 nm as a function of N. (b) Calculated contrast of graphene as a function of oxide thickness and excitation wavelength. Dotted lines trace the quarter-wavelength condition. c) Optical micrograph of multilayer with 1, 2, 3, and 6 layers. (d) Raman spectra as a function of number of layers. From [75].

The Raman spectrum of graphite was measured 42 years ago [81]. Since then Raman spectroscopy has become one of the most used characterization techniques in carbon science and technology, being the method of choice to probe disordered and amorphous carbons, fullerenes, nanotubes, diamonds, carbon chains, and polyconjugated molecules [82]. The Raman spectrum of graphene was measured 6 years ago [79]. This triggered a huge effort to understand phonons [79,80], electron-phonon [79,80,83], magneto-phonon [84,85] and electron-electron [86] interactions, and the influence on the Raman process of number [79] and orientation [79,80] of layers, electric [87,88,89] or magnetic [90,91] fields, strain [92,93], doping [94, 95], disorder[80], quality [96] and types[96] of edges, functional groups [97]. This provided key insights in the related properties of all sp^2 carbon allotropes, graphene being their fundamental building block. Raman spectroscopy has also huge potential for layered materials other than graphene.

Liquid phase exfoliation; Graphene flakes can be produced by exfoliation of graphite via chemical wet dispersion followed by ultrasonication, both in aqueous [98, 99,100,101] and non-aqueous solvents [6,7,101,102]. This technique has the advantage of low cost and scalability. Graphene flakes with lateral sizes ranging from few nm to a few microns can now be produced with concentration up to a few mg/ml in up to litre batches [102,103]. Control of lateral size and number of layers is achieved via separation in centrifugal fields. Up to ~70% SLG can be achieved by mild sonication in bile salts followed by sedimentation based-separation [100,104]. LPE also allows isolation of flakes with controlled thickness, when combined with density gradient ultracentrifugation (DGU) with ~80% SLG yield (Fig.12) [99].

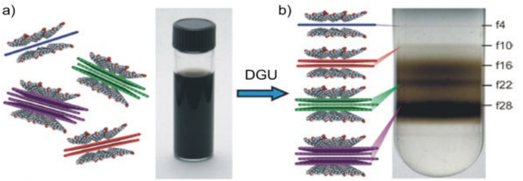


Figure 12. Sorting of graphite flakes using DGU. a) Schematic illustration of surfactant encapsulated graphene sheets and photograph of an unsorted aqueous. b) Photograph of a centrifuge tube following DGU marked with the main bands of monodisperse graphene [99].

Other routes based on chemical wet dispersion have been investigated, such as exfoliation of fluorinated graphite [105], intercalated compounds [106], expandable graphite [107] ultrasonication of graphite in ionic liquid [103] and non-covalent functionalization of graphite with 1-pyrenecarboxylic acid [108].

LPE is an essential tool for the production of composite materials, thin films and conducting inks, with no need of expensive growth substrates. Graphene inks have been already demonstrated to be a viable route for the production of ink-jet printed thin film transistors [6]. Furthermore, many applications in photonics and optoelectronics, such as transparent conductors, third generation solar cell electrodes and optical graded graphene-based polymer composites will benefit from graphene produced by LPE [104]. LPE is also a useful for the production of graphene nanoribbons (GNR) [109]. LPE does not require transfer techniques and the resulting material can be deposited on different substrates (rigid and flexible) following different strategies such as, dip and drop casting, spin, spray and rod coating, ink-jet printing, etc.

LPE can also be used to exfoliate and disperse any other layered materials, such as chalcogenides and transition metal oxides

(TMOs), BN, MoS_2, Ws_2 etc. [110]. The development of a sorting strategy both in lateral dimensions and number of layers will be essential for the full exploitation of their optical and electronic properties.

Segregation form silicon carbide; Acheson reported a method for producing graphite from SiC in as early as 1896 [111]. Recently this approach has been perfected to yield SLG and FLG [112,113,114,115] (crystallites >10µm, small number of defects). Electronic decoupling from the underlying SiC substrate can be achieved by hydrogen treatment [116]. During the process, silicon is thermally desorbed at temperatures between 1250°C [112] and 1550°C [114,115]. This process is more controllable and scalable when compared to mechanical cleaving. In fact, graphene transistors can be manufactured from epitaxial graphene on a wafer scale [117]. Similar to exfoliated graphene, it has been demonstrated that single epitaxial graphene layers can be identified by Raman spectroscopy [118]. In addition Raman spectroscopy revealed that these layers are compressively strained [118]. A major disadvantage of epitaxial graphene is the high cost of SiC wafers, their limited size compared to Si wafers, and the high processing temperatures, well above current CMOS limits.

Chemical vapor deposition (CVD); SLG and FLG can be grown by CVD on metals, such as nickel [119,120,121,122], ruthenium [123] iridium [124,125] or copper [3,126]. Several methods of transferring the CVD graphene films onto target non-metallic substrates have been suggested [3,121,122], including the use of disposable Poly(methyl methacrylate) (PMMA) [121] or Polydimethylsiloxane (PDMS) [122] films.

CVD has now almost reached maturity for mass-production. Samples over 50 cm in size have been grown and transferred on target substrates [3].

Decisive progresses were made in the last few years towards the understanding of the growth processes, the characterization of the graphene/metal interaction, the tailoring of graphene's properties by tuning this interaction, or the design of novel hybrid structures with unique functionalities for spintronics, nanomagnetism, or catalysis. Europe occupies a special position in this respect, with a number of theory and surface science groups having pioneered the field.

Although CVD growth on Cu-foils is the most popular approach to date; there are other alternative schemes to produce wafer-scale graphene which yet require an active phase of research. Amongst these, are CVD on insulating substrates [127, 128, 129, 130, 131, 132, 133], Plasma Enhanced CVD (PECVD) [134] and molecular beam epitaxy (MBE) growth [135] .

Carbon segregation from metal substrates; This method exploits the solubility of carbon in transition metals (thin films of nickel), that subsequently segregates graphene at the metal surface. The graphene quality and the number of layers are strongly dependent on the growth and annealing conditions. The advantage of this method over standard CVD is that the graphene quality is controlled by the carbon source and annealing conditions. To get large metal grains with appropriate crystalline orientation (111) [136], a first step annealing of the metal surface is often performed. The carbon diffusion is simultaneously occurring during the crystalline orientation of nickel.

All the process steps occur in fully semiconductor compatible environment. Europe semiconductor industry can, then, reasonably take benefit of the versatility of this method toward the integration of graphene in their technological process flow.

6.1 Graphene growth by carbon segregation in Europe

This section exemplifies the leading and active position of Europe in graphene growth by carbon segregation. The first section deals with the study of the structural properties of graphene, the second addresses the investigation of the electronic, magnetic, and mechanical properties, the third focuses on the design of graphene/metal hybrid structures with novel functionalities, and the last gives an overview of Europe's efforts towards the production of graphene *via* growth on metals.

6.2 Structural properties of graphene/metals

Ref. 137 reported a pioneering atomic-scale characterization of SLG with scanning tunnelling microscopy (STM) in 1992, well before the “rise” of graphene. The study was performed for graphene grown on a Pt(111) crystal by chemical vapour deposition [137]. A number of European groups have employed this technique to study the structure of graphene on other metal surfaces, like Ir(111) (Fig. 13a) [138,139], Ru(0001) [140,141] or Ni(111) [142,143,144].

Ref. 145 conducted surface X-ray diffraction (SXRD) measurements of SLG, and revealed a surprisingly large (ca 5 nm) commensurate graphene/Ru. Recent experiments also revealed that incommensurate structures may be found as well, on graphene/Ir [147]. The question of commensurability of graphene onto metals is of fundamental nature. It has deep consequences, a wealth of intriguing phenomena related to the physics of phase transitions in two dimensions being expected. The graphene-metal distance and the nano-rippling of graphene on its metallic substrate, which follows the graphene-metal so-called moiré superstructure, are hallmarks of graphene-metal interaction: metals with a strong affinity with carbon are expected to induce a low graphene-metal distance [146], and a strong nano-rippling, which eventually can disrupt the conical band structure around the Fermi level and induce charge transfers.

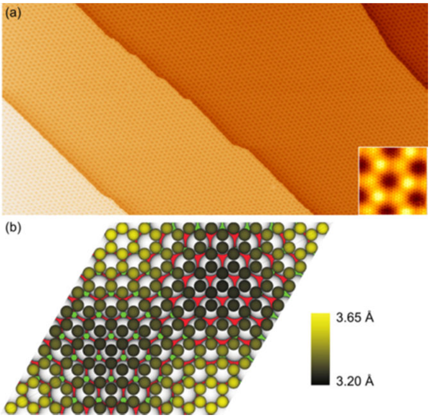


Figure 13. (a) 250×125 nm^2 STM topograph of graphene/Ir, showing the moiré superstructure spanning over four atomically flat terraces (from Ref. [124]); inset: atomic resolution STM topography showing the centre of carbon rings as dark spots, and the moiré superstructure, from [125]. (b) Top-view of the relaxed geometrical structure of graphene/Ir obtained by DFT including van der Waals interactions (from Ref. [147]).

This question fuelled an active debate in the literature. The contribution of Europe is decisive, and has much enriched the picture of the graphene/metal interaction thanks to the involvement of different groups with complementary expertises, ranging from STM [140,141], density functional theory (DFT) calculations [147,145,146,148,149], electron diffraction [150], He diffraction [151], SXRD [145], and more recently, X-ray standing waves [147].

There exist a long-lasting tradition of DFT simulations of carbon materials in Europe and this holds for graphene on metals. A pioneering contribution was in Ref. 136, who targeted the study of graphene on Ni(111). Large supercells (several hundred atoms) were considered in Ref. 147. This is an unprecedented fine description of the graphene-metal electronic interaction [149]. Europe maintains its leading position, notably by its efforts towards taking into account van der Waals interactions in DFT [152,153], the most recent achievement being the use of a fully-consistent treatment of several hundred atoms supercells (Figure 13b) [147]. These interactions, often eluded in DFT calculations, are known to have prominent contribution to the graphene bonding on metals in many cases. Their implementation in DFT now provides a good description of the structure of graphene/metals, which agrees with the latest state-of-the-art measurements.

The production of high quality graphene via growth on metals first requires that defects in graphene are identified, then controlled, and whenever possible avoided. European groups have addressed, in some cases initiated, the study of a number of defects in graphene/metals: grain boundaries, pentagon-heptagon pairs [124], point defects [154], wrinkles [155], or local deformations [146].

6.3 Foreseen progress/evolution

The full understanding of the influence of defects on the properties of graphene has not been achieved yet. Benefiting from a strong expertise in defect characterization, Europe can play a crucial role in this respect. Answering the debated question of carbon magnetism due to vacancies in graphene would for instance be a major advance. Better controlling their formation and eventually avoiding them is of prime importance in view of producing ultra-high quality graphene. Another field where Europe could largely contribute to, based on its experience, is towards the graphene band structure engineering with the help of super-potentials induced by the graphene/metal epitaxy. Ordered vacancy lattices or antidot lattices, triangular or anisotropic moiré patterns, periodic strain patterns, etc, were proposed as efficient routes in this respect. Only a few of these routes were explored by experimentalists so far. Another area where Europe should continue is the understanding of the graphene/metal interaction, which drives the structure, electronic properties, and growth of graphene. A unified and predictive picture is still missing.

6.4 Electronic, magnetic, and mechanical properties of graphene/metals

It was realized a few years ago that the moiré pattern arising between graphene and metal substrate can act as a varying electronic potential for *n* [156]. This could induce nanometre-scale electron/hole pockets for graphene/Ru [141]. The origin for these inhomogeneities is thought to be local charge transfers and change of hybridization [157]. Fainter modulations were found in graphene/Ir [158], where superpotential effects were evidenced by angle-resolved photoelectron spectroscopy (ARPES) (Fig. 14a) [158]. It was shown that the band structure can be further disturbed, up to the point where graphene π-bands become anisotropic, by metal cluster growth on graphene/Ir [156].

The study of the metal-graphene interactions started some years ago with ARPES [158]. Until 2009 however, only those metals which strongly interact with graphene were addressed. European groups conducted the first studies of graphene decoupled from its substrate [159].

An almost intact Dirac cone, with a Dirac point almost matching the Fermi level (marginal charge transfer), was achieved for graphene on Ni intercalated by an Au monolayer (Fig. 14b) [159]. A similar observation was done for graphene on Ir (Fig. 14a) [158]. This pushed a number of groups worldwide to consider this system as a reasonable realization of free-standing graphene. Effective manipulating of graphene's band structure was put in evidence in this system, H adsorption inducing a bandgap, as high as 450 meV, at the Dirac point (Figure 14c) [160]; similar results were obtained for graphene/Au/Ni [161].

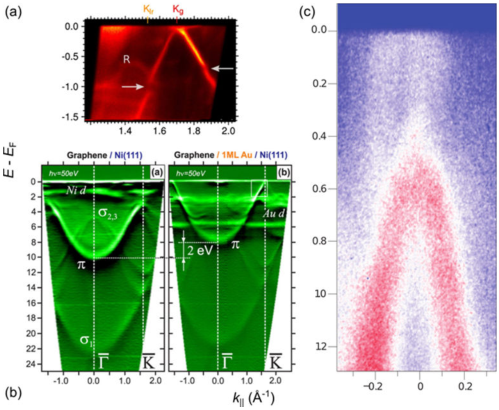


Figure 14. *Energy (E) verus in-plane wave vectore ($k_{||}$) cuts in the band structure of graphene in the vicinity of the K point of graphene. The origin for the energy axis is taken at the Fermi level (E_F). (a) Graphene on Ir(111), showing a conical dispersion, marginal charge transfer, mini-band gaps (arrows) and a replica band, arising for moiré superpotential effects (from Ref. 158]), (b) graphene on Ni(111) (left) and with an intercalated Au layer (right), for which the conical dispersion of graphene is recovered (from Ref. [159]), (c) H-adsorbed graphene on Ir(111), characterized by the presence of a large band gap at the Dirac point (from Ref. [160]).*

Spin-polarization of the π-bands could open the route to graphene-based spintronics. There has been a noticeable effort in this direction, restricted to Europe, which led to interesting debates. It was first argued that strong Rashba (spin-orbit) splitting of the π-bands could be induced in epitaxial graphene on Ni [144]. From other works, it is concluded that whether on Co or Ni, the Rashba splitting can only be marginal [162], while few 10 meV splitting was obtained via Au contact, which still corresponds to an enhancement of the spin-orbit constant in graphene by a factor of 100. The study of the thermal expansion coefficient of epitaxial graphene started recently [163]. Core level electron spectroscopy and *ab initio* molecular dynamics revealed an increase of the carbon bond length in a large range of temperature [164], and, counter-intuitively, an increase of the nano-rippling amplitude against heating [164]. SXRD confirmed that the graphene-metal epitaxy, even when governed by weak interactions, renders the thermal expansion coefficient different from that of isolated graphene, but does not follow that of the metal [146], possibly due to slippage.

The study of the nanomechanical properties of epitaxial graphene is again led by European groups. Atomic-scale resolution scanning probe microscopies, atomic force microscopy (AFM) [165] and STM [166] provided insights into local variations of the interaction between a metal tip and the graphene surface. The chemical inhomogeneity, which follows the Moiré and is due to varying interactions between graphene and the substrate, were shown to play an important role. DFT calculations provided details of the electronic interaction between graphene and its metallic support. Many efforts in treating the spin degree of freedom in these calculations were pioneered by European groups [136,167,168,169]. This allowed addressing proximity induced magnetism, magnetic moment enhancement at the graphene/metal interface, or spinning filtering.

6.5 Foreseen progress/evolution

Beyond the exceptional thermal conduction of free-standing graphene, it is necessary to develop a good understanding of the thermal properties of graphene contacted to a metal, for instance in graphene/metal hybrid structures, or to elucidate the influence of metal electrodes contacted to graphene.

Epitaxial graphene on metals provides in certain cases model systems mimicking free-standing graphene. This is the case for graphene/Ir or Au intercalated graphene/Ni. The European community well understood this unique opportunity of taking benefit of the powerful tool-kit offered by surface science to probe the basic properties of graphene. Some of the properties remain mostly unexplored in epitaxial graphene, and it is reasonable to expect that Europe's state-of-the-art instrumentation should allow filling this gap.

6.6 Graphene/metal hybrid structures

The first proposals for graphene based spin-valves were reported in Europe [167]. Ref. 170 predicted that one or several graphene layers sandwiched between two epitaxial ferromagnetic leads (Figure 15a), was could offer high magnetoresistance and low resistance×area product [170] in the current-perpendicular-to-the-plane (CPP) geometry.

The latter feature is desirable for high density magnetic storage where small area ferromagnet/graphene/ferromagnet bits would have low resistance: low power consumption devices could thus be triggered. These theoretical works stimulated a strong interest in the community. Several groups are aiming at the experimental realization of the set-up. Along this view, a first step was made by a European group, with the demonstration of spin polarization in graphene on Ni [143].

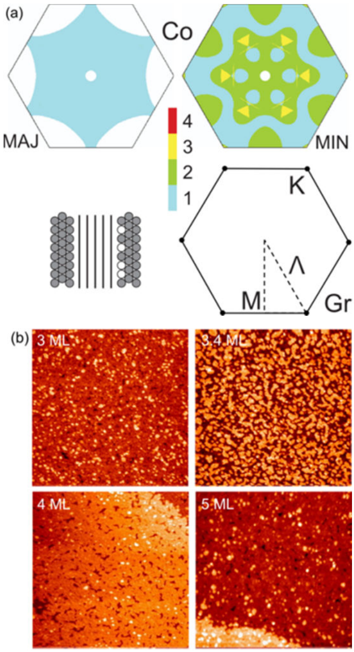


Figure 15. *(a) Fermi surface (colour are for the number of Fermi surfaces) for Co minority and majority spin electrons (top), Fermi surface of graphene (bottom right), and schematic side-view of a graphene/Co spin valve (from Ref. [167]). (b) Layer-by-layer growth of Co by pulsed laser deposition on graphene/Ir, as seen by STM (100×100 nm^2 topographs), for increasing Co thickness, expressed in monolayers (ML) (from Ref. [169]).*

The growth of flat and continuous layers of a ferromagnet on graphene is a difficult task since usually clustered films are formed. Using pulsed laser deposition it was found that high quality epitaxial ultrathin Co films could be prepared (Fig. 15b) [169]. Spin-valves in the CPP geometry now appear within reach.

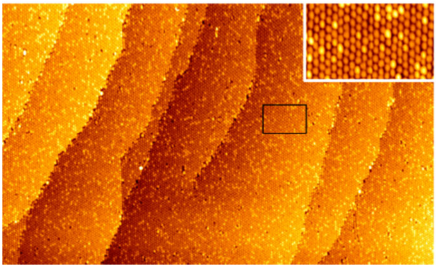


Figure 16. *500*300 nm^2 STM topograph of Ir nanoclusters self-organized on the triangular moiré (2.5 nm pitch) of graphene/Ir(111). The inset shows a blow-up of the black-framed region (From Ref. [163]).*

Ref [138] has shown that epitaxial graphene may be decorated with dense arrays of equally sized nanoclusters, under the influence of the graphene/Ir moiré (Figure 13). Later the same group showed that a variety of materials could be organized on the moiré [163] (see Fig. 16), and other European groups reported that the method is also efficient on the graphene/Rh [171] and graphene/Ru [172] moirés. Not only these new systems pave way to the study of size dependent magnetic [40] or catalytic properties on a graphene substrate (*i.e.* potentially mediating exchange interactions or inert against catalytic reactions), but also the clusters may allow to manipulate the graphene band structure, as recently shown on graphene/Ir, were anisotropic Dirac cones were accordingly engineered [156]. Worth noting also is the recent demonstration of supramolecular assemblies on epitaxial graphene [40,173], which could allow to engineer novel functionalities thanks to appropriate molecules.

6.7 Foreseen progress/evolution

Intercalation of a variety of elements between graphene and its metallic substrate has been studied for decades [174]. A few European groups started to make use of this effect in view of building-up novel graphene-based layered structures [159,168,169], either for protecting metal layers from atmosphere oxidation, or for tailoring graphene's band structure (band-gap, spin-splitting). Many progresses are expected in this direction, and novel complex heterostructures could be developed accordingly. The study of small-size effects (for instance catalytic or magnetic) and of the influence of the graphene substrate of cluster/graphene hybrids has just started.

Europe occupies a leading position in this field. The interaction between physicists and chemists proved very efficient, as exemplified by the achievement and control of supramolecular networks on epitaxial graphene. Such fruitful interactions could extend to the surface chemical modification of graphene, which will provide new opportunities for tailoring the properties of graphene.

7. Graphene mass production

The investigation of the basic processes during graphene growth on metals is crucial in view of controlled growth of defect-free graphene over large areas. Europe, USA, Korea, Singapore, Japan and China are in strong and constructive competition in this field. Extensive STM work guided the achievement of centimetre-scale, single crystallographic orientation epitaxial graphene on Ir [124,175] or Ni[176], Pt[176], Ru[123,176]. Low-energy electron microscopy

(LEEM), photoemission electron microscopy (PEEM) and spot profile low-energy electron diffraction (SPALEED) allowed to determine optimum growth conditions [155, 177, 178, 179]. Europe also offers unique STM instrumentation, with environmental microscopes operating at temperatures as high as 1000 K. This allowed real-time imaging of growth with nanometre resolution [180,181].

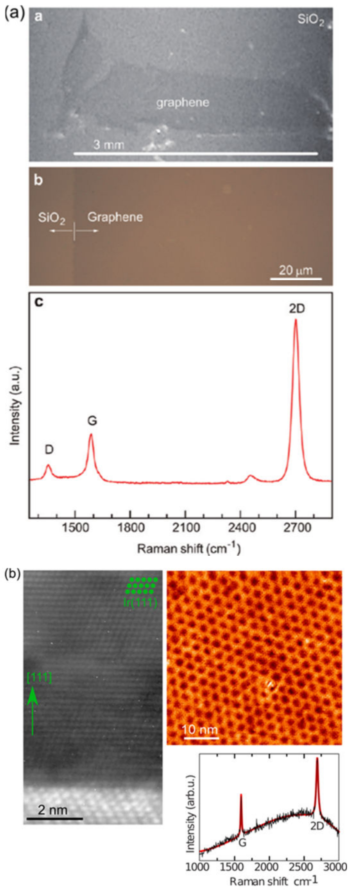


Figure 17. *(a) Graphene transferred from its high quality Ni thin film on MgO: optical micrographs (top and middle) and Raman spectrum of graphene transferred on a Si/SiO$_2$ wafer (from Ref. [181]). (b) Transmission electron microscope cross-section of a single crystalline Ir(111) thin film on C-plane sapphire (left), STM topograph of a graphene layer on top of this film (top right), and Raman spectrum of graphene/Ir (bottom right) (from Ref. [168]).*

A recent evolution in the field of graphene production on metals consists in substrate engineering. The defects in the substrate are believed to influence the formation of defects in graphene. Low-cost preparation of large area graphene cannot afford bulk single-crystals as substrate. Almost simultaneously, a few research groups in US at University of Texas (R.S. Ruoff) [126], MIT (J. Kong) [121], in Korea at SAINT (B.H. Hong [122] and Sungkyunkwan University (J.H. Ahn) [3], together with two European teams [182,183] demonstrated the preparation of high quality graphene on thin, high quality metal films prepared on wafers.

Europe has a unique expertise in simulations of graphene (and CNT) growth on metal surfaces. The approach has been optimized along years and relies on tight binding Monte Carlo calculation. It allows tracking the initial stages of growth, and putting in evidence the formation precursors. Refs. [184,185] explored the temperature-dependent surface segregation of carbon contained in Ni [184,185], while Ref. 186 studied healing mechanisms for defects during growth [186].

European groups [182, 187, 188, 189, 190, 191, 192, 193, 194, 195] have contributed to the optimization of chemical vapour deposition of graphene in low-cost conditions, *i.e.* at atmospheric pressures or slightly below. This preparation route efficiently provides large-area graphene of reasonable quality, after transfer to a suitable support. Given the few-months period required for preparation conditions optimization, it is expected that a number of additional reports/patents will be issued within Europe in the coming months. Controlled graphene nano-structuration is a long-standing quest which is motivated by the prospect for band gap creation in graphene. This is a prerequisite for logic graphene transistors. Ref. 196 suggested surface polymerization at metal surfaces. The next step consists in transferring GNRs to appropriate supports. Even if CVD on metal is a very promising mass production technique, the transfer step could be considered as an issue. Polymer transfer (by PMMA and PDMS) may leave some impurities.

Moreover, the Cu foil which is mostly used to produce large SLG is expensive and can impact the whole process specification. An efficient Cu recycling strategy needs to be devised.

Europe can play a major role in looking for rapid, cheap and versatile fabrication methods. Europe leads LPE of graphene [7]. This technique was developed there, and several advances have been achieved [98,100,102,103,104,106]. LPE needs to be improved to reach control on-demand of number of layers, flakes thickness and lateral size, as well as the rheological properties of the graphene dispersions. Modelling is needed to fully understand the exfoliation process in different solvents, in order to better separate flakes in centrifugal fields, so to achieve SLG and FLG with well defined morphological properties at a high rate.

7.1 Foreseen progress /evolution

Europe is strongly involved in *in situ* studies of the growth of epitaxial graphene. It is possible that that this will allow Europe to be a key player in the highly competitive field of graphene growth of metals. Noteworthy, growth monitoring *in operando*, *i.e.* close to 1000°C, either under UHV or atmospheric conditions, is being pursued by several EU labs.

7.2 Europe position in graphene chemistry

Europe is strong in graphene chemistry research, with several groups leading the fields of covalent and supramolecular functionalization. The recent production of mono-dispersed, tuneable graphene nano-ribbons with controlled edge terminations by bottom-up chemical synthesis [28] is a major, all-European advancement in the field. Another recent European advance is the selective chemical functionalization of the graphene edges [35]. Graphene chemistry is also strongly pursued by major European companies, collaborating in different FP7 projects.

7.3 Bottom-up graphene design

Precise control of the GNR edge structure is essential to avoid defect induced scattering [28]. One promising route is bottom-up growth via polymerisation of polyaromatic oligomers (Figure 18). Ref. 197 successfully produced a variety of GNRs using metal assisted coupling of molecular precursors into linear polyphenylenes, followed by cyclodehydrogenation.

While there are currently scalability issues with this approach, nevertheless it shows great promise, especially in view of controllable edge site chemical functionalization, for chemical fine tuning of nanoribbon electronic properties.

Alternative routes to control edge chemistry are under development, for example top-down approaches exploiting metal nanoparticles to selectively etch graphene with crystallographic orientation [198,165] or via STM lithography [199,166]. Ribbon edge and defect chemistry is being driven in Europe by first principles electronic structure modelling [200,167]. Edge chemistry and structure dominates the band gap of GNRs [201,168], with out-of-plane distortions stabilizing the edges [202,203,169,170]. Selective edge functionalisation was proposed as a route to nanojunction design in GNRs [204,171], while quantum transport modelling suggests that controlled GNR doping with light element impurities, such as Ni and B may be a route to new types of switching devices [167,205,172]. Further work on defect modelling is summarised in a recent review [205].

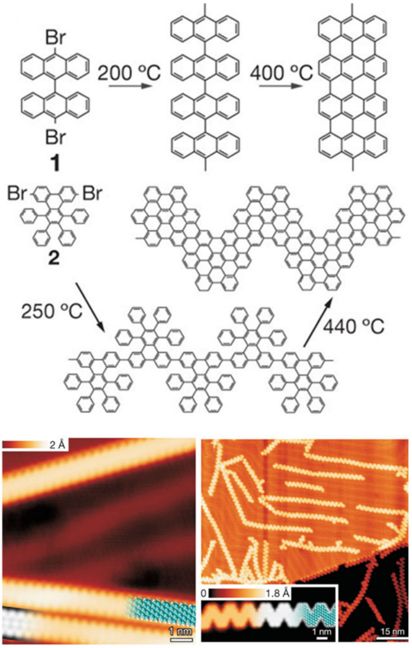


Figure 18. (top) Reaction schemes for producing straight and chevron-type graphene nanoribbons on metal surfaces using different molecular precursors, (bottom left) High resolution STM with overlaid molecular model (blue) of resultant graphene nanoribbon (T=5K, U=-0.1V, I=0.2nA), (bottom right) Overview STM image of chevron-type graphene nanoribbons fabricated on a Au(111) surface (T=35K, U=−2V, I=0.02nA). The inset shows a high-resolution STM image (T=77K, U=−2V, I=0.5nA) and a DFT-based simulation of the STM image (greyscale) with partly overlaid molecular model of the ribbon (blue, carbon; white, hydrogen). From [28].

The combination in Europe of a well established community of atomic scale modelling, with strong expertise in controlled nanocarbon chemistry offers an exciting potential for bottom-up design of graphene based materials and devices.

7.4 Nomenclature and classification

As the graphene field matures and becomes increasingly applications driven, new standards and classifications will be needed, for which the integrated research community within Europe is well placed to act as a driving force.

Low cost 'industrial graphene' for composite applications may contain multi-layer material, whilst ICT-grade graphene requirements will be more stringent. Flake size, impurity content, degree of poly-crystallinity and chemical post-treatment will all need to be incorporated in such a classification. As for any other carbon material [206], Raman spectroscopy [207,208,209] may be the ideal tool to provide a standard reference.

8. Graphene photonics and optoelectronics

Graphene is emerging as a viable alternative to conventional optoelectronic, plasmonic and nanophotonic materials [104]. It has decisive advantages such as near-wavelength-independent absorption, tunability via electrostatic doping, large charge-carrier concentration, low dissipation rates, extraordinary electronic properties and the ability to confine electromagnetic energy to unprecedented small volumes. Graphene can be produced in large quantities and large areas, a key ingredient towards future graphene-based photonics. In addition, it can also be integrated with Si technology on a wafer-scale. Combined, these aspects constitute fundamental advantages to produce photonic devices with performance superior to other materials, especially in less-conventional wavelength ranges, thus far limited by the unavailability of appropriate optical materials.

8.1 Transparent conductors/contacts

Graphene and other 2d layered materials, will have a disruptive impact on current optoelectronics devices based on conventional materials, not only because of cost/performance advantages, but also because they can be manufactured in more flexible ways, suitable for a growing range of applications. In particular, human interface technology requires the development of new applications based on stretchable electronics and optoelectronics, such as flexible displays, touch-screens, light emitting diodes, conformal biosensors, photodetectors and new generation solar cells. Such devices are mostly based on transparent conducting electrodes (TCEs) that require materials with low Rs and high T throughout the visible region, other than physical and chemical stability, appropriate work function, uniformity, thickness, durability, toxicity and cost [210].

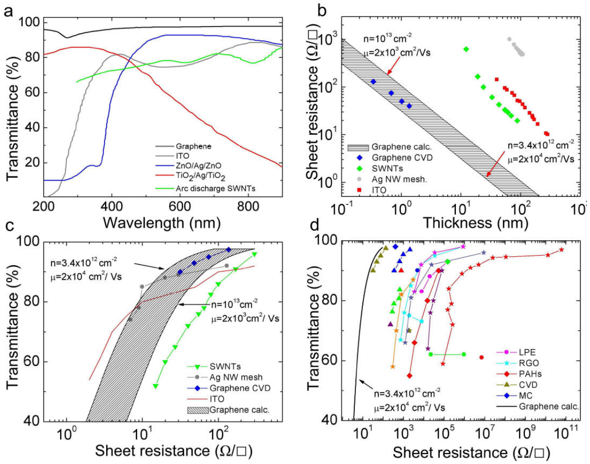
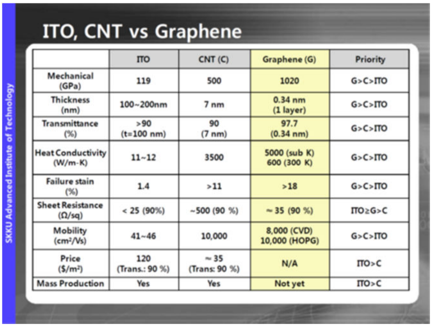


Figure 19. a) Transmittance of graphene compared to different transparent conductors; b) Thickness dependence of Rs for graphene compared to some common materials; c) T vs Rs for different transparent conductors compared to graphene; d) T vs Rs for GTCFs grouped according to production strategies: CVD, micro-mechanical cleavage (MC), organic synthesis using poly-aromatic hydrocarbon (PAHs), LPE of pristine graphene or graphene oxide (GO). A theoretical line is also plotted for comparison [227].

The dominant material used in TC applications is ITO [211]. This has limitations: an ever increasing cost due to In scarcity [211], processing requirements, difficulties in patterning [211,212], sensitivity to acidic and basic environments. Moreover, ITO is brittle and can wear out or crack when bending is involved, such as touch screens and flexible displays [213]. Metal grids [214], metallic nanowires [215], or other metal oxides [212] have been explored as alternative. Metal nanowires, e.g. Ag NWs have been demonstrated as TCEs on polymeric substrates using different methods, such as vacuum filtration, rod coating, transfer printing, and spray deposition. However, they suffer from stability and adhesion issues. On the other hand, 2d layered materials are ideal candidates offering a cost-effective, flexible alternative to ITO and other transparent conductors.

Graphene in principle can combine high T with high conductivity, maintaining these properties even under extreme bending and stretching, ideal for easy integration in polymeric and flexible substrates. In many cases (e.g. touch screens or OLEDs), this increases fabrication flexibility, in addition to having economic advantages. For instance, present liquid-crystal-based devices face high fabrication costs associated with the requirement for large transparent electrodes. The move to a graphene-based technology could make them more viable. New forms of graphene-based TCEs on flexible substrates for solar cells add value and operational flexibility, not possible with current TCs and rigid glass substrates.

Doped graphene offers comparable T and Rs to ITO on flexible substrates [212]. Graphene films have higher T over a wider wavelength range with respect to CNT films [216,217,218], thin metallic films [214,215], and ITO [212], Fig. 19a. However, the bi-dimensional dc conductivity $\sigma_{2d,dc}$ does not go to zero, but assumes a constant value [12] $\sigma_{2d,dc}$~$4e^2/h$, resulting in Rs ~6kΩ for an ideal intrinsic SLG with T ~97.7%. Thus, ideal intrinsic SLG would beat the best ITO only in terms of T, not Rs. However, real samples deposited on substrates, or in thin films, or embedded in polymers are never intrinsic. Exfoliated SLG has typically $n \geq 10^{12}cm^{-2}$ (see e.g. Ref [219]), and much smaller Rs. Figs. 19b,c show that graphene can achieve the same Rs as ITO, ZnO-Ag-ZnO [220], $TiO_2/Ag/TiO_2$ and CNTs with a much reduced thickness (Fig 19b) and a similar, or higher T. Fig. 19c plots T versus Rs for ITO [214], Ag nanowires [214], CNTs [216] and the best graphene-based TCFs reported to date [3], again showing that the latter is superior. For instance, taking $n=3.4\times10^{12}cm^{-2}$ and $\mu=2\times10^4cm^2/Vs$, achievable in CVD sample, it is possible to get T=90% and Rs = 20Ω/□ [104] with graphene, values already achieved with hybrid graphene-metal grids [221].



ITO, CNT vs Graphene

SKKU Advanced Institute of Technology

	ITO	CNT (C)	Graphene (G)	Priority
Mechanical (GPa)	119	500	1020	G>C>ITO
Thickness (nm)	100~200nm	7 nm	0.34 nm (1 layer)	G>C>ITO
Transmittance (%)	>90 (t=100 nm)	90 (7 nm)	97.7 (0.34 nm)	G>C>ITO
Heat Conductivity (W/m-K)	11~12	3500	5000 (sub K) 600 (300 K)	G>C>ITO
Failure stain (%)	1.4	>11	>18	G>C>ITO
Sheet Resistance (Ω/sq)	< 25 (90%)	~500 (90 %)	~ 35 (90 %)	ITO≥G>C
Mobility (cm²/Vs)	41~46	10,000	8,000 (CVD) 10,000 (HOPG)	G>C>ITO
Price ($/m²)	120 (Trans.: 90 %)	~ 35 (Trans: 90 %)	N/A	ITO>C
Mass Production	Yes	Yes	Not yet	ITO>C

Figure 20. Comparison between performances of ITO, carbon nanotubes and graphene (by courtesy of ByungHee Hong Seoul National.

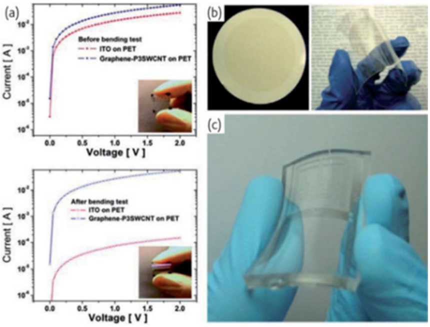


Figure 21. Preserving electrical conductivity under stress is an important property for TCFs. (a) Upon flexing the conductivity of indium tin oxide decreases 3 orders of magnitude, while the conductivity of a G-CNT hybrid electrode remains stable. From [222].

Different strategies were explored to prepare graphene-based TCFs: spraying [46], dip [223] and spin coating [44], vacuum filtration [224], roll-to-roll processing [3]. Huge progresses were made since the first TCs using GO [224]. A key strategy to improve performance is stable chemical doping. For instance, Ref. [3]

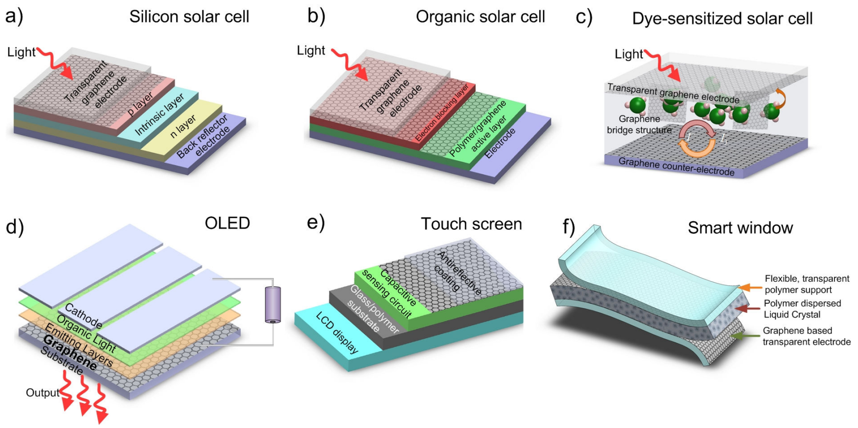


Figure 22. Graphene-based optoelectronics. Schematics of inorganic (a), organic (b) and dye-sensitized (c) solar cells, organic LED (d) capacitive touch screen (e) and smart window (f) [104].

achieved Rs ~30Ω/□; T~90% by nitric acid treatment of GTCFs derived from CVD grown flakes, which is one order of magnitude lower in terms of Rs than previous GTCFs from wet transfer of CVD films. Acid treatment permitted to decrease the Rs of solution processed nanotubes-graphene hybrid film till 100Ω/□ for T=80% [225]

Figure 19d is an overview of current graphene-based TCs. It shows that GTCFs derived from CVD, combined with doping, could outperform ITO, metal wires and SWNTs.

Note that GTCFs and GOTCFs produced by other methods, such as LPE, albeit presently with higher Rs at T=90%, have already been tested in organic light emitters [226], solar cells [223] and flexible smart window [104]These are a cheaper and easier scalable alternative to CVD films, and need be considered in applications where cost reduction is crucial. Figure 20 summarizes the main properties of graphene TCEs comparing the performances with respect to ITO and CNTs [227].

The aforementioned performances of graphene-based TCEs are extremely promising in view of commercial applications, especially in bendable and stretchable devices (see fig.21), e.g. as window electrode in inorganic (Fig. 22a), organic (Fig. 22b) and dye-sensitized solar cells (Fig. 22c) other than in OLED (Fig. 22d) touch screen (Fig. 22e) smart window (Fig. 22f), etc.

8.2 Photovoltaic devices

The direct exploitation of solar radiation to generate electricity in photovoltaic (PV) devices is at the centre of an ongoing research effort to utilize the renewable energy. Si currently dominates the market of PV devices [228], with energy conversion efficiency (η) up to ~25% [229]. However, regardless of significant development over the past decades [230], the high cost of Si-based solar cells is a bottleneck for the implementation of solar electricity on large scale (in absence of government subsidies). The development of new PV materials and concepts is thus fundamental to reduce the overall costs and increase efficiency.

Graphene can fulfil multiple functions in photovoltaic devices: TC window, antireflective layer, photoactive material, cannel for charge transport and catalyst [104]. GTCFs can be used as window electrodes in inorganic [231], organic [232] and dye-sensitized solar cells (DSSCs) [223], see Fig. 22 a,b,c respectively. The best performance achieved to date has η≈ 1.2% using CVD graphene as the TC, with Rs values of 230Ω/□ and T=72% [233]. However, further optimization is certainly possible, considering that GTCFs with Rs=30Ω/□ and T=90% have already been demonstrated [3] and graphene-hybrids have been reported with even better results (Rs 20Ω/□, T=90%) [221].

GO dispersions were also used in bulk heterojunction photovoltaic devices, as electron-acceptors achieving η≈1.4% [234]. Theoretically η~12% should be possible with graphene as photoactive material [235].

Graphene can cover an even larger number of functions in DSSCs. Indeed, other than as TC window [223], graphene can be incorporated into the nanostructured TiO_2 photoanode to enhance the charge transport rate, preventing recombination, thus improving the internal photocurrent efficiency [236]. An efficiency of ~7%, higher than conventional nanocrystalline TiO_2 photoanodes in the same experimental conditions, was demonstrated in Ref. [236]. Graphene quantum dots with tuneable absorption have been designed, produced and demonstrated as promising photoactive materials in DSSCs [237]. Further optimization is required for the optimum adsorption of these molecules with TiO_2 nanoparticles by covalently attaching binding groups to the quantum dots in order to improve charge injection. Another option is to use graphene, with its high surface area [238], as substitute for the platinum (Pt) counter-electrode. A hybrid poly(3,4 ethylenedioxythiophene):poly(styrenesulphonate) (PEDOT:PSS) graphene oxide composite was used as counter-electrode, to obtain η = 4.5%, comparable to the 6.3% for a Pt counter-electrode tested under the same conditions [239] but now with a cheaper material. More importantly, it was recently demonstrated that graphene can be used as counter-electrode material to replace simultaneously both Pt as catalyst and the TC oxide as conductive electrode [240]. This is a fundamental step towards cost reduction and large scale integration of DSSCs.

Current solar cell technologies use only a small part of the solar spectrum [212], due to their intrinsic band gap limiting the maximum detectable wavelength. The absence of a band-gap in graphene translates into the absence of this detectable wavelength limit. This means that solar radiation over a much wider spectral range could be converted to energy.

The combination of graphene with plasmonic nanostructures can also be used to increase the light harvesting properties in solar cells [241].

8.3 Organic Light Emitting Diodes

Organic light-emitting diodes (OLEDs) are a class of optoelectronic devices that can take advantage of graphene. Low power consumption and ultra-thin OLEDs have been developed more than 20 years ago [242], and are now applied in ultra-thin televisions and other displays, such as those on digital cameras and mobile phones.

OLED have an electroluminescent layer between two charge- injecting electrodes, at least one of which transparent. In these diodes, holes are injected into the highest occupied molecular orbital (HOMO) of the polymer from the anode, and electrons into the lowest unoccupied molecular orbital (LUMO) from the cathode. For efficient injection, the anode and cathode work functions should match the HOMO and LUMO of the light-emitting polymer. Traditionally, ITO is used as the transparent conductive film. However, it has a number of disadvantages. First, ITO may be too expensive for use in OLEDs for lighting because of the increasing cost and the low throughput deposition process. Second, metal oxides such as ITO are brittle and therefore of limited use on flexible substrates. Third, In is known to diffuse into the active layers of OLEDs, which leads to a degradation of performance over time. There is a clear need for alternative TCEs with optical and electrical performance similar to ITO but without its drawbacks. Graphene has a work function of 4.5 eV, similar to ITO. This, combined with its promise as a flexible and cheap transparent conductor, makes it an ideal candidate for an OLED anode (Fig. 22d), while also eliminating issues related to In diffusion.

Ref [243] developed an OLED with a few nanometers of graphene as transparent conductor. Ref [244] reported a flexible OLED based on a modified graphene anode having a high work function and low Rs. The performance (37.2 lm W^{-1} in fluorescent OLEDs, 102.7 lm W^{-1} in phosphorescent OLEDs) outperforms optimized devices with an ITO anode (24.1 lm W^{-1} in fluorescent OLEDs, 85.6 lm W^{-1} in phosphorescent OLEDs) [244].

These results pave the way for inexpensive OLED mass production on large-area low-cost flexible plastic substrates, which could be rolled up like wallpaper and applied to any substrate

8.4 Touch screens

Touch panels are used in a wide range of applications, such as cell phones and cameras, and where keyboard and mouse do not allow a satisfactory, intuitive, quick, or accurate interaction with the display content.

Resistive and capacitive (see Fig. 22e) touch panels are the most common. A resistive touch panel comprises a conductive substrate, a LCD front-panel, and a TCF [245]. When pressed by a finger or pen, the front-panel film comes into contact with the bottom TC and the coordinates of the contact point are calculated on the basis of their resistance values. The TC requirements for resistive screens are Rs ~500–2000Ω/□ and T>90% at 550nm [245]. Favourable mechanical properties, including brittleness and wear resistance, high chemical durability, no toxicity, and low production costs are also important. GTCFs can satisfy the requirements for resistive touch screens in terms of T and Rs, when combined with large area uniformity. Ref. [3] reported a graphene-based touch panel by screen-printing a CVD sample. Considering the Rs and T required by analogue resistive screens, GTCF or GOTCF produced via LPE also offer a viable alternative, and further cost reduction.

Capacitive touch screens are emerging as the high-end version, especially since the launch of Apple’s iPhone. These consist of an insulator such as glass, coated with ITO [245]. As the human body is also a conductor, touching the surface of the screen results in electrostatic field distortion, measurable as a change in capacitance. Although capacitive touch screens do not work by poking with a pen, thus mechanical stresses are lower with respect to resistive ones; the use of GTCFs can improve performance and reduce costs.

However, these solutions do not yet provide 100% satisfaction in terms of user experience, as touch screens tend to be inert in the way they interact with a user. Also, the proliferation of icons, virtual keys and densely packed browsing menus on mobile touch screen displays require increasing cognitive efforts from the user in order to be located, distinguished and manipulated. Solutions for low-cognitive effort user interfaces (UI), such as vibration enabled tactile feedback, are currently gaining market momentum by improving usability, interaction interoperability, and user acceptance.

Thus far, most active tactile feedback solutions have been implemented through simple monolithic vibrations of the entire device driven by a single or very few vibrating actuators, typically electromechanical or piezoelectric [246]. The types of tactile feedback that can be provided by such traditional techniques are limited to relatively basic feedback patterns which are only partially correlated to finger position, perceived audio-visual information and actions. Such solutions do not yet provide complete satisfaction in terms of user experience. Key to this is the inability of monolithic vibrations to provide localized tactile feedback associated with visual images, and this is related to the difficulty in implementing tactile feedback directly from a display surface. To address the problem of providing localized tactile feedback directly from the display of a device, a flexible and optically transparent graphene-based programmable electrostatic tactile (ET) system was developed [247] capable of delivering localized tactile information to the user's skin, directly from the display's surface and in accordance with the displayed visual information. The device is based on the electrovibration a phenomenon [248] that can be explained through electrostatic interaction between the touch surface and the user finger [249].

8.5 Graphene photodetectors

Photodetectors measure photon flux or optical power by converting the absorbed photon energy into electrical current. They are widely used in a range of devices [250], such as integrated optoelectronic circuits, televisions, DVD players, biomedical imaging, remote sensing and control, optical communications, and quantum information technology. Most exploit the internal photoeffect, in which the absorption of photons results in carriers excited from the valence to the conduction band, outputting an electric current. The spectral bandwidth is typically limited by the absorption [250]. Graphene absorbs from the UV to THz [24,251,252,253]. As a result, graphene-based photodetectors (GPD) (Fig.23) could work over a much broader wavelength range. The response time is ruled by the carrier mobility. Graphene has huge mobilities, so it can be ultrafast [251]. Graphene's suitability for high-speed photodetection was demonstrated in an comms link operating at 10Gbit s^{-1} [254].

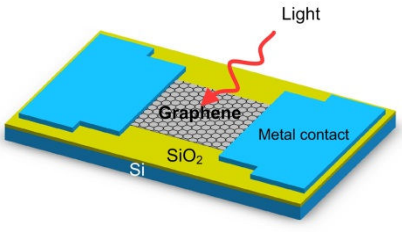


Figure 23. Graphene-based photodetector [104].

The photoelectrical response of graphene has been investigated both experimentally and theoretically [254,255,256,257,258]. Although the exact mechanism for light to current conversion is still debated [256,259,260], a p–n junction is usually required to separate the photo-generated e–h pairs. Such p–n junctions are often created close to the contacts, because of the difference in the work functions of metal and graphene [148,261]. Responses at wavelengths of 0.514, 0.633, 1.5 and 2.4µm have been reported [255]. Much broader spectral detection is expected because of the graphene ultrawideband absorption [258]. The operating bandwidth of GPDs is mainly limited by their time constant resulting from the device resistance, R, and capacitance, C. An RC-limited bandwidth of about 640 GHz was reported for graphene [258], comparable to traditional photodetectors [262]. However, the maximum possible operating bandwidth is typically restricted by their transit time, the finite duration of the photogenerated current [250]. The transit-time-limited bandwidth of graphene photodetectors could be over 1,500 GHz [258].

Although an external electric field can produce efficient photocurrent generation with an electron–hole separation efficiency>30% [256], zero source–drain bias and dark current operations could be achieved by using the internal electric field formed near the metal electrode–graphene interfaces [254,223]. However, the small effective area of the internal electric field could decrease the detection efficiency [214,262], as most of the generated electron–hole pairs would be out of the electric field, thus recombining, rather than being separated. The internal photocurrent efficiencies (15−30% [256,257] and external responsivities (generated electric current for a given input optical power) of ~6.1 mA/W, much higher than the so far reported [254] for GPDs are relatively low compared with current photodetectors [250]. This is mainly due to limited optical absorption when only one SLG is used, short photocarrier lifetimes and small effective areas (~200 nm [258]).

Future work will target the low light absorption of graphene (2.3% of normal incident light [24,263]), the difficulty of extracting photoelectrons (only a small area of the p–n junction contributes to current generation); and the absence of a photocurrent for the condition of uniform flood illumination on both contacts of the device. Unless the contacts are made of different materials, the voltage/current produced at both contacts will be of opposite polarity for symmetry reasons, resulting in zero net signal [254,256,264].

The optimization of the contacts needs to be pursed both theoretically and experimentally. Other possible ways of overcoming these restrictions is to utilize plasmonic nanostructures placed near the contacts as recently demonstrated [241]. Such a field enhancement, exactly in the area of the p–n junction formed in graphene, can result in a significant performance improvement.

The significant photothermoelectric contribution to the photocurrent in graphene p-n junctions was recently pointed out [260]. This regime, which features a long-lived and spatially distributed hot carrier population, may offer a path to hot carrier–assisted thermoelectric technologies for efficient solar energy harvesting.

Recently, a novel hybrid graphene-quantum dot phototransistor with ultrahigh gain has been demonstrated [265]. The proposed device takes advantage of the strong light absorption in quantum dots and the two-dimensionality and high mobility [20] of graphene to merge these materials into a hybrid system for photodetection with extremely high sensitivity [265]. The graphene-quantum dot phototransistor has shown ultrahigh gain of 10^8 and ten orders of magnitude larger responsivity with respect to pristine graphene photodetectors [265]. Moreover, the hybrid graphene-quantum dot phototransistors exhibit spectral selectivity from infrared to visible, gate-tunable sensitivity, and can be integrated with current circuit technologies [265].

Graphene was also demonstrated to be ideal for the enclosure within a planar λ/2 optical microcavity [266]. The latter is a photonic structure that confines optical fields between two highly reflecting mirrors with a spacing of only one half wavelength of light [267]. The optical confinement provide a powerful means to control both the otherwise featureless optical absorption [24] and the spectrally broad thermal emission [268,269] of graphene. The monolithic integration of a graphene transistor with a planar optical microcavity permitted the control on photocurrent generation. Tuning the excitation wavelength on resonance with the optical microcavity, an enhancement of ~20 in photocurrent was measured with respect to the out of resonance excitation [266]. In the same condition (spectral interval) a non-confined graphene transistor has shown a photocurrent increase of only 2. This demonstrates that the mocrocavity-controlled graphene transistor acts as light detector with spectral selectivity [266].

Moreover, electrically excited, thermal light emission of graphene can be controlled by the spectral properties of the microcavity. Indeed, the thermal emission spectrum of a microcavity-controlled graphene transistor displays a single, narrow peak at λ_{cavity}= 925nm having a fullwidth-at-half-maximum of 50 nm, providing a 140-fold spectral narrowing with respect to the simulated free-space thermal spectrum at T = 650 K [266].

Moreover, the integrated graphene transistor electrical transport characteristic is profoundly modifies by the optical confinement of graphene by the optical microcavity [266]. The modifications of the electrical transport can be related to the microcavity-induced enhancement or inhibition of spontaneous emission of thermal photons [266]. The concept of optical confinement of graphene enables a new class of functional devices as, for example, spectrally selective and highly directional light emitters, detectors, and modulators.

8.6 Graphene saturable aborbers

Materials with nonlinear optical and electro-optical properties are needed in most photonic applications. Laser sources producing nano- to sub-picosecond pulses are key components in the portfolio of leading laser manufacturers. Regardless of wavelength, the majority of ultrafast lasers use a mode-locking technique, where a nonlinear optical element, called a saturable absorber, turns the continuous-wave output into a train of ultrafast optical pulses [270]. The key requirements are fast response time, strong nonlinearity, broad wavelength range, low optical losses, high power handling, low power consumption, low cost and ease of integration into an optical system. Currently, the dominant technology is based on semiconductor saturable absorber mirrors (SESAM) [270,271]. However, these have a narrow tuning range, and require complex fabrication and packaging [270,272]. The linear dispersion of the Dirac electrons in graphene offers an ideal solution: for any excitation there is always an electron–hole pair in resonance. The ultrafast carrier dynamics [273,274] combined with large absorption [24,75] and Pauli blocking, make graphene an ideal ultrabroadband, fast saturable absorber [253,272]. Unlike SESAM and CNTs, there is no need for bandgap engineering or chirality/diameter control [253,272].

Since its first demonstration in 2009 [272], the performance of ultrafast lasers mode-locked by graphene has improved significantly (Fig.24). For example, the average output power has increased from a few mW [272] to 1 W [275]. Some of the aforementioned production strategies (e.g. LPE [101,253, 272,276,277,278], CVD [279,280], carbon segregation [281], mechanical exfoliation [282,283]) have been used for graphene saturable absorber (GSA) fabrication. So far, GSAs have been demonstrated for pulse generation at 1µm [275,284], 1.2µm [285], 1.5µm [253,272,279, 280,282,286] and 2µm [287]. The most common wavelength so far is ~1.5µm, not due to GSAs wavelength restriction, but because this is the standard wavelength of optical telecommunications. Ref. [288] reported a widely tunable fiber laser mode-locked with a GSA demonstrating its "full-band" operation performance. For fiber lasers, the simplest and most economical approach to GSA integration is sandwiching it between two fiber connectors (Fig.24) [253, 272, 279, 280, 282, 283, 288]. Other GSA integration approaches (e.g. evanescent-wave based integration [287]) have been demonstrated for high-power generation. Sub-200fs pulses have been achieved using a stretched-pulse design, where the cavity dispersion is balanced to stretch the pulse for the limitation of nonlinear effects [276].

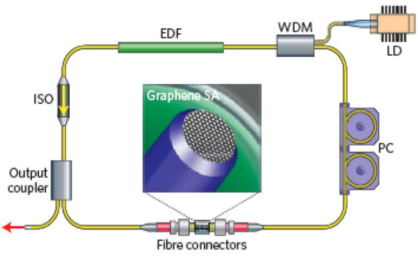


Figure 24. Graphene mode-locked fiber. WDM, wavelength division multiplexer; PC, polarization controller; EDF, erbium-doped fiber; ISO, isolator [77].

Solid-state lasers are typically used for high-power output, as alternative to fiber lasers [289]. GSAs have also been demonstrated to mode-lock solid-state lasers [284,285,290]. In this case, CVD graphene (>1cm^2) has been directly transferred to quartz for solid-state laser mode-locking [285]. Ref. [285] reported 94fs pulses with 230mW output power. Another approach for GSA fabrication relies in spin-coating LPE graphene either on quartz substrates or high-reflectivity mirrors. GSA can then be inserted into a solid-state cavity for ultrafast pulse generation achieving average power up to 1W using a solid-state Nd: YVO4 laser [275]. The output wavelength is ~1 µm with power energy of ~14nJ.

8.7 Optical limiters and frequency converters

Optical limiters are devices that have high transmittance for low incident intensity and low transmittance for high intensity [291]. There is a great interest in these for optical sensors and human eye protection, as retinal damage can occur when intensities exceed a certain threshold [291]. Passive optical limiters, which use a nonlinear optical material, have the potential to be simple, compact and cheap [291]. However, so far no passive optical limiters have been able to protect eyes and other common sensors over the entire visible and near-infrared range [291]. Typical materials include semiconductors (i.e. ZnSe, InSb), organic molecules (i.e. phthalocyanines), liquid crystals and carbon-based materials (i.e. carbon-black dispersions, CNTs and fullerenes) [291,292]. In graphene-based optical limiters the absorbed light energy converts into heat, creating bubbles and microplasmas [292], which results in reduced transmission. Graphene dispersions can be used as wideband optical limiters covering visible and near-infrared. Broad optical limiting (at 532 and 1,064 nm) by LPE graphene was reported for nanosecond pulses [292]. It was also shown [293] that functionalized graphene dispersions could outperform C60 as an optical limiter.

Optical frequency converters are used to expand the wavelength accessibility of lasers (for example, frequency doubling, parametric amplification and oscillation, and four-wave mixing) [291]. Calculations suggest that nonlinear frequency generation in graphene (harmonics of input light, for example) should be possible for sufficiently high external electric fields (>100 V cm^{-1}) [294].

Second-harmonic generation from a 150fs laser at 800nm has been reported for a graphene film [295]. In addition, four-wave mixing to generate near-infrared wavelength tunable light has been demonstrated using SLG and FLG [296]. Graphene's third-order susceptibility $|\chi 3|$ was measured to be $\sim 10^{-7}$ e.s.u. [296]—up to one order of magnitude larger than CNTs [296]. Other features of graphene, such as the possibility of tuning the nonlinearity by changing the number of layers, and wavelength-independent nonlinear susceptibility [296] could be used for various applications (optical imaging, for example).

9. Graphene transistors and electronics applications

Figure 25 shows an artist drawing of a future graphene integrated circuit, in which, after initial wafer scale integration, further lithography, chemical treatments, would be used to engineer active and passive electronic, phononic or spintronics components. This illustrates graphene as a suitable platform to crosslink the nanoscale to conventional microelectronics.

One can envision integrating on the same chip advanced functionalities including chemical sensing, nano-electromechanical resonators, thermal management, and electronic functions. Spintronics will also offer a co-integration of memory and computation functions on the same substrate.

This section overviews the current status of graphene transistors as potential supplement to CMOS technology.

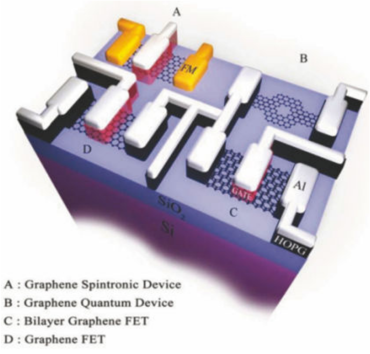


Figure 25. A futuristic graphene integrated circuit (not to scale), wherein the desirable properties of various thicknesses of graphene layers are utilized along with strategic oxides (SiO_2, ferroelectric, ferromagnetic, multiferroic, etc.) in response to various external stimuli, such as electric or magnetic fields. In the present illustration, the device structure is fabricated from a very thin single-crystal graphite sheet after subsequent patterning/selective ablation. The remaining graphite acts as a good ohmic contact and interconnection between the top Al metallization (which also acts as a self-aligned mask, protecting the underlying graphite) and the variable-thickness graphene-based devices. Extract from [297].

9.1 Band gap opening in graphene

Creating a band gap in graphene is one of the major challenges for employing graphene in conventional device circuits, both for analog and digital applications. For digital applications a band gap is mandatory as on/off ratios larger 10^4 are required [298]. For analog applications however, a band gap is not required *per-se*, but the lack of drain current saturation in graphene based FETs and the resulting low voltage gain are major obstacles. A small band-gap~100meV would improve the situation.

9.2 Macroscopic graphene field effect transistors

The most straightforward device application of graphene may seem to be as a replacement channel material for silicon MOSFETs. Fig. 26a shows a schematic of such a graphene FET, including a top gate electrode, gate dielectric and source and drain metal contacts. Fig. 26b shows a top view optical micrograph of a macroscopic graphene FET on SiO_2 [299]. The fabrication of graphene FETs follows standard Si process technology once the graphene is deposited and identified. This includes the use of photo- or e-beam lithography, reactive ion etching and thin film deposition for the gate insulators and contacts. Details of typical fabrication processes are described in Refs. [300,301,302].

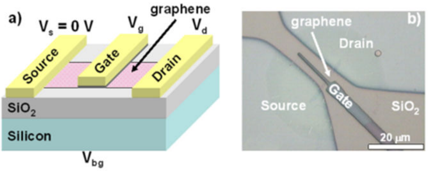


Figure 26. a) Schematic cross section and b) optical top-view micrograph of a graphene field effect transistor [299].

The transfer characteristics (here: drain current Id vs. back gate voltage V_{bg}) of a typical graphene transistor is shown in Fig. 27. It reveals a major drawback of macroscopic graphene MOSFETs: the absence of a band gap severely limits the current modulation in the graphene FET and, in addition, leads to ambipolar behaviour.

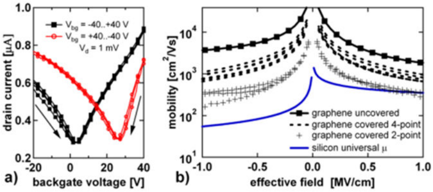


Figure 27. a) Drain current versus back gate voltage of a graphene FET. The change of the sweep direction results in considerable hysteresis of 22 V. b) Mobility versus electric field in graphene FETs. Covering graphene with a gate insulator leads to mobility reduction. Contacts have a considerable influence on graphene FETs [299]. Universal mobility of silicon included as reference after Takagi [303].

The best current modulation reported to date has been about 40, measured at room temperature for water gated graphene [95]. Furthermore, in conjunction with randomly distributed oxide charges the zero band gap leads to a finite minimum charge density even without any applied gate voltage [304]. Consequently, macroscopic graphene transistors conduct substantial current even at their point of minimum conductance (also referred to as Dirac point or charge neutrality point), preventing their application as Si MOSFET replacement. Fig. 27a further shows hysteresis as the gate voltage is swept from negative to positive and vice versa. This typical behaviour occurs despite measuring in vacuum conditions ($P=5x10^{-3}$ mbar) and is a strong indicator of charge traps near the graphene/insulator interface. While suspended graphene measured in ultra high vacuum has been shown to have mobilities exceeding 1000000 cm^2/Vs [20], realistic graphene FETs are limited by substrates and top gates.

Nonetheless, the mobilities in top gated devices exceed those of Si and are typically on the order of several hundred to a thousand cm^2/Vs, even though graphene/ insulator interfaces have not at all been optimized yet [299,300,301,302,305,306]. Fig. 27b shows electron and hole mobilities extracted from several top gated devices, both in 2-point and by 4-point probe configuration.

9.3 Graphene nanoribbon transistors

A potential method to create a band gap in graphene is to cut it into narrow ribbons of less than a few tens of nanometers.

GNRs can be armchair or zig-zag edge terminated. In armchair GNRs, the transition from 2D graphene to 1D GNRs leads to quantum confinement and a bandgap that is roughly inversely proportional to the GNR width ($E_g \sim 1/W$) [307,308]. The precise value of the band gap is further predicted to depend on the number N of carbon atoms across the ribbon [307,308,309,310]. This is demonstrated in Fig. 28a, where the simulated density of states (DOS) versus energy for three different hydrogen-terminated armchair GNRs with N = 11, 12 and 13 is shown [14,311].

While the GNR with N = 11 is semi-metallic, the ribbons with 12 and 13 atoms are semiconducting (generally armchair ribbons are semi-metallic at $N = 3m-1$, where m is an integer [312]). In hydrogen-terminated zig-zag GNRs, however, the situation is more complicated. Ref. [307] predicted that localized edge states near the Fermi level lead to semi-metallic behaviour, regardless of the number of carbon atoms. On the other hand, Ref. 309 calculated *ab initio* that edge magnetization causes a staggered sublattice potential on the graphene lattice that induces a band gap. Finally, GNRs with other chiral orientation have been considered, including a mix of edges along a ribbon, adding to the complexity of this option [313,314,315, 316,317,318,319]. In summary, the simulated results for any form of GNRs should be regarded with care, as they typically share an optimistic assumption of well controlled termination of dangling bonds. In reality, there is likely a great variety of chemical groups terminating the GNR edges. A first detailed discussion has been recently published to address these issues [320], but it is probably reasonable to consider the nature of “real life” zig-zag GNRs still an open question. The predicted presence of a band gap in specific GNRs has been experimentally confirmed.

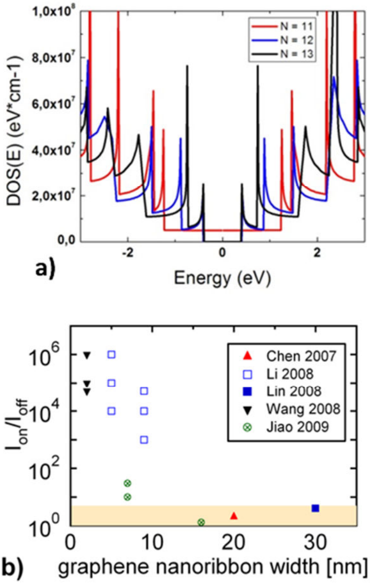


Figure 28. *a) Simulated DOS vs. energy of hydrogen terminated armchair GNRs for various numbers of electrons N across the ribbon [14]. b) Experimental Ion/Ioff ratios versus GNR width taken from literature. None of the GNRs thus far has shown metallic behavior. The lower colored part of the graph indicates Ion/Ioff values of typical macroscopic graphene FETs; From [14].*

First evidence was reported by Refs. [321,322], where GNRs were structured by e-beam lithography and etched in oxygen plasma with minimum widths~20 nm. The band gaps of these GNRs where in the range of ~30 meV and resulted in field effect transistors with I_{on}/I_{off} ratios of about 3 orders of magnitude at low temperatures (1.7–4 K), reduced to~ 10 at room temperature. These investigations support theoretical predictions that sub-10 nm GNRs are required for true field effect transistor action at room temperature. More importantly, the experiments revealed a band gap regardless of the chiral orientation of the GNRs [321]. This latter result was attributed to a strong influence of edge states [319,321,323], which dominate over the chirality of the band structure. To date, two examples of sub-10 nm GNRs have been shown experimentally. Ref. 324 fabricated GNRs with a minimum width~1 nm and a band gap of about 500meV using e-beam lithography and repeated, careful over-etching. The resulting transistors consequently switched off at room temperature to “no measurable conductance” [324]. An alternative fabrication process for GNRs was presented by Ref. [109]. Here, GNRs were solution derived from graphite by thermal exfoliation, ultrasonication and ultracentrifugation. The resulting dispersions were deposited onto substrates and GNRs were identified with AFM. The devices exhibited well behaved transistor action at room temperature with $I_{on}/I_{off}>10^6$ [109,325].

The experimental I_{on}/I_{off} ratios reported to date are summarized in Fig. 28b. While they clearly support theoretical predictions and show promise for GNR electronics, they also show an urgent need for further research in this field: Statistical data is scarce and the discrepancies between theory and experiment need to be addressed. The necessity of controllable sub-10nm feature sizes and great uncertainties in chirality control as well as edge state definition remain tremendous challenges. To this end, a recently developed technique, helium ion beam microscopy, has been shown to have potential for precise nano-patterning [326,327].

9.4 Bilayer graphene

Another viable approach to obtain a band gap in graphene is to break its symmetry. Ref. [328] proposed that macroscopic BLG would display a suitable band gap if a transverse electric field was applied to break the layer symmetry. Ref. [328] predicts a roughly linear dependence of the gap on applied displacement field, with each 0.1V/nm adding~10 meV and a subsequent saturation at about 300meV.

This prediction was experimentally confirmed by Ref. 329 for BLG on SiC through angle-resolved photoemission spectroscopy (ARPES). In their work, they used potassium doping to modify the carrier density, which lead to changes in the electronic band gap [329]. The size of the created band gap was also confirmed by means of infrared spectroscopy [330,331].Ref. [332] took this approach a step further by applying an electrostatic field through a double gate configuration with individually controlled back and top-gate electrodes. However the band gap in their devices could not be utilized to increase the on/off ratio at room temperature due to the presence of intergap states [332]. Only at low temperatures they observed an insulating behaviour in BLG with a perpendicular applied electric displacement field. By optimizing the process technology Refs [258,333] reduced the intergap states in BLG-FETs significantly so that they were able to increase the on/off ratio up~100 at room temperature by applying an electrical displacement field. This is comparable to the on/off ratio in small band-gap III/V transistors and sufficient for most analog applications. The channel resistance of a double-gated BLG FET is depicted in Fig. 29 [333].

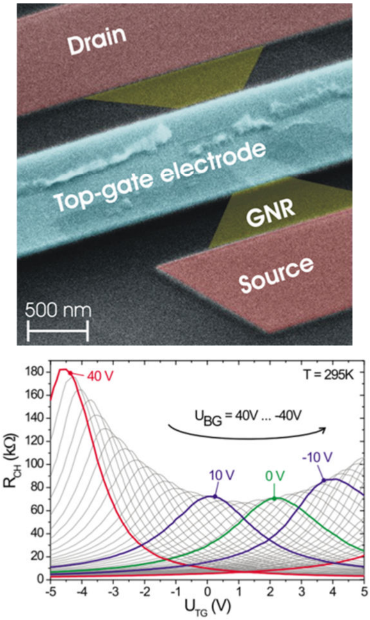


Figure 29. Top:SEM image (false color) of a double-gated bilayer graphene FET [333]. Bottom:Channel Resistance of a double-gated bilayer FET as a function of the applied top-gate voltage for different back-gate voltages [333].

In this device the resistance modulation is 8 at zero applied back-gate and increases to 80 at an applied back-gate of 40V. However, using a double gate structure, with two individually controlled gates, increases complexity, which is not desired in applications. Recently it has been shown that the static gate can be replaced by adsorbate doping [334]. In this work a band gap could be obtained and utilized to increase the on/off ratio with only one gate electrode [334].

Using BLG with a perpendicular electric field Ref.335 realized logic gates. By combining a p-type and an n-type BLG FET with an induced band gap, Ref. 335 realized NAND and NOR gates, fundamental building blocks for digital logic circuits. The operation of NOR gates and the resulting operation of the BLG based NOR gate are depicted in Fig. 30

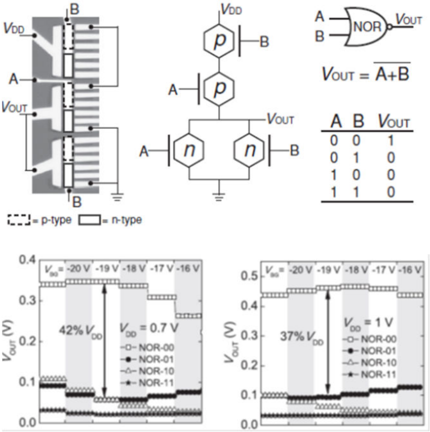


Figure. 30. Top: Device wiring used for realizing a NOR gate; corresponding circuit diagram and the truth table of the operation (taken from [194]). Bottom: The operation at a drive voltage 0.7 V and 1.0 V, respectively (taken from [335]).

9.5 Summary band gap engineering in graphene

Over the past few years different approaches were explored for creating a band gap in graphene, whereof confinement to GNRs and BLG are the most promising. Using graphene in switches for digital operation requires a band gap>400meV, hence confining graphene to GNRs is necessary. Using bottom-up synthesis on/off ratios larger 10^6 are achievable using GNRs [325].

The challenges is to develop industrially compatible top-down methods for the fabrication of such small structures. In contrast, in BLGs a band gap could be realized using standard top-down fabrication, but as the theoretical limits of the band gap in BLG are~300 meV an application to digital circuits will be challenging. However analog applications can strongly benefit from this band gap, which is tuneable by electric means.

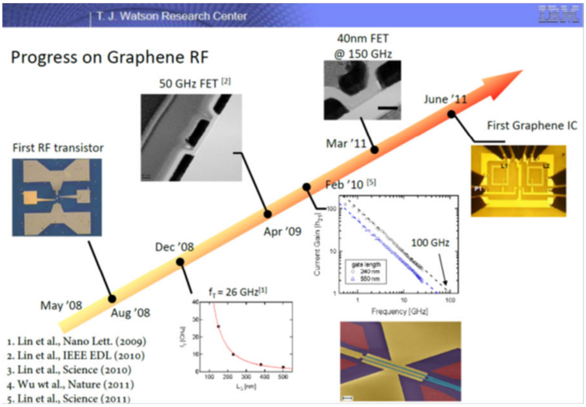


Figure 31. Summary of published graphene RF transistor data (Courtesy of Yu Min Lin, IBM, USA).

9.6 RF Transistors

Numerous communication systems rely on electromechanical devices, such as filters, resonators, and RF switches. Their miniaturization will strongly affect the development of future communication systems. The ultimate limit to this miniaturization is represented by graphene electromechanical devices.

Graphene combines exceptional electronic properties with excellent mechanical properties. Its ambipolar transport properties, ultra thin and flexible, and electrostatic doping offer a new degree of freedom for the development of advanced electronic devices with many potential applications in communications and RF electronics.

For RF analog applications a high on-off ratio is desirable but not mandatory. Instead, most relevant for good RF performance is a FET channel with excellent carrier transport properties (high mobility and maximum velocity) [336], combined with a small scale length, which improves strongly as the channel material thickness is reduced [337]. Graphene RF FETs have been investigated, both using exfoliated [306,338] and epitaxial materials [339,340]. Graphene transistors with a 240nm gate operating at frequencies up to 100 GHz were demonstrated in early 2010 [341]. This cut-off frequency is already higher than those achieved with the best silicon MOSFET having similar gate lengths [342].

Higher f_T can be expected for optimized devices with shorter gate lengths as demonstrated by the progress achieved by the IBM group that in 2 years improved the performances of their Graphene-based RF transistor passing from 26 GHz[306] to 155 GHz[343] (Fig. 31). The latter result was achieved with CVD graphene was grown on copper film and transferred to a wafer of diamond-like carbon. This once more emphasizes the need for graphene/insulator interface engineering.

Cut-off frequency over 300 GHz were demonstrated with a 140 nm channel length [344], comparable with the very top high-electron-mobility transistors (HEMTs) with similar gate length [345], see Fig.32. These results are impressive, considering that RF graphene research has been done for a fraction of the time devoted thus far to conventional devices. As shown in Fig. 32, the progress in graphene-based high frequency devices has been impressive. This progress opens new horizons for quick development of plethora of applications in RF communications.

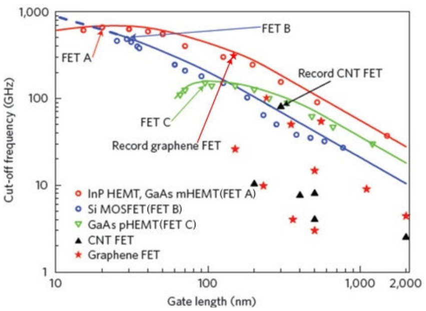


Figure 32. Comparing cut-off frequency versus gate length for graphene MOSFETs, nanotube FETs and three types of radiofrequency FET (Adapted from ref. 321).

Compared to conventional Si and III-V materials, ambipolar graphene electronics has many advantages. The higher mobility allows higher operating frequencies for frequency doubling and mixing. In addition, ambipolar devices can significantly reduce the number of transistors needed. Simpler circuits mean less power consumption and smaller chip area. Graphene is also an ideal material for flexible electronics integration.

To take advantage of the full potential of graphene devices, basic research needs to be combined with improved material growth and device technology. A better understanding of parameters such as breakdown voltage, electron velocity, and saturation current is needed to allow a complete benchmark and evaluation of this material. Once the growth and fabrication technology of these new devices matures, their integration with conventional Si electronics, and/or flexible and transparent substrates has the potential to transform communications. Thus graphene can be seen, rather than as a replacement of Si technology, as a complement to it in a “More than Moore” [346] perspective.

9.7 Non-conventional graphene switches

A number of concepts for (non-volatile) graphene switches have emerged based on mechanisms other than the classic field effect. Even though a thorough review is beyond the scope of this leaflet, they are briefly introduced in this section. A first concept are graphene/GO Schottky barrier MOSFETs [347], where semiconducting GO acts as the transistor channel. Another approach relies on creating nanoscale gaps by electric fields [348]. These are reversibly opened and closed by breaking and re-forming the carbon atomic chains [348].

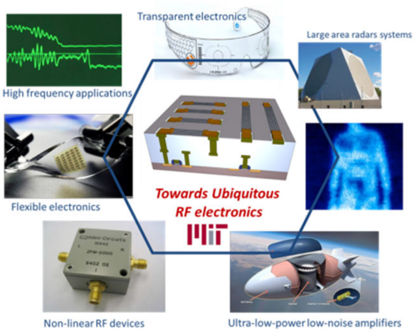


Figure 33. Possible applications of graphene RF transistor (Courtesy of Tomas Palacios, MIT, USA).

Chemical surface modification affects strongly the electronic band structure of graphene [349]. The electrostatical control of drain current can be reversibly modified in a graphene FET by controlled chemisorption [350]. Ferroelectric gating has been shown to electrostatically dope graphene and change the drain currents in a non-volatile way [351]. While these early concepts are far from mature, they nevertheless demonstrate the potential of graphene for nanoelectronics applications that might not be anticipated today.

9.8 Atomistic simulations of transistors

Due to the novelty of the graphene research field, device design principles have not yet been extensively elaborated, and different design options must be explored, evaluated and optimized. From this perspective, numerical simulations can greatly help.

When dealing with the investigation of device electrical behaviour, atomistic features of the material, such as for example the lattice potential, disappear behind a series of synthetic parameters like the effective mass tensor. The price to pay is however the lack of accuracy at the atomic level, which can be obtained through *ab-initio* simulations, at the expense of huge computational requirements, especially when the number of atoms is of the order of few thousands like in realistic FETs.

The strategy is then to find a trade-off, leveraging on atomistic simulations based on the Non-Equilibrium Green's Function (NEGF) formalism, which can provide physical insight at the atomic level, but with fewer computational burden as compared to DFT calculations.

Efforts towards the understanding of BLG for next-generation devices have been first addressed in [352], where a double gate FET was simulated by means of the self-consistent solution of the 2D Poisson and Schrödinger equation with open-boundary conditions, within NEGF. Strong band-to-band tunnelling heavily limits device performance, since the current in the off-state is too large for digital applications, when applying drain-to-source voltages complying with the International Technology Roadmap for Semiconductors (ITRS) [298], i.e. approximately 0.5 V.

The large tunnelling component, instead of being detrimental like in thermionic devices, can be turned into an advantage in tunnel FETs [353], whose main appeal is represented by a sub-threshold swing well below those achievable in thermionic devices (<60mV/dec) [354]. This would allow reducing the supply voltage for digital logic applications, and consequently the power consumption. It is indeed well known that power dissipation is nowadays the most limiting factor in integrated circuits, so that all future approaches need be directed towards the design of low power devices, the so-called "Green Transistors"[355]. From this perspective, BLG tunnel FET (see Fig.34) represents a viable option, because of its large I_{on}/I_{off} ratios (large than 10^3), even when applying ultra-low power supply (0.1 V) [353]. An alternative FET, based on graphene heterostructures with atomically thin boron nitride acting as a tunnel barrier, was recently demonstrated [356].

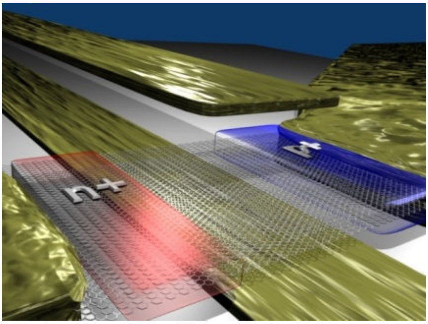


Figure 34. Sketch of the bilayer graphene tunnel FET proposed in [353].

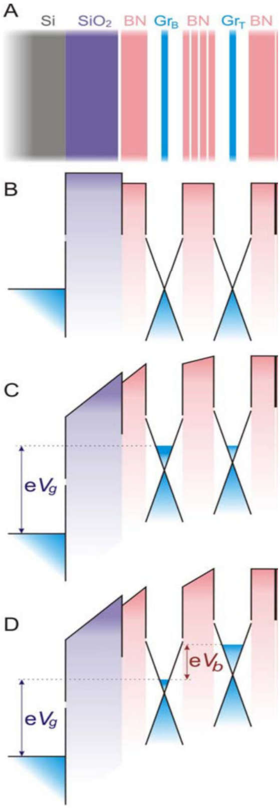


Figure 35. *(a) Schematic structure of the graphene heterostructure FET. The corresponding band structure with (b) no gate voltage and (c) finite gate voltage Vg and zero bias Vb applied. (d) Band structure when both Vg and Vb are finite. The cones illustrate graphene's Dirac-like spectrum and, for simplicity, the tunnel barrier for electrons is considered [adapted from ref. 322].*

The operation of the device (see Fig. 35) relies on the voltage tunability of the tunnelling density of states and of the effective height of the tunnel barrier adjacent to the graphene electrode [356]. The device exhibits room temperature switching ratios of ~50. However, this value can be improved by optimizing the device structure and up to 10^5 was recently reported by using MoS_2 instead of BN [357].

Lateral confinement, as in GNRs, is another approach widely addressed in the last year to induce an energy gap. Simulations have provided relevant information regarding the potential and the limits of this approach [358,359]. In particular, GNRs smaller than 3 nm are needed to comply with ITRS, which is very difficult to achieve with state-of-the-art electron beam lithography [360]. Things get even worse when considering sources of non-idealities, such as line-edge roughness or single vacancy defects, which strongly limit electron mobility in GNRs, another important figure of merit for digital applications [361]. However, even when dealing with perfect edges, mobility in narrow devices (W<2nm) is strongly limited by electron-phonon coupling, leading to similar mobility as the Si counterpart [362].

Chemical functionalization is a viable route toward bandgap engineering. Ref. [363] exposed graphene to a stream of hydrogen atoms leading to a material close to the ideal graphane. DFT suggests that [364] graphane would have a 5.4 eV gap, while it reduces to 3.2 eV in 50% hydrogenated graphene. A recent study (Fig. 36) [365] suggested that such devices can provide large currents as well as I_{on}/I_{off} ratios, and can represent a promising option for future technology nodes.

Probably more than towards digital applications, research should be focus on analog electronics, where the lack of a bandgap does not represent an issue, and high performance in terms of cutoff frequency in RF applications can be achieved [366], and negative differential resistance [367,368] can be exploited in a range of applications, such as oscillators, fast switching logic, and low power amplifiers.

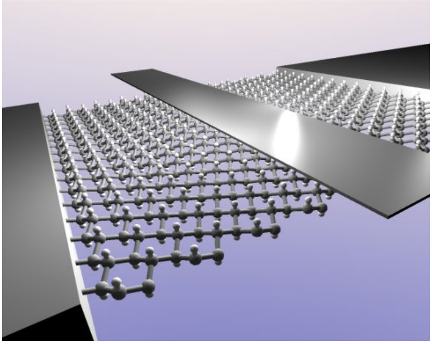


Figure 36. Sketch of the functionalized graphene based transistor

10. Conclusion

Graphene has already demonstrated high potential to impact most areas of electronic information technology, ranging from top end high performance applications in ultrafast information processing, to consumer applications using transparent or flexible electronic structures. This is testified by the increasing number of chip-makers now active in graphene research.

The combination of its unique optical and electronic properties, in addition to flexibility, robustness and environmental stability, make graphene an extremely interesting material for future photonic and optoelectronic devices.

Graphene can successfully replace many materials (*i.e.* ITO) in several existing applications, but certainly, the combination of its unique properties will inspire completely new applications and is where future research should focus (i.e. creating new technologies exploiting the uniqueness of graphene and related inorganic 2d crystals, rather than just try to displace existing and established technologies).

Graphene may allow high-speed, compact-footprint electro-optical modulators, switches and photodetectors integrated with waveguides or plasmonic circuits. Moreover, the mechanical flexibility of graphene will also enable integration with bendable substrates and plastic waveguides.

Graphene can detect light beyond the current limit set by the band gap of traditional semiconductors, opening new applications in the far-infrared (terahertz, THz) and mid-infrared regimes (e.g. bolometers and cameras), and provides the potential for ultrafast pixelated detection with ballistic transport of generated *n*. This could enable portable terahertz sensors for remote detection of dangerous agents, environmental monitoring or wireless communication links with transmission rates above 100 Gbit/s. Moreover, it can be exploited for photocurrent generation by providing a gain mechanism where multiple carriers are created from one incident photon.

The compatibility of graphene with standard CMOS processes at wafer scale makes it a promising candidate for future electronics, particularly for high data-rate (inter- and intra-chip) interconnects. While macroscopic graphene transistors are not suitable for logic applications, due to the lack of band gap, graphene RF transistors seem promising and feasible. Graphene nanoribbons, on the other hand, show promise as a CMOS compatible approach, but their extreme sensitivity at an atomic level to both geometric and edge termination variations may well render their practical use extremely challenging. Non-classic switching mechanisms may eventually lead to a co-integration of graphene into silicon technology, even though details are not yet clear today. In addition to these device related issues, there is the imperative need of a large area, CMOS compatible deposition or placement technique. As CVD and related methods are being explored, many device related questions are being addressed using the existing manufacturing methods. These insights will be transferable as soon as industrially relevant production and placement technologies will become available.

Acknowledgements

CPE thanks COST MP0901 “NanoTP” for support, as well as ANR NANOSIM-GRAPHENE. JC acknowledges financial support from the Alexander von Humboldt Foundation, the French ANR (NMGEM project) and the EC (GRENADA project). A. C. F. acknowledges funding from EU grants GRAPHENE-CA, NANOPOTS, GENIUS, RODIN, EPSRC grants EP/GO30480/1 and EP/F00897X/1, and a Royal Society Wofson Research Merit Award. FB and ACF acknowledge Paul Beecher, Tawfique Hasan, Zoran Radivojevic and Zhipei Sun for useful discussion.

11. References

[1] Novoselov, K. S., Castro Neto, A. New directions in science and technology: two-dimensional crystals Rep. Prog. Phys. 74 082501 (2011)

[2]http://www.nobelprize.org/nobel_prizes/physics/laureates/ 2010/press.html.

[3] Bae, S. et al. Roll-to-roll production of 30-inch graphene films for transparent electrodes Nature Nanotech. 5, 1 (2010).

[4] http://research.nokia.com/morph

[5] Lin, Y-M et al., Wafer-Scale Graphene Integrated Circuit Science 332, 1294 (2011).

[6] Torrisi, F., et al., Ink-Jet Printed Graphene Electronics. arXiv:1111.4970v1 (2011).

[7] Hernandez, Y., et al. High-yield production of graphene by liquid-phase exfoliation of graphite. Nature Nanotech. 3, 563 (2008).

[8] Tannock, Q., Exploiting carbon flatland, Nat. Mater. 11, 2 (2012).

[9] Harrison, W.A., ed. Electronic Structure and Properties of Solids: the Physics of the Chemical Bond. 1989, Dover Publications.

[10] Charlier, J.C., et al. Electron and phonon properties of graphene: Their relationship with carbon nanotubes Topics. Appl. Physics 111, 673 (2008).

[11] Wallace, P. R., The Band Theory of Graphite Phys. Rev. 71, 622 (1947).

[12] Geim, A.K. and K.S. Novoselov, The rise of graphene. Nature Mater.6, 183 (2007).

[13] Ando, T., The electronic properties of graphene and carbon nanotubes. NPG Asia Mater. 1, 17 (2009).

[14] Lemme M., Current status in graphene transistors. Solid State Phenom., 499 156 (2010).

[15] Novoselov, K.S., et al., Two-dimensional gas of massless Dirac fermions in graphene. Nature 438, 197 (2005).

[16] Berger, C., et al., Electronic confinement and coherence in patterned epitaxial graphene. Science, 312 1191 (2006).

[17] Bolotin, K.I., et al., Ultrahigh electron mobility in suspended graphene. Solid State Communications 146, 351 (2008).

[18] Morozov, S.V., et al., Giant Intrinsic Carrier Mobilities in Graphene and Its Bilayer. Phys. Rev. Lett., 100, 016602 (2008).

[19] Du, X., et al., Approaching ballistic transport in suspended graphene. Nature Nanotech. 3, 491 (2008).

[20] Castro, E. V., et al., Limits on Charge Carrier Mobility in Suspended Graphene due to Flexural Phonons. Phys. Rev. Lett. 105, 266601 (2010).

[21] Moser, J., Barreiro, A., Bachtold, A. Current-induced cleaning of graphene. Appl. Phys. Lett. 91, 163513 (2007).

[22] Balandin, A.A., et al., Superior Thermal Conductivity of Single-Layer Graphene. Nano Lett. 8, 902 (2008).

[23] Ghosh, S., et al., Extremely high thermal conductivity of graphene: Prospects for thermal management applications in nanoelectronic circuits. Appl. Phys. Lett. 92, 151911 (2008).

[24] Nair, R. R., et al. Fine structure constant defines transparency of graphene. Science 320, 1308 (2008).

[25] Lee, C., et al. Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene Science 321, 385, (2008).

[26] Booth, T.J., et al., Macroscopic Graphene Membranes and Their Extraordinary Stiffness. Nano Letters 8, 2442 (2008).

[27] Baughman, R. H., Zakhidov, A. A., de Heer, W. A. Carbon Nanotubes—the Route Toward Applications Science 297, 787 (2002).

[28] Cai, J., P. et al., Atomically precise bottom-up fabrication of graphene nanoribbons Nature 466, 470 (2010).

[29] Brodie, B.C., Sur le poids atomique du graphite Ann. Chim. Phys., 55, 466 (1860).

[30] Hummers, W.S. and R.E. Offeman, Preparation of graphite oxide J. Am. Chem. Soc. 80, 1339 (1958).

[31] Staudenmaier, L., Ber. Deut. Chem. Ges., 31, 1481 (1898).

[32] Titelman, G. I., et al. Characteristics and microstructure of aqueous colloidal dispersions of graphite oxide Carbon 43, 641 (2005).

[33] Liscio, A., et al., Charge transport in graphene–polythiophene blends as studied by Kelvin Probe Force Microscopy and transistor characterization J. Mater. Chem. 21, 2924 (2011).

[34] Treossi, E., M. et al., High-contrast visualization of graphene oxide on dye-sensitized glass, quartz and silicon by fluorescence quenching J. Am. Chem. Soc., 131, 15576 (2009).

[35] Quintana, M., A., et al., Selective organic functionalization of graphene bulk or graphene edges Chem. Comm. 47, 9330 (2011).

[36] Melucci, M., E. et al., Facile covalent functionalization of graphene oxide using microwaves: bottom-up development of functional graphitic materials J. Mater. Chem., 20, 9052 (2010).

[37] Matsuo, Y., et al. Silylation of graphite oxide, Carbon, 42, 2117 (2004).

[38] Englert, J.M., et al. Covalent bulk functionalization of graphene Nature Chem. 3, 279 (2011).

[39] Backes, C., et al., Nanotube surfactant design: the versatility of water-soluble perylene bisimides. Adv. Mater., 22, 788 (2010).

[40] Wang, Q.H. and Hersam, M.C. Room-temperature molecular-resolution characterization of self-assembled organic monolayers on epitaxial graphene. Nature Chem. 1, 206 (2009).

[41] Mattevi, C. et al. Evolution of electrical, chemical, and structural properties of transparent and conducting chemically derived graphene thin films. Adv. Funct. Mater. 19, 2577 (2009).

[42] Erickson, K., R. et al., Determination of the local chemical structure of graphene oxide and reduced graphene oxide Adv. Mater, 22, 4467 (2010).

[43] Eda, G., Chhowalla, M., Chemically Derived Graphene Oxide: Towards Large-Area Thin-Film Electronics and Optoelectronics. Adv. Mater. 22, 2392 (2010).

[44] Becerril, H.A., et al., Evaluation of solution-processed reduced graphene oxide films as transparent conductors. ACS Nano, 2, 463 (2008).

[45] Stankovich, S., et al., Synthesis of graphene-based nanosheets via chemical reduction of exfoliated graphite oxide. Carbon, 2007, 45, 1558-1565.

[46] Gilje, S., et al., A chemical route to graphene for device applications. Nano Lett., 7, 3394 (2007).

[47] Zhou, M., et al., Electrochemically Reduced Graphene Oxide Films. Chemistry-a European Journal, 15, 6116 (2009).

[48] Yao, P.P., et al., Electric Current Induced Reduction of Graphene Oxide and Its Application as Gap Electrodes in Organic Photoswitching Devices. Adv. Mater. 22, 5008 (2010).

[49] Bagri, A., et al., Structural evolution during the reduction of chemically derived graphene oxide, Nature Chem. 2, 581 (2010).

[50] Pang, S.P., et al. Patterned Graphene Electrodes from Solution-Processed Graphite Oxide Films for Organic Field-Effect Transistors Adv. Mater. 21, 3488 (2009).

[51] Eda, G. and Chhowalla, M. Graphene-based Composite Thin Films for Electronics. Nano Letters, 9, 814 (2009).

[52] Wu, J.B., et al., Organic solar cells with solution-processed graphene transparent electrodes. Appl. Phys. Lett. 92, 263302 (2008).

[53] Yang, N.L., et al., TiO2 Nanocrystals Grown on Graphene as Advanced Photocatalytic Hybrid Materials. ACS Nano, 4, 887 (2010).

[54] Zhu, X.J., et al., Nanostructured reduced graphene oxide/Fe2O3 composite as a high-performance anode material for lithium ion batteries. ACS Nano, 5, 3333 (2011).

[55] Wei, Z.Q., et al., Nanoscale Tunable Reduction of Graphene Oxide for Graphene Electronics. Science, 328, 1373 (2010).

[56 Alaboson, J.M.P., et al., Conductive Atomic Force Microscope Nanopatterning of Epitaxial Graphene on SiC(0001) in Ambient Conditions. Adv. Mater., 23, 2181 (2011).

[57] Mativetsky, J.M., et al., Local Current Mapping and Patterning of Reduced Graphene Oxide. J. Am. Chem. Soc., 132, 14130 (2010).

[58] He, S. J., et al., A Graphene Nanoprobe for Rapid, Sensitive, and Multicolor Fluorescent DNA Analysis. Adv. Funct. Mater. 20, 453 (2010).

[59] Merchant, C. A., et al., DNA Translocation through Graphene Nanopores. Nano Lett. 10, 2915 (2010).

[60] Schneider, G.F., et al., DNA Translocation through Graphene Nanopores, Nano Lett. 10, 3163 (2010).

[61] Rochefort, A. and Wuest, J.D. Interaction of Substituted Aromatic Compounds with Graphene Langmuir, 2009, 25, 210-215.

[62] Roos, M., et al., Hierarchical Interactions and Their Influence upon the Adsorption of Organic Molecules on a Graphene Film. J. Am. Chem. Soc. 133, 9208 (2011).

[63 Gierz, I., et al. Atomic Hole Doping of Graphene. Nano Lett. 8, 4603 (2008).

[64] Wehling, T.O., et al., Molecular doping of graphene. Nano Lett. 8, 173 (2008).

[65] Lauffer, P., et al., Molecular and electronic structure of PTCDA on bilayer graphene on SiC(0001) studied with scanning tunneling microscopy. Phys. Stat. Solidi B-Basic Solid State Physics 245, 2064 (2008).

[66 Zhang, Y.H., et al. Tuning the electronic structure and transport properties of graphene by noncovalent functionalization: effects of organic donor, acceptor and metal atoms. Nanotechnology 21, (2010).

[67] Matte, H., et al., Quenching of fluorescence of aromatic molecules by graphene due to electron transfer. Chem. Phys. Lett., 506, 260 (2011).

[68] Swathi, R. S. and Sebastiana K. L. Resonance energy transfer from a dye molecule to graphene J. Chem. Phys. 129, 054703 (2008).

[69] Treossi, E., et al., High-Contrast Visualization of Graphene Oxide on Dye-Sensitized Glass, Quartz, and Silicon by Fluorescence Quenching. J. Am. Chem. Soc. 131, 15576 (2009).

[70] Wang, Y.B., et al., Fluorescence Quenching in Conjugated Polymers Blended with Reduced Graphitic Oxide. J. Phys. Chem. C, , 114, 4153 (2010).

[71 Kim, J., et al. Graphene Oxide Sheets at Interfaces. J. Am. Chem. Soc. 132, 260 (2010).

[72] Loh, K.P., et al., Graphene oxide as a chemically tunable platform for optical applications. Nature Chem. 2, 1015 (2010).

[73] Rao, C.N.R. and Voggu, R. Charge-transfer with graphene and nanotubes. Materials Today 13, 34 (2010).

[74] Novoselov, K.S., et al., Electric Field Effect in Atomically Thin Carbon Films. Science 306, 666 (2004).

[75] Casiraghi, C., et al., Rayleigh Imaging of Graphene and Graphene Layers. Nano Lett. 7, 2711 (2007).

[76] Blake, P., et al., Making graphene visible. Appl. Phys. Lett. 91, 063124 (2007.).

[77] Abergel, D.S.L., A. Russell, and V.I. Fal'ko, Visibility of graphene flakes on a dielectric substrate. Appl. Phys. Lett. 91, 063125 (2007).

[78] Ni, Z.H., et al., Graphene Thickness Determination Using Reflection and Contrast Spectroscopy. Nano Lett. 7, 2758 (2007).

[79] Ferrari, A.C., et al., Raman Spectrum of Graphene and Graphene Layers. Phys. Rev.Lett. 97, 187401 (2006).

[80] Ferrari, A.C., Raman spectroscopy of graphene and graphite: Disorder, electron-phonon coupling,

doping and nonadiabatic effects. Solid State Comm. 143, 47 (2007).

[81] Tuinstra, F. and Koenig, J. L. Raman Spectrum of Graphite J. Chem. Phys. 53, 1126 (1970).

[82] Ferrari, A.C. and Robertson, J., Raman of amorphous, nanostructured, diamond-like carbon and nano-diamond. Philos. Trans. R. Soc. Ser. A 362, 2477 (2004).

[83] J. Yan, et al., Electric Field Effect Tuning of Electron-Phonon Coupling in Graphene. Phys. Rev. Lett. 98, 166802 (2007).

[84] Ando, T. , Magnetic Oscillation of Optical Phonon in Graphene J. Phys. Soc. Jpn. 76, 024712 (2007).

[85] Goerbig, M.O. et al., Filling-Factor-Dependent Magnetophonon Resonance in Graphene Phys. Rev. Lett. 99, 087402 (2007).

[86] Basko, D.M., et al., Electron-electron interactions and doping dependence of the two-phonon Raman intensity in graphene. Phys. Rev. B 80, 165413 (2009).

[87] Das, A., et al., Monitoring dopants by Raman scattering in an electrochemically top-gated graphene transistor. Nature Nanotechnology 3, 210 - 215 (2008).

[88] Malard, L. M. et al., Probing the electronic structure of bilayer graphene by Raman scattering. Phys. Rev. B 76, 201401 (2007).

[89] Pisana, S. et al., Breakdown of the adiabatic Born–Oppenheimer approximation in graphene. Nature Mater. 6, 198 (2007).

[90] Yan, J., et al., Observation of Magnetophonon Resonance of Dirac Fermions in Graphite. Phys. Rev. Lett. 105, 227401 (2010).

[91] Faugeras, C., et al., Magneto-Raman Scattering of Graphene on Graphite: Electronic and Phonon Excitations. Phys. Rev. Lett. 107, 036807(2011).

[92] Mohiuddin, M. G., et al., Uniaxial strain in graphene by Raman spectroscopy: G peak splitting, Grüneisen parameters, and sample orientation. Phys. Rev. B 79, 205433 (2009).

[93] Ferralis,N. Maboudian, R. and Carraro, C., Evidence of Structural Strain in Epitaxial Graphene Layers on 6H-SiC(0001). Phys. Rev. Lett. 101, 156801 (2008).

[94] Casiraghi, C., et al., Raman Fingerprint of Charged Impurities in Graphene. Appl. Phys. Lett. 91, 233108 (2007).

[95] Das, A.,et al., Monitoring dopants by Raman scattering in an electrochemically top-gated graphene transistor. Nature Nanotech. 3, 210 (2008).

[96] Casiraghi, C,. et al., Raman spectroscopy of graphene edges. Nano Lett. 9, 1433 (2009).

[97] Ferrari A. C. et al., Resonant Raman spectroscopy of disordered, amorphous, and diamondlike carbon. Phys. Rev. B 64, 075414 (2001).

[98] Lotya, M. et al. Liquid phase production of graphene by exfoliation of graphite in surfactant/water solutions. J. Am. Chem. Soc. 131, 3611

[99] Green, A. A. & Hersam, M. C. Solution phase production of graphene with controlled thickness via density differentiation. Nano Lett. 9, 4031 (2009).

[100] Maragò, O. M., et al., Brownian motion of graphene. ACS Nano 4, 7515 (2010).

[101] Hasan, T., et al. Solution-phase exfoliation of graphite for ultrafast photonics. Phys. Status Solidi B 247, 2953 (2010)

[102] Khan, U., et al. High-Concentration Solvent Exfoliation of Graphene.Small 6, 864 (2010).

[103] Nuvoli, D. et al. High concentration few-layer graphene sheets obtained by liquid phase exfoliation of graphite in ionic liquid. J.Mater. Chem. 21, 3428 (2011).

[104] Bonaccorso F., et al., Graphene photonics and optoelectronics. Nature Photon. 4, 611 (2010).

[105] Lee, J. H., et al., One-Step Exfoliation Synthesis of Easily Soluble Graphite and Transparent Conducting Graphene Sheets. Adv. Mater. 21, 4383 (2009).

[106] Valles, C., et al., Solutions of negatively charged graphene sheets and ribbons. J. Am. Chem. Soc. 130, 15802 (2008).

[107] Li, D. et al. Processable aqueous dispersions of graphene nanosheets. Nature Nanotech. 3, 101 (2008).

[108] An, X. et al. Stable Aqueous Dispersions of Noncovalently Functionalized Graphene from Graphite and their Multifunctional High-Performance Applications. Nano Lett. 10, 4295 (2010).

[109] Li, X., et., Chemically Derived, Ultrasmooth Graphene Nanoribbon Semiconductors. Science 319, 1229 (2008).

[110] Coleman, J. N., et al. , Two-Dimensional Nanosheets Produced by Liquid Exfoliation of Layered Materials. Science 331, 568 (2011).

[111] Acheson, E. G., Production of artifi cial crystalline carbonaceous materials; article of carborundum and process of the manufacture thereof carborundum. US patent 615,648 (1896).

[112] Berger, C., et al., Ultrathin epitaxial graphite: 2D electron gas properties and a route toward graphene-based nanoelectronics. J. Phys. Chem. B 108, 19912 (2004).

[113] Berger, C., et al., Electronic confinement and coherence in patterned epitaxial graphene. Science 312, 1191 (2006).

[114] De Heer, W.A., et al., Epitaxial graphene. Solid State Communications. 143, 92 (2007).

[115] Emtsev, K. V., et al., Towards wafer-size graphene layers by atmospheric pressure graphitization of silicon carbide. Nature Mater. 8, 203 (2009).

[116] Riedl, C. et al. Quasi-free-standing epitaxial graphene on SiC obtained by hydrogen intercalation. Phys. Rev. Lett. 103, 246804 (2009).

[117] Kedzierski, J., et al., Epitaxial Graphene Transistors on SiC Substrates. Electron Devices, IEEE Transactions. 55, 2078 (2008).

[118] Rohrl, J., et al., Raman spectra of epitaxial graphene on SiC(0001). Appl. Phys. Lett. 92, 201918 (2008).

[119] Obraztsov, A. N., et al., Chemical vapor deposition of thin graphite films of nanometer thickness. Carbon 45, 2017 (2007).

[120] Yu, Q., et al., Graphene segregated on Ni surfaces and transferred to insulators. Appl. Phys. Lett. 93, 113103 (2008).

[121] Reina, A., et al., Large Area, Few-Layer Graphene Films on Arbitrary Substrates by Chemical Vapor Deposition. Nano Lett. 9, 30 (2009).

[122] Kim, K.S., et al., Large-scale pattern growth of graphene films for stretchable transparent electrodes. Nature 457, 706 (2009).

[123] Sutter, P.W., J.-I. Flege, and E.A. Sutter, Epitaxial graphene on ruthenium. Nature Mater. 7, 406 (2008).

[124] Coraux, J., et al., Structural Coherency of Graphene on Ir(111). Nano Lett. 8, 565 (2008).

[125] N'Diaye, A.T., et al., Structure of epitaxial graphene on Ir(111). New Journal of Physics 10, 043033 (2008).

[126] Li, X., et al., Large-Area Synthesis of High-Quality and Uniform Graphene Films on Copper Foils. Science 324, 1312 (2009).

[127] Rummeli, M. H., et al. Direct Low-Temperature Nanographene CVD Synthesis over a Dielectric Insulator. ACS nano 4, 4206 (2010).

[128] Hwang, J., et al., Epitaxial growth of graphitic carbon on C-face SiC and Sapphire by chemical vapor deposition (CVD). J. Crystal Growth 312, 3219 (2010).

[129] Michon, A. , et al., Direct growth of few-layer graphene on 6H-SiC and 3C-SiC/Si via propane chemical vapor deposition. Appl. Phys. Lett. (2010) 97, 171909.

[130] Strupinski, W., et al., Graphene Epitaxy by Chemical Vapor Deposition on SiC. Nano Lett. 11, 1786 (2011).

[131] Fanton, M. A., et al., Characterization of Graphene Films and Transistors Grown on Sapphire by Metal-Free Chemical Vapor Deposition. ACS Nano 5, 8062 (2011).

[132] Sun, J., et al., Large-area uniform graphene-like thin films grown by chemical vapor deposition directly on silicon nitride. Appl. Phys. Lett. 98, 252107 (2011).

[133] Scott, A., et al., The catalytic potential of high-κ dielectrics for graphene formation.Appl. Phys. Lett. 98, 073110 (2011).

[134] Dato, A. et al., Substrate-Free Gas-Phase Synthesis of Graphene Sheets Nano Lett. 8, 2012 (2008).

[135] Al-Temimy, A., et al., Low temperature growth of epitaxial graphene on SiC induced by carbon evaporation. Appl. Phys. Lett. 95, 231907 (2009).

[136] Bertoni, G., et al., First-principles calculation of the electronic structure and EELS spectra at the graphene/Ni(111) interface. Phys. Rev. B 71, 075402 (2004)

[137] Land, T. A., et al., STM investigation of single layer graphite structures produced on Pt(111) by hydrocarbon decomposition Surf. Sci. 264, 261 (1992).

[138] N'Diaye, A. T., et al., Two-Dimensional Ir Cluster Lattice on a Graphene Moiré on Ir(111). Phys. Rev. Lett. 97, 215501 (2006).

[139] Klusek, Z., et al., Local electronic edge states of graphene layer deposited on Ir(1 1 1) surface studied by STM/CITS. Appl. Surf. Sci. 252, 1221 (2005).

[140] Marchini, S., Günther, S., Wintterlin, J., Scanning tunneling microscopy of graphene on Ru(0001). Phys. Rev. B 76, 075429 (2007).

[141] Vázquez de Parga, A. L., et al., Periodically Rippled Graphene: Growth and Spatially Resolved Electronic Structure. Phys. Rev. Lett. 100, 056807 (2007).

[142] Rosei, R., et al., Structure of graphitic carbon on Ni(111): A surface extended energy-loss fine-structure study. Phys. Rev. B 28, 1161–1164 (1983).

[143] Dedkov, Y. S., Fonin, M., Laubschat, C., A possible source of spin-polarized electrons: The inert graphene/Ni(111) system. Appl. Phys. Lett. 92, 052506 (2008).

[144] Dedkov Y. S., et al., Rashba Effect in the Graphene/Ni(111) System. Phys. Rev. Lett. 100, 107602 (2008).

[145] Martoccia, D., et al., Graphene on Ru(0001): A 25×25 Supercell. Phys. Rev. Lett. 101, 126102 (2008).

[146] Blanc, N., et al., submitted

[147] Busse, C., et al., Graphene on Ir(111): Physisorption with Chemical Modulation. Phys. Rev. Lett., 107, 036101 (2011).

[148] Giovannetti, G., et al. Doping Graphene with Metal Contacts Phys. Rev. Lett.101, 026803 (2008).

[149] Wang, B., et al., Chemical origin of a graphene moiré overlayer on Ru(0001). Phys. Chem. Chem. Phys. 10, 3530 (2008).

[150] Morits, W., et al., Structure Determination of the Coincidence Phase of Graphene on Ru(0001) Phys. Rev. Lett. 104, 136102 (2010).

[151] Borca, B., et al., Electronic and geometric corrugation of periodically rippled, self-nanostructured graphene epitaxially grown on Ru(0001) New J. Phys. 12, 093018 (2010).

[152] Vanin, M., et al., Graphene on metals: A van der Waals density functional study. Phys. Rev. B 81, 081408(R) (2010).

[153] Stradi, D., et al., Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Phys. Rev. Lett. 106, 186102 (2011).

[154] Ugeda, M. M., et al., Missing Atom as a Source of Carbon Magnetism. Phys. Rev. Lett. 104, 096804 (2010).

[155] N'Diaye, A. T., et al., In situ observation of stress relaxation in epitaxial graphene. New J. Phys. 11, 113056 (2009)

[156] Rusponi, S., et al., Highly Anisotropic Dirac Cones in Epitaxial Graphene Modulated by an Island Superlattice. Phys. Rev. Lett. 105, 246803 (2010)

[157] Gyamfi, M., et al., Inhomogeneous electronic properties of monolayer graphene on Ru(0001) Phys. Rev. B 83, 153418 (2011)

[158] Pletikosić, I., et al., Dirac Cones and Minigaps for Graphene on Ir(111) Phys. Rev. Lett. 102, 056808 (2009).

[159] Varykhalov, A., et al., Electronic and Magnetic Properties of Quasifreestanding Graphene on Ni. Phys. Rev. Lett. 101, 157601 (2008).

[160] Balog, R., et al., Bandgap opening in graphene induced by patterned hydrogen adsorption. Nature Mater. 9, 315 (2010).

[161] Haberer, D., et al., Tunable Band Gap in Hydrogenated Quasi-Free-Standing Graphene. Nano Lett. 10, 3360 (2010).

[162] Rader, O., et al., Is There a Rashba Effect in Graphene on 3d Ferromagnets? Phys. Rev. Lett. 102, 057602 (2009).

[163] N'Diaye, A. T., et al., A versatile fabrication method for cluster Superlattices. New J. Phys. 11, 103045 (2009).

[164] Pozzo, M., et al., Thermal Expansion of Supported and Freestanding Graphene: Lattice Constant versus Interatomic Distance Phys. Rev. Lett. 106, 135501 (2011).

[165] Sun, Z., et al., Topographic and electronic contrast of the graphene moiré on Ir(111) probed by scanning tunneling microscopy and noncontact atomic force microscopy Phys. Rev. B 83, 081415(R) (2011).

[166] Altenburg, S. J. , et al., Graphene on Ru(0001): Contact Formation and Chemical Reactivity on the Atomic Scale Phys. Rev. Lett. 105, 236101 (2010).

[167] Hill, E.W., et al., Graphene Spin Valve Devices. IEEE TRANSACTIONS ON MAGNETICS, VOL. 42, 2694 (2006).

[168] Weser, M., et al., Electronic structure and magnetic properties of the graphene/Fe/Ni(111) intercalation-like system Phys. Chem. Chem. Phys. 13, 7534 (2011).

[169] Vo-Van, C., et al., Ultrathin epitaxial cobalt films on graphene for spintronic investigations and applications New J. Phys. 12, 103040 (2010).

[170] Yazyev, O. V., Pasquarello, A., Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride. Phys. Rev. B 80, 035408 (2009).

[171] Sicot, M., et al., Nucleation and growth of nickel nanoclusters on graphene Moiré on Rh(111) Appl. Phys. Lett. 96, 093115 (2010).

[172] Donner, K. , Jakob, P., Structural properties and site specific interactions of Pt with the graphene/Ru(0001) moiré overlayer. J. Chem. Phys. 131, 164701 (2010).

[173] Pollard, A. J., et al., Supramolecular Assemblies Formed on an Epitaxial Graphene Superstructure. Angew. Chem. Int. Ed. 49, 1794 (2010).

[174] Tontegode, A. Y. , Carbon on transition metal surfaces Prog. Surf. Sci. 38, 201 (1991).

[175] Coraux, J., et al., Growth of graphene on Ir(111) New J. Phys. 11, 023006 (2009).

[176] Gao, M., et al., Tunable interfacial properties of epitaxial graphene on metal substrates Appl. Phys. Lett. 96, 053109 (2010).

[177] van Gastel, R., et al., Selecting a single orientation for millimeter sized graphene sheets. Appl. Phys. Lett. 95, 121901 (2009).

[178] Günther, S., et al., Single Terrace Growth of Graphene on a Metal Surface. Nano Lett. 11, 1895 (2011).

[179] Hattab, H., et al., Growth temperature dependent graphene alignment on Ir(111) Appl. Phys. Lett. 98, 141903 (2011).

[180] Dong, G. et al. (in press)

[181] Iwasaki, T., et al., Long-Range Ordered Single-Crystal Graphene on High-Quality Heteroepitaxial Ni Thin Films Grown on MgO(111). Nano Lett. 11, 79 (2011)

[182] Vo-Van, C., et al., Epitaxial graphene prepared by chemical vapor deposition on single crystal thin iridium films on sapphire Appl. Phys. Lett. 98, 181903 (2011).

[183] Park, H. J., et al., Growth and properties of few-layer graphene prepared by chemical vapor deposition. Carbon 48, 1088 (2009).

[184] Amara, H., Bichara, C. , Ducastelle, F., Formation of carbon nanostructures on nickel surfaces: A tight-binding grand canonical Monte Carlo study. Phys. Rev. B 73, 113404 (2006).

[185] Amara H., et al., Tight-binding potential for atomistic simulations of carbon interacting with transition metals: Application to the Ni-C system. Phys. Rev. B 79, 014109 (2009).

[186] Karoui, S., et al., Nickel-Assisted Healing of Defective Graphene.
ACS Nano 4, 6114 (2010).

[187] Thiel, S., et al., Engineering polycrystalline Ni films to improve thickness uniformity of the chemical-vapor-deposition-grown graphene films. Nanotechnology 21, 015601 (2010).

[188] Baraton, L. et al., Europhys. Lett., in press

[189] Dervishi, E., et al., The role of hydrocarbon concentration on the synthesis of large area few to multi-layer graphene structures. Chem. Phys. Lett. 501, 390 (2011).

[190] Hesjelda, T., Continuous roll-to-roll growth of graphene films by chemical vapor deposition. Appl. Phys. Lett. 98, 133106 (2011).

[191] Mattevi, C., Kim, H., Chhowalla, M., A review of chemical vapour deposition of graphene on copper. J. Mater. Chem. 21, 3324 (2011).

[192] Oznuler, T., et al., Synthesis of graphene on gold. Appl. Phys. Lett. 98, 183101 (2011).

[193] Robertson, A. W., Warner, J. H., Hexagonal Single Crystal Domains of Few-Layer Graphene on Copper Foils. Nano Lett. 11, 1182 (2011).

[194] Wu, Y. A., et al., Aligned Rectangular Few-Layer Graphene Domains on Copper Surfaces. Chem. Mater. 23, 4544 (2011).

[195] Lherbier, A., et al., Charge Transport in Chemically Doped 2D Graphene. Phys. Rev. Lett. 101, 036808 (2008).

[196] Bieri, M., et. al. Porous graphenes: two-dimensional polymer synthesis with atomic precision. Chem Commun. 2009 , 6919-6921.

[197] Booth, T., et al, Discrete Dynamics of Nanoparticle Channelling in Suspended Graphene. Nano Lett. 11, 2689 (2011).

[198] Tapaszto, L., et al., Tailoring the atomic structure of graphene nanoribbons by scanning tunnelling microscope lithography. Nature Nanotech. 3, 397-401 (2008).

[199] Wagner, P., Bezanilla, A., Roche, S., Ivanovskaya, V. V., Rayson, M. J., Ewels, C. P. in preparation (2011)

[200] Cervantes-Sodi, F., et al., Edge-functionalized and substitutionally doped graphene nanoribbons: Electronic and spin properties. Phys. Rev. B. 77, 165427 (2008).

[201] Ivanovskaya, V. V., et al, Low-energy termination of graphene edges via the formation of narrow nanotubes. Phys. Rev. Lett., 107, 065502 (2011).

[202] Wagner, P., et al, Ripple edge engineering of graphene nanoribbons. arXiv:1107.1977v1 (2011).

[203] Cocchi, C., et al., Designing All-Graphene Nanojunctions by Covalent FunctionalizationJ. Phys. Chem. C, 115, 2969 (2011).

[204] Biel, B., et al., Anomalous Doping Effects on Charge Transport in Graphene Nanoribbons. Phys. Rev. Lett. 102, 096803 (2009).

[205] Banhart, F., Kotakoski, J. Krasheninnikov, A. V., Structural Defects in Graphene. ACS Nano 5, 26 (2011).

[206] Ferrari, A. C. and Robertson, J. (eds), Raman spectroscopy in carbons: from nanotubes to diamond, Theme Issue, Phil. Trans. Roy. Soc. A 362, 2267-2565 (2004).

[207] Nemanich, R.J., Solin, S. A., Martin, R.M., Light-scattering study of boron nitride microcrystals, Phys. Rev. B 23, 6348 (1981).

[208] Reich, S., et al., Resonant Raman scattering in cubic and hexagonal boron nitride. Phys. Rev B 71, 205201 (2005).

[209] Russo V. et al. Raman spectroscopy of Bi-Te thin films. J. Raman Spectrosc. 39, 205 (2008)

[210] Gordon, R. J., Criteria for Choosing Transparent Conductors. MRS Bulletin 8, 53 (2000).

[211] Hamberg, I. and Granqvist, C. G., Evaporated Sn-doped In2O3 films: basic optical properties and applications to energy-efficient windows. J. Appl. Phys. 60, R123 (1986).

[212] Granqvist, C. G., Transparent conductors as solar energy materials: a panoramic review. Sol. Energy Mater. Sol. Cells 91, 1529–1598 (2007).

[213] Sheraw, C. D., et al., Organic thin-film transistor-driven polymer dispersed liquid crystal displays on flexible polymeric substrates. Appl. Phys. Lett. 80, 1088 (2002).

[214] Lee, J. Y., et al., Solution-processed metal nanowire mesh transparent electrodes. Nano Lett. 8, 689 (2008).

[215] De, S., et al. Silver nanowire networks as flexible, transparent, conducting films: extremely high dc to optical conductivity ratios. ACS Nano 3, 1767 (2009).

[216] Geng, H. Z., et al., Effect of acid treatment on carbon nanotube-based flexible transparent conducting films. J. Am. Chem. Soc. 129, 7758 (2007).

[217] Wu, Z., et al., Transparent, conductive carbon nanotube films. Science 305, 1273 (2004).

[218] De, S. and Coleman, J. N,. Are there fundamental limitations on the sheet resistanceand transmittance of thin graphene films? ACS Nano 4, 2713 (2010).

[219] Casiraghi, C., et al., Raman fingerprint of charged impurities in graphene Appl. Phys. Lett. 91, 233108 (2007)

[220] Sahu, D. R., Lin, S. Y. and Huang, J. L., ZnO/Ag/ZnO multilayer films for the application of a very low resistance transparent electrode. Appl. Surf. Sci. 252, 7509 (2006).

[221] Zhu, Y., et al., Rational Design of Hybrid Graphene Films for High-Performance Transparent Electrodes. Acs Nano 5, 6472 (2011).

[222] Tung, V. C., et al,. Low-temperature solution processing of graphene-carbon nanotube hybrid materials for high-performance transparent conductors. Nano Lett. 9, 1949 (2009).

[223] Wang, X., Zhi, L., and Mullen, K., Transparent, conductive graphene electrodes for dye-sensitized solar cells. Nano Lett. 8, 323 (2007).

[224] Eda, G., Fanchini, G. & Chhowalla, M., Large-area ultrathin films of reduced graphene oxide as a transparent and flexible electronic material. Nature Nanotech. 3, 270 (2008).

[225] King, P. J., et al.,Improvement of Transparent Conducting Nanotube Films by Addition of Small Quantities of Graphene. ACS Nano 4, 4238 (2010).

[226] Matyba, P., et al., Graphene and mobile ions: the key to all-plastic, solution processed light-emitting devices. ACS Nano 4, 637 (2010).

[227] Bonaccorso, F., Graphene photonics and optoelectronic. ArXiv1006.4854v1.

[228] Chapin, D. M., Fuller, C. S. and Pearson, G. L., A new silicon p-n junction photocell for converting solar radiation into electrical power. J. Appl. Phys. 25, 676 (1954).

[229] Green, M. A., et al., Solar cell efficiency tables. Prog. Photovolt. Res. Appl. 7, 321 (1999).

[230] Peter, L. M., Towards sustainable photovoltaics: the search for new material. Phil. Trans. R. Soc. A 369, 1840 (2011).

[231] Li, X., et al., Graphene-On-Silicon Schottky Junction Solar Cells. Adv. Mater. 22, 2743,(2010).

[232] Wang, X., et al., Transparent carbon films as electrodes in organic solar cells. Angew. Chem. 47, 2990 (2008).

[233] De Arco, L. G., et al., Continuous, highly flexible, and transparent graphene films by chemical vapor deposition for organic photovoltaics" ACS Nano 4, 2865 (2010).

[234] Liu, Z., et al., Organic photovoltaic devices based on a novel acceptor material: Graphene. Adv. Mater. 20, 3924 (2008).

[235] Yong, Y., Tour, J. M., Theoretical efficiency of nanostructured graphene-based photovoltaics. Small 6, 313 (2009).

[236] Yang, N., et al., Two-dimensional graphene bridges enhanced photoinduced charge transport in dye-sensitized solar cells ACS Nano 4, 887 (2010).

[237] Yan, X., et al., "Large, Solution-Processable Graphene Quantum Dots as Light Absorbers for Photovoltaics" Nano Lett., 10, 1869, (2010).

[238] Stoller, M. D., et al., Graphene-based ultracapacitor. Nano Lett., vol. 8, 3498 (2008).

[239] Hong, W., et al., Transparent graphene/PEDOT-PSS composite fi lms as counter electrodes of dye sensitized solar cells" Electrochem. Commun. 10, 1555 (2008).

[240] Bonaccorso, F., et al., Graphene-based Natural Dye-Sensitized Solar Cells" Graphene 2011, Imaginenano 11-14 April, Bilbao, (Spain).

[241] Echtermeyer, T.J., et al. Strong plasmonic enhancement of photovoltage in graphene. Nature Comm. 2, 458 (2011).

[242] Burroughes, J. H., et al. Light-emitting diodes based on conjugated polymers. Nature 347, 539–541 (1990).

[243] Wu, J., et al. Organic light-emitting diodes on solution-processed graphene transparent electrodes. ACS Nano 4, 43–48 (2009).

[244] Han, T-H., et al., Extremely efficient flexible organic light emitting diodes with modified graphene anode. Nature Photon. 6, 105 (2012).

[245] Pickering, J. A., Touch-sensitive screens: the technologies and their applications. Int. J. Man. Mach. Stud. 25, 249 (1986).

[246] Silfverberg, M. 5th International Symposium, Mobile HCI 2003, Udine, Italy, 2003.

[247] Beecher, P., et al., Material Choices For Haptic Interfaces. Material Research Society 2011 Spring Meeting April 26-29, 2011 San Francisco, California (USA).

[248] E. Mallinckrodt, A. L. Hughes, W., Sleator Science, 118, 277 (1953)

[249] Kaczmarek, K. A. et al., Polarity Effect in Electrovibration for Tactile Display," Biomedical Engineering. IEEE Transactions on, 53, 2047 (2006).

[250] Saleh, B. E. A. & Teich, M. C. Fundamentals of Photonics Ch. 18, 784–803 (Wiley, 2007).

[251] Dawlaty, J. M., et al. Measurement of the optical absorption spectra of epitaxial graphene from terahertz to visible. Appl. Phys. Lett. 93, 131905 (2008).

[252] Wright, A. R., Cao, J. C. and Zhang, C., Enhanced optical conductivity of bilayer graphene nanoribbons in the terahertz regime. Phys. Rev. Lett. 103, 207401 (2009).

[253] Sun, Z., et al. Graphene mode-locked ultrafast laser. ACS Nano 4, 803–810 (2010).

[254] Mueller, T., Xia, F. and Avouris, P., Graphene photodetectors for high-speed optical communications. Nature Photon. 4, 297 (2010).

[255] Vasko, F. T., and Ryzhii, V., Photoconductivity of intrinsic graphene. Phys. Rev. B 77, 195433 (2008).

[256] Park, J., Ahn, Y. H. and Ruiz-Vargas, C., Imaging of photocurrent generation and collection in single-layer graphene. Nano Lett. 9, 1742 (2009).

[257] Xia, F. N., et al. Photocurrent imaging and effi cient photon detection in a graphene transistor. Nano Lett. 9, 1039 (2009).

[258] Xia, F., et al., Ultrafast graphene photodetector. Nature Nanotech. 4, 839 (2009).

[259] Xu, X. D., et al., Photo-thermoelectric eff ect at a graphene interface junction. Nano Lett. 10, 562 (2010).

[260] Gabor, N. M., et al., Hot Carrier–Assisted Intrinsic Photoresponse in Graphene. Science 334, 648 (2011)

[261] Blake, P., et al. Influence of metal contacts and charge inhomogeneity on transport properties of graphene near the neutrality point. Solid State Commun.149, 1068 (2009)

[262] Kang, Y. M. , et al. Monolithic germanium/silicon avalanche photodiodes with 340 GHz gain–bandwidth product. Nature Photon. 3, 59 (2009)

[263] Kuzmenko, A. B., et al., Universal optical conductance of graphite. Phys. Rev. Lett. 100, 117401 (2008).

[264] Lee, E. J. H., et al. Contact and edge effects in graphene devices. Nat. Nanotechnol. 3, 486 (2008)

[265] Konstantatos, G., et al., Hybrid graphene-quantum dot phototransistors with ultrahigh gain. ArXiv. 1112.4730v1

[266] Engel, M., et al.,Light-matter interaction in a microcavity-controlled graphene transistor. arXiv:1112.1380v1.

[267] Vahala, K. J., Optical microcavities. Nature 424, 839 (2003).

[268] Freitag, M., et al., Thermal infrared emission from biased graphene. Nat. Nanotechnol. 5, 497 (2010).

[269] Berciaud, S., et al., Electron and Optical Phonon Temperatures in Electrically Biased Graphene. Phys. Rev. Lett. 104, 227401 (2010).

[270] Keller, U., Recent developments in compact ultrafast lasers. Nature 424, 831 (2003).

[271] Okhotnikov, O., Grudinin, A., Pessa, M., Ultra-fast fibre laser systems based on SESAM technology: new horizons and applications. New J. Phys. 6, 177 (2004)

[272] Hasan, T., et al. Nanotube–polymer composites for ultrafast photonics. Adv. Mater. 21, 3874 (2009).

[273] Breusing, M., Ropers, C. and Elsaesser, T., Ultrafast carrier dynamics in graphite. Phys. Rev. Lett. 102, 086809 (2009).

[274] Sun, D., et al., Ultrafast Relaxation of Excited Dirac Fermions in Epitaxial Graphene Using Optical Differential Transmission Spectroscopy. Phys. Rev. Lett. 101, 157402, (2008).

[275] Sun, Z., et al., High-power ultrafast solid-state laser using graphene based saturable absorber, in The Conference on Lasers and Electro-Optics(Baltimore, US, 2011), JWA79.

[276] Popa, D., et al., Sub 200fs pulse generation from a graphene mode-locked fiber laser. Appl. Phys. Lett. 97, 203106 (2010)

[277] Popa, D., et al., Graphene Q-switched, tunable fiber laser”. Appl. Phys. Lett. 98, 073106 (2011)

[278] Popa, D., et al., Sub 200fs pulse generation from a graphene mode-loched fiber laser. Appl. Phys. Lett. 97, 203106 (2010).

[279] Zhang, H., et al. Vector dissipative solitons in graphene mode locked fiber lasers. Opt. Commun. 283, 3334 (2010).

[280] Zhang, H., et al. Compact graphene mode-locked wavelength-tunable erbium-doped fiber lasers: from all anomalous dispersion to all normal dispersion. Laser Phys. Lett. 7, 591 (2010).

[281] Yu, H., et al. Large Energy Pulse Generation Modulated by Graphene Epitaxially Grown on Silicon Carbide. ACS Nano 4, 7582 (2010).

[282] Chang, Y. M.,et al., Multilayered graphene efficiently formed by mechanical exfoliation for non linear saturable absorbers in fiber mode locked lasers. Appl. Phys. Lett. 97, 211102 (2010).

[283] Martinez, A., Fuse, K. and Yamashita, S., Mechanical exfoliation of graphene for the passive mode-locking of fiber lasers. 99, 121107 (2011).

[284] Tan, W. D., et al., Mode locking of ceramic Nd:yttrium aluminum garnet with graphene as a

saturable absorber. Appl. Phys. Lett. 96, 031106 (2010).

[285] Cho, W. B. et al., High-quality, large-area monolayer graphene for efficient bulk laser mode-locking near 1.25 um. Opt. Lett., 36, 4089-4091 (2011)

[286] Martinez, A., et al., Optical deposition of graphene and carbon nanotubes in a fiber ferrule for passive mode-locked lasing. Opt. Express 18, 23054 (2010).

[287] Wang, F. ,et al., ~2um Graphene Q-switched Thulium Fiber Laser. Submitted (2011).

[288] Sun, Z., et al., A stable, wideband tunable, near transform-limited, graphene-mode-locked, ultrafast laser. Nano Res. 3, 404 (2010).

[289] W. Koechner, Solid-State Laser Engineering (Springer, New York, 2006).

[290] Lee, C.-C. et al., Ultra-Short Optical Pulse Generation with Single-Layer Graphene. J. Nonlinear Opt. Phys. Mater. 19, 767-771 (2010).

[291] Bass, M., Li, G. and Stryland, E. V. Handbook of Optics IV (McGraw-Hill, 2001).

[292] Wang, J. et al., Broadband nonlinear optical response of graphene dispersions. Adv. Mater. 21, 2430 (2009).

[293] Xu, Y., et al. A graphene hybrid material covalently functionalized with porphyrin: synthesis and optical limiting property. Adv. Mater. 21, 1275 (2009).

[294] Mikhailov, S. A. Non-linear electromagnetic response of graphene. Europhys. Lett. 79, 27002 (2007).

[295] Dean, J. J. and van Driel, H. M., Second harmonic generation from graphene and graphitic films. Appl. Phys. Lett. 95, 261910 (2009).

[296] Hendry, E., et al., Strong nonlinear optical response of graphene flakes measured by four-wave mixing. Phys. Rev. Lett. 105, 097401 (2010).

[297] Dhar, S. et al., A new route to graphene layers by selective laser ablation AIP ADVANCES 1, 022109 (2011).

[298] ITRS roadmap 2009, www.itrs.net (2011).

[299] Lemme, M.C., et al., Towards Graphene Field Effect Transistors. ECS Transactions, 11, 413 (2007).

[300] Lemme, M.C., et al., A Graphene Field-Effect Device. Electron Device Letters, IEEE, 28, 282 (2007).

[301] Echtermeyer, T. J., et al., Graphene field-effect devices. European Physical Journal-Special Topics. 148, 19 (2007)

[302] Williams, J.R., Di Carlo, L. and Marcus, C.M., Quantum Hall Effect in a Gate-Controlled p-n Junction of Graphene. Science 317, 638 (2007).

[303] Takagi, S., et al., On the universality of inversion layer mobility in Si MOSFET's: Part I-effects of substrate impurity concentration. Electron Devices, IEEE Transactions 41, 2357 (1994).

[304] Martin, J., et al., Observation of electron-hole puddles in graphene using a scanning single-electron transistor. Nature Phys. 4, 144 (2008).

[305] Lemme, M.C., et al., Mobility in graphene double gate field effect transistors. Solid-State Electronic 52, 514 (2008).

[306] Lin, Y.-M., et al., Operation of Graphene Transistors at Gigahertz Frequencies. Nano Lett. 9, 422 (2009).

[307] Nakada, K., et al., Edge state in graphene ribbons: Nanometer size effect and edge shape dependence. Physical Review B. 54, 17954 (1996).

[308] Barone, V., Hod, O., and Scuseria G.E., Electronic Structure and Stability of Semiconducting Graphene Nanoribbons. Nano Lett. 6, 2748 (2006).

[309] Son, Y.-W., Cohen, M.L. and Louie S.G., Energy Gaps in Graphene Nanoribbons. Phys. Rev. Lett. 97, 216803 (2006).

[310] Obradovic, B., et al., Analysis of graphene nanoribbons as a channel material for field-effect transistors. Appl. Phys. Lett. 88, 142102 (2006).

[311] Yang, L., et al., Band-gap change of carbon nanotubes: Effect of small uniaxial and torsional strain. Phys. Rev. B, 60, 13874 (1999).

[312] Fujita, M., et al., Peculiar Localized State at Zigzag Graphite Edge. J. Phys. Soc. Jpn. 65, 1920 (1996).

[313] Huang, B., et al., Making a field effect transistor on a single graphene nanoribbon by selective doping. Appl. Phys. Lett.. 91, 253122 (2007).

[314] Yan, Q., et al., Intrinsic Current-Voltage Characteristics of Graphene Nanoribbon Transistors and Effect of Edge Doping. Nano Lett. 7, 1469 (2007).

[315] Kan, E.-J., et al., Will zigzag graphene nanoribbon turn to half metal under electric field? Appl. Phys. Lett. 91, 243116 (2007).

[316] Hod, O., et al., Enhanced Half-Metallicity in Edge-Oxidized Zigzag Graphene Nanoribbons. Nano Lett. 7, 2295 (2007).

[317] Kudin, K.N., Zigzag Graphene Nanoribbons with Saturated Edges. ACS Nano 2, 516 (2008).

[318] Yoon, Y. and Guo, J. Effect of edge roughness in graphene nanoribbon transistors. Appl. Phys. Lett. 91, 073103 (2007).

[319] Sols, F., Guinea, F. and Neto A.H.C., Coulomb Blockade in Graphene Nanoribbons. Phys. Rev. Lett. 99, 166803 (2007).

[320] Cervantes-Sodi, F., et al., Edge-functionalized and substitutionally doped graphene nanoribbons: Electronic and spin properties. Phys. Rev. B 77, 165427 (2008).

[321] Han, M.Y., et al., Energy Band-Gap Engineering of Graphene Nanoribbons. Phys. Rev. Lett. 98 206805 (2007).

[322] Chen, Z., et al., Graphene nano-ribbon electronics. Physica E: Low-dimensional Systems and Nanostructures 40, 228 (2007).

[323] Han, M.Y., et al., Electron Transport in Disordered Graphene Nanoribbons Phys. Rev. Lett.104, 056801 (2010).

[324] Ponomarenko, L.A., et al., Chaotic Dirac Billiard in Graphene Quantum Dots. Science 320, 356 (2008).

[325] Wang, X., et al., Room-Temperature All-Semiconducting Sub-10-nm Graphene Nanoribbon Field-Effect Transistors. Phys. Rev. Lett. 100, 206803 (2008).

[326] Lemme, M.C., et al., Etching of Graphene Devices with a Helium Ion Beam. ACS Nano, 3, 2674 (2009).

[327] Bell, D.C., et al., Precision Cutting and Patterning of Graphene with He Ions. Nanotechnology 20, 455301 (2009).

[328] McCann, E., Asymmetry gap in the electronic band structure of bilayer graphene. Physical Review B (Condensed Matter and Materials Physics) 74, 161403 (2006).

[329] Ohta, T., et al., Controlling the Electronic Structure of Bilayer Graphene. Science 313, 951 (2006).

[330] Mak K. F., et al., Observation of an Electric-Field-Induced Band Gap in Bilayer Graphene by Infrared Spectroscopy Phys. Rev. Lett. 102, 256405 (2009).

[331] Zhang, Y. T. et al., Direct observation of a widely tunable bandgap in bilayer graphene. Nature 459, 820 (2009).

[332] Oostinga, J.B., et al., Gate-induced insulating state in bilayer graphene devices. Nature Mater. 7, 151 (2008).

[333] Szafranek, B. N. et al., Electrical observation of a tunable band gap in bilayer graphene nanoribbons at room temperature Appl. Phys. Lett. 96, 112103 (2010).

[334] Szafranek, B. N. et al., High On/Off Ratios in Bilayer Graphene Field Effect Transistors Realized by Surface Dopants. Nano Lett. 11, 2640 (2011).

[335] Li, S-L., et al., Complementary-like Graphene Logic Gates Controlled by Electrostatic Doping. Small 7, 1552 (2011).

[336] Schwierz, F. and Liou, J.J., RF transistors: Recent developments and roadmap toward terahertz applications. Solid-State Electronics. 51, 1079 (2007).

[337] Frank, D.J., Taur, Y. and Wong, H.S.P., Generalized scale length for two-dimensional effects in MOSFETs. Electron Device Letters, IEEE. 19, 385 (1998).

[338] Meric, I., et al. RF performance of top-gated, zero-bandgap graphene field-effect transistors. in Electron Devices Meeting, 2008. IEDM 2008. IEEE International. 2008.

[339] Moon, J.S., et al., Epitaxial-Graphene RF Field-Effect Transistors on Si-Face 6H-SiC Substrates. Electron Device Letters, IEEE. 30, 650 (2009).

[340] Palacios, T., Hsu, A., and Wang H. Applications of graphene devices in RF communications. Communications Magazine, IEEE 48, 122 (2010).

[341] Lin, Y-M., et al., 100-GHz Transistors from Wafer-Scale Epitaxial Graphene. Science 327, 662 (2010).

[342] Schwierz, F. and Liou, J. J. Modern Microwave Transistors – Theory, Design, and Performance (Wiley, 2003).

[343] Wu, Y., et al., High-frequency, scaled graphene transistors on diamond-like carbon, Nature 472, 74 (2011).

[344] Liao, L., et al.High-speed graphene transistors with a self-aligned nanowire gate. Nature 467, 305 (2010).

[345] Schwierz, F., Graphene transistors. Nature Nanotech. 5, 487 (2010)

[346] http://www.itrs.net/Links/2010ITRS/IRC-ITRS-MtM-v2%203.pdf

[347] Wu, X., et al., Epitaxial-Graphene/Graphene-Oxide Junction: An Essential Step towards Epitaxial Graphene Electronics. Phys. Rev. Lett. 101, 026801 (2008).

[348] Standley, B., et al., Graphene-Based Atomic-Scale Switches. Nano Letters, 2008. 8(10): p. 3345-3349.

[349] Boukhvalov, D.W. and Katsnelson, M.I. , Tuning the gap in bilayer graphene using chemical functionalization: Density functional calculations. Phys. Rev. B 78, 085413 (2008).

[350] Echtermeyer, T.J., et al., Nonvolatile Switching in Graphene Field-Effect Devices. Electron Device Letters, IEEE. 29, 952 (2008).

[351] Zheng, Y., et al., Gate-controlled nonvolatile graphene-ferroelectric memory. Appl. Phys. Lett. 94, 163505 (2009).

[352] Fiori, G., Iannaccone, G., On the possibility of tunable-gap bilayer graphene FET, IEEE Electron Device Letters, Vol. 30, pp. 261-264, 2009.

[353] Fiori, G., Iannaccone, G., Ultralow-Voltage Bilayer graphene tunnel FET, IEEE Electron Device Letters, Vol. 30, pp.1096-1098, 2009.

[354] Chang, L., et al., Extremely Scaled Silicon Nano-CMOS Device. Proceedings of the IEEE, 91, 1860 (2003).

[355] Hu, C., et al., Green Transistor - A VDD Scaling Path for Future Low Power ICs. IEEE VLSI Technology, Systems and Applications, 2008. VLSI-TSA 2008.

[356] Britnell, L., et al., Field-effect tunneling transistor based on vertical graphene heterostructures. ArXiv1112.4999

[357] Geim, A.K., QED in a Pencil Trace KITP Graphene Workshop 01-09-07.

[358] Fiori, G., Iannaccone, G. Simulation of Graphene Nanoribbon Field-Effect Transistors. IEEE, Electron Device Letters 28, 760 (2007).

[359] Yoon, Y., et al., Performance Comparison of Graphene Nanoribbon FETs With Schottky Contacts and Doped Reservoirs. IEEE Transaction on Electron Devices 55, 2314 (2008).

[360] Grassi, R., et al., Hierarchical modeling of carbon nanoribbon devices for CNR-FETs engineering, Device Research Conference, 2008.

[361] Betti, A., Fiori, G., Iannaccone, G., Atomistic Investigation of Low-Field Mobility in Graphene Nanoribbons ,IEEE Trans. Electr. Dev., available at: ieeexplore.ieee.org

[362] Ferry, D. K., Semiconductor transport London: Taylor & Francis, 2000. Technology & Engineering ISBN 0-7484-0865-7.

[363] Elias, D. , et al., Control of Graphene's Properties by Reversible Hydrogenation: Evidence for Graphane. Science 323, 610 (2009).

[364] Lebègue, S., et al., Accurate electronic band gap of pure and functionalized graphane from GW calculations. Phys. Rev. B 79, 245117 (2009).

[365] Fiori, G., et al., Simulation of hydrogenated graphene field-effect transistors through a multiscale approach. Phys. Rev. B, 82, 153404 (2010).

[366] Chauhan, J., and Guo, J., Assessment of High-Frequency Performance Limits of Graphene Field-Effect Transistors. Nano Res. 4, 571 (2011).

[367] Nam Do, V., et al., Electronic transport and spin-polarization effects of relativisticlike particles in mesoscopic graphene structures, J. Appl. Phys. 104, 063708 (2008).

[368] Hung Nguyen, V., et al., Quantum transport of dirac fermions in graphene field effect transistors, SISPAD 2010, p.9.

Modeling

We are presently witnessing the final phase of the downscaling of MOS technology and, at the same time, the rise of a multiplicity of novel device concepts based on properties of matter at the nanoscale and even at the molecular scale. Ultra-scaled MOS devices and nanodevices relying on new physical principles share the reduced dimensionality and, as a result, many of the modelling challenges. In addition, new materials and process steps are being included into MOS technology at each new node, to be able to achieve the objectives of the Roadmap; these changes make traditional simulation approaches inadequate for reliable predictions. So far modelling at the nanoscale has been mainly aimed at supporting research and at explaining the origin of observed phenomena. In order to meet the needs of the MOS industry and to make practical exploitation of new device and solid-state or molecular material concepts possible, a new integrated approach to modelling at the nanoscale is needed, as we will detail in the following. A hierarchy of multi-scale tools must be set up, in analogy with what already exists for microelectronics, although with a more complex structure resulting from the more intricate physical nature of the devices and the intrinsically multi-physics nature of the problems to be solved. A dedicated effort in the field of modelling is apparent in the United States, where significant funding has been awarded to the Network for Computational Nanotechnology, which is coordinating efforts for the development of simulation tools for nanotechnology of interest both for the academia and for the industry. Although the required integrated platforms need to be developed, the efforts made in the last few years by the modelling community have yielded significant advances in terms of quantitatively reliable simulation and of ab-initio capability, which represent a solid basis on which a true multi-scale, multi-physics hierarchy can be built. The combination of

Position Paper on Modeling

M. Macucci[1], S. Roche[2], A. Correia[3], J. Greer[4], X. Bouju[5], M. Brandbyge[6], J. J. Saenz[7], M. Bescond[8], D. Rideau[9], P. Blaise[10], D. Sanchez-Portal[11], J. Iñiguez[12], X. Oriols[13], G. Cuniberti[14], and H. Sevincli[14]

[1] Dipartimento di Ingegneria dell'informazione, Università di Pisa, Pisa, Italy

[2] CIN2 (ICN-CSIC) and UAB, Catalan Institute of Nanotechnology, Barcelona, Spain

[3] Phantoms Foundation, Madrid, Spain

[4] Tyndall National Institute, Lee Maltings, Cork, Ireland

[5] Centre d'Élaboration de Matériaux et d'Études Structurales (CEMES), Nanosciences Group, Toulouse, France

[6] DTU Nanotech, Department of Micro and Nanotechnology, Technical University of Denmark, Kongens Lyngby, Denmark

[7] Universidad Autónoma de Madrid, Departamento de Física de la Materia Condensada, Madrid, Spain

[8] IM2NP, UMR CNRS 6242, Marseille, France

[9] STMicroelectronics, Crolles, France

[10] CEA, LETI, MINATEC, Grenoble, France

[11] Centro de Fisica de Materiales CSIC-UPV/EHU, Materials Physics Center MPC, San Sebastián, Spain

[12] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Bellaterra, Spain

[13] Dept. of Electron. Eng., Univ. Autonoma de Barcelona, Barcelona, Spain

[14] Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden, Germany

This is a further update of the position paper for the Theory and Modelling Working Group, including the results of the last two meetings, one held in Pisa during the IWCE conference, in October 2010, and the other held in Bilbao, during the IMAGINENANO conference, in April 2011.

While the previous update (in 2009) of the original 2008 document was substantially focused on the main issues on which collaboration within the modelling community is needed and on an analysis of the situation in Europe in comparison with that in the rest of the world, the present update primarily deals with the actual needs of the industry in terms of modelling, with the relevance of physics-based modeling, with time-dependent analysis, with new computational approaches, and with issues rising in the simulation of wide-bandgap semiconductors.

1. Introduction

We are presently witnessing the final phase of the downscaling of MOS technology and, at the same time, the rise of a multiplicity of novel device concepts based on properties of matter at the nanoscale and even at the molecular scale.

Ultra-scaled MOS devices and nanodevices relying on new physical principles share the reduced dimensionality and, as a result, many of the modelling challenges. In addition, new materials and process steps are being included into MOS technology at each new node, to be able to achieve the objectives of the Roadmap; these changes make traditional simulation approaches inadequate for reliable predictions. So far modelling at the nanoscale has been mainly aimed at supporting research and at explaining the origin of observed phenomena.

In order to meet the needs of the MOS industry and to make practical exploitation of new device and solid-state or molecular material concepts possible, a new integrated approach to modelling at the nanoscale is needed, as we will detail in the following. A hierarchy of multi-scale tools must be set up, in analogy with what already exists for microelectronics, although with a more complex structure resulting from the more intricate physical nature of the devices and the intrinsically multi-physics nature of the problems to be solved.

A coordinated effort in the field of modelling is apparent in the United States, where significant funding has been awarded to the Network for Computational Nanotechnology, which is coordinating efforts for the development of simulation tools for nanotechnology of interest both for the academia and for the industry.

Although the required integrated platforms need to be developed, the efforts made in the last few years by the modelling community have yielded significant advances in terms of quantitatively reliable simulation and of ab-initio capability, which represent a solid basis on which a true multi-scale, multi-physics hierarchy can be built. The combination of these new advanced software tools and the availability of an unprecedented computational power (in particular considering the recent advances in terms of GPU-based general purpose computing, and the very recent development of software environments, such as OPENACC that allow an almost automated porting of legacy codes to hybrid GPU-CPU platforms) make the time ripe for a real leap forward in the scope and performance of computational approaches for nanotechnology and nanosciences.

2. Current Status of MOS simulation and industrial needs

The continuous downscaling of MOSFET critical dimensions, such as the gate length and the gate oxide thickness, has been a very successful process in current manufacturing, as testified, e.g., by the ITRS requirements. However, conventional scaling down of MOSFET channel length is declining as the physical and economic limits of such an approach are coming closer. Novel solutions are increasingly being used in MOSFET channel engineering within the industry.

Among the new technological features of very advanced devices, high-k dielectrics, the archetype of which is hafnium oxide, can significantly reduce gate leakage. Mechanical strain applied in the channel and substrate orientation can also significantly improve carrier mobility. Moreover, alternative geometries, such as double-gated devices, in which the channel doping level is relatively low, must be evaluated within the perspective of an industrial integration. In particular, the subsequent effects of the high-k gate dielectric and of the double-gate geometry on channel mobility must be clearly quantified.

Technology Computer-Aided Design (TCAD) refers to the use of computer simulations to develop and optimize semiconductor devices. State-of-the-art commercial TCAD device simulators are currently working using the Drift-Diffusion (DD) approximation of the

Boltzmann transport equation. Quantum effects are accounted for using the Density Gradient approximation, that works well for traditional bulk devices, but that can be unreliable for advanced devices such as the double-gated-MOS structure or for new materials. Moreover, emerging materials also significantly challenge the conventional DD-based tools, mostly due to a lack of appropriate models and parameters.

It is indeed important to understand what would make large semiconductor companies really interested in advanced modeling tools: an answer recurrent from people with experience in the industry is that a simulation code should be able to provide insight into why a given advanced device does not work, an answer that often cannot be obtained from existing commercial codes. In particular, it would be important to have a model that, even though not quantitatively reliable, could tell when things are not going according to intuition. This would be far more important for industry developers than having a very complex code that shows that there is just a small correction with respect to the behavior of the device that could be predicted just by intuition or by means of standard simulators.

If the real added value in a sophisticated model is to predict a behavior that differs from what intuition would tell us, rather than providing quantitatively exact results, the question arises whether drift-diffusion is all the industry needs, because with small changes it has been adapted to successive generations of devices, always yielding acceptable results. In reality, this is not true, because adaptation of drift-diffusion have often been made "a posteriori," once the actual behavior of the device was known from measurements or from more sophisticated models. Very simple models, such as drift-diffusion, although quite efficient when dealing with a well established technology, cannot be of great help when trying to determine what effect a change of parameters will have in a new technology.

It becomes urgent to develop new physically-based models with a view of integrating them into a standardized simulation platform that can be efficiently used in an industrial environment. For this purpose, tight collaborations between world-class universities and research institutions, CAD vendors and industrial partners must be established. Within the framework of these collaborations, there will be the best chances of success, both in terms of academic model development and theoretical achievements, but also in terms of concrete implementations and benchmarks of new models in TCAD tools. Innovative concepts based on nano-materials or molecular devices, new models and simulation tools would provide our ICT industries a competitive advantage for device development and optimization in terms of time-cycle and wafer-costs.

3. Commercial vs. academic quantum-transport solvers

In response to the industrial need of new simulation tools, a class of quantum and transport solvers is emerging. These commercial state-of-the-art solvers can be divided into two categories. In the first category, one can find the quantum-transport solvers, such as those based on the Non-Equilibrium Green Function Method, in which carrier transport is treated using the full quantum Green function formalism. In the second category one can include the Monte Carlo Solvers, that model carrier transport via the Boltzmann equation. This equation is solved in a stochastic way, using a classical description of the free fly of the electrons but a quantum description of the interactions. The currently available high-level NEGF[1] and

MC solutions [2] are still in the development phase, and no ready-to-use industrial solutions are available so far to meet the requirements of the 22 nm node and beyond.

From the point of view of technology development support, the Monte Carlo simulators should be able to provide reliable electrical results on a regular basis for 22 nm MOS devices. However the need for full-band Monte-Carlo codes together with bandstructure solvers that account for strain and are capable of dealing with new materials must be highlighted. Indeed, some commercial 3D Schroedinger solvers[1] combined with NEGF solvers start being available. These solvers can be used to model ballistic quantum transport in advanced devices with strong transverse confinement. However, they do not include any inelastic scattering mechanism, and thus are not suitable for the calculation of transport properties in the 22 nm node devices and near-future nodes.

On the other hand, high-level device simulation tools are at an early stage of development in universities and research institutions. These codes generally include advanced physical models, such as strain-dependent bandstructure and scattering mechanisms, and should provide accurate predictions in complex nano-systems. However, such simulation tools are in general difficult to use in an industrial environment, in particular because of a lack of documentation, support and graphical user interface, although an increasing number of academic codes are now including graphic tools [3,4]. Taking advantage of these ongoing research projects, it should be possible to integrate such high-level codes into industrial TCAD tools or to use them to obtain calibrated TCAD models useful for the industry. Concerning this latter point, the quantum drift-diffusion-based solution must be ``customized,'' in order to make fast and accurate simulations of advanced devices possible. For instance, the effect of the high-k gate dielectric stack on device performance must be addressed with a particular attention to its impact on carrier transport properties. This is definitely one of the most challenging issues in semiconductor industry at present.

Efficient modelling tools, as well as accurate physics highlights, would certainly bring a significant competitive advantage for the development and the optimization of the 22 nm CMOS technology and for future technologies, including molecular devices.

4. Importance of modelling variability

Near the end of the current edition of the International Technology Roadmap for Semiconductors (ITRS) in 2018, transistors will reach sub-10 nm dimensions [5]. In order to maintain a good control of the electrical characteristics, new transistor architectures have to be developed. It is widely recognized that quantum effects and intrinsic fluctuations introduced by the discreteness of electronic charge and atoms will be major factors affecting the scaling and integration of such devices as they approach few-nanometer dimensions [6-11].

For instance, in conventional one-gate nanotransistors, variations in the number and position of dopant atoms in the active and source/drain regions make each nano-transistor microscopically different from its neighbors [12-16]. In nanowire MOS transistors the trapping of one single electron in the channel region can change the current by over 90% [17,18]. Interface roughness of the order of 1-2 atomic layers introduces variations in gate tunneling, quantum confinement and surface/bulk mobility from device to device. The inclusion of new materials such as SiGe will induce additional sources of fluctuations associated with random variations in the structure, defects, strain and inelastic scattering [19,20]. These intrinsic fluctuations will have an important impact on the functionality and reliability of the corresponding circuits at a time when fluctuation margins are shrinking due to continuous reductions in supply voltage and increased transistor count per chip [7,8].

The problem of fluctuations and disorder is actually more general and affects fundamental aspects of information storage and processing as device size is scaled down. The presence of disorder limits the capability of patterning by introducing a spatial variance: when the pattern size approaches the spatial variance, patterns are unavoidably lost. An analogous problem exists as a result of time fluctuations (shot noise) associated with the granularity of charge: as current levels are reduced, the signal power decreases faster (quadratically with current) than the shot noise power (linear with current), leading to a progressive degradation of the signal-to-noise power ratio.

Disorder has demonstrated all of its disruptive power on nanodevices in the case of single-electron transistors: as a result of their extreme charge sensitivity, stray charges, randomly located in the substrate, are sufficient to completely disrupt their operation.

Fluctuations associated with the granularity of charge and spatial disorder are fundamental roadblocks that affect any effort towards handling information on an increasingly small scale.

It is thus of strategic importance to develop device simulation tools that are capable of efficiently exploring the extremely large parameter space induced by such variability and evaluate the actual performance limits of new nanodevices. Strategies to decrease the amount of naturally occurring disorder or to cope with it need to be devised as emerging devices are developed into new technologies aiming at the limits of the downscaling process.

5. Integration between material and device simulation

Both for decananometric MOSFETs and for most emerging devices, the distinction between material and device simulation is getting increasingly blurred, because at low dimensional scales the properties of the material sharply diverge from those of the bulk or of a thin film and become strongly dependent on the detailed device geometry. Such a convergence should start being reflected also in research funding, because, at the dimensional scale on which research is currently focused, a project cannot possibly take into consideration only one of these two aspects. This was not the case until a few years ago, when a material could be investigated within the field of chemistry or material science and then parameters were passed on to those active in the field of device physics and design, who would include them in their simulation tools.

Fortunately, the nanoelectronics simulation community is not starting from scratch in terms of atomic scale materials computations. Computational physics and quantum chemistry researchers have been developing sophisticated programs, some with on the order of millions of lines of source code, to explicitly calculate the quantum mechanics of solids and molecules from first principles. Since quantum mechanics determines the charge distributions within materials, all electrical, optical, thermal and mechanical properties, in fact any physical or chemical property can in principle be deduced from these calculations.

However, these programs have not been written with nanoelectronic TCAD needs in mind, and substantial theoretical and computational problems remain before their application in process and device modeling reaches maturity. However, the coupling of electronic structure theory programs to information technology simulations is occurring now, and there is nothing to suggest this trend will not continue unabated.

Quantum electronic structure codes come in essentially two flavors: those using plane wave expansions (or real-space grids) and those using basis sets of atomic orbitals to span the electronic wave functions. Plane wave codes are suitable for solid state calculations and have been mainly developed within the Solid State Physics community. Codes using atomic orbitals were initially developed within the Quantum Chemistry community, although recently have also become popular within the Materials Physics community. Quantum Chemistry codes rely heavily on the expansion of the atomic orbitals in terms of Gaussian functions. This is mainly due to the fact that, with the use of Gaussians, the four-center-integrals associated with Coulomb and exchange interactions become analytic and easy to calculate. However, within the framework of Density Functional Theory, due to non-linear dependence of the exchange-correlation energy and potential with the density, the evaluation of such contributions to the energy and Hamiltonian has to be necessarily performed numerically and the advantage of using Gaussian functions is mainly lost. This has opened the route for the use of other types of localized basis sets optimized to increase the efficiency of the calculations. For example, localized basis orbital can be defined to minimize the range of the interactions and, therefore, to increase the efficiency of the calculation, the storage, and the solution of the electronic Hamiltonian [21]. In particular, so-called order-N or quasi-order-N methodologies have been developed over the last two decades that, using the advantages of such local descriptions, allow for the calculation of the electronic structure of very large systems with a computational cost that scales linearly or close to linearly with the size of the system [22,23]. This is in contrast with traditional methods that typically show a cubic scaling with the number of electrons in the system. Order-N schemes are particularly powerful and robust for insulators and large biomolecules. However, the design of efficient and reliable order-N methods for metallic systems is still a challenge.

The most widely used codes for ab initio simulations of solids and extended systems rely on the use of the Density Functional Theory, rather than on Quantum Chemistry methods. Many of them have been developed in Europe, and some of them are commercial, although their use is mostly limited to the academic community. Among the commercial code, we can cite the plane-wave codes VASP [24] and CASTEP [25], and the Hartree-Fock/DFT code CRYSTAL [26] that utilizes Gaussian basis functions. Other widely used plane-wave codes are the public domain CP2K [27] and Abinit [28]. Abinit is distributed under GNU license and has become a very complete code with a rapidly growing community of developers. Among the most popular DFT codes using local atomic orbitals as a basis set we can mention the order-N code SIESTA [21,29], which uses a basis set of numerical atomic orbitals, and Quickstep [30], that uses a basis set of Gaussian functions.

One of the reasons why codes using basis sets of atomic orbitals have recently become very popular is that they provide the ideal language to couple with transport codes based on Non-Equilibrium-Green’s functions (NEGFs) to study transport properties in molecular junctions and similar systems. Using the local language implicit behind the use of atomic orbitals (with tight-binding-like Hamiltonians) is trivial to partition the system in different regions that can be treated on different footings. For example, it becomes relatively simple to combine information from a bulk calculation to describe the electrodes with information obtained from a simulation that explicitly considers the active part of the device. Again Europe has taken the lead along this path. Two of the most popular simulation tools for ballistic transport using NEGFs combined with DFT have been developed based on the SIESTA code: tranSIESTA [31] and Smeagol [32]. In particular, tranSIESTA was developed by a collaboration of Danish and Spanish research groups and, although there is a public domain version that will be distributed with the latest version of the SIESTA code (siesta.3.0), it has also given rise to a commercial simulation package called QuantumWise [33].

Electronic structure theory represents the lowest and most sophisticated level of computation in our simulation hierarchy. At this level there are many different degrees of rigor and associated errors in the computations. The most accurate results are provided by post-Hartree-Fock Quantum Chemical methods. Unfortunately, they are extremely demanding and not well suited for simulations of solids and condensed matter systems. As already mentioned, the most popular approach to study such systems is Density Functional Theory, which provides a good balance between the computational cost and the accuracy of the results. However, even at the DFT level, ab initio calculations are computationally too demanding to perform realistic simulations of devices. Therefore, it is necessary to develop more approximate methods and, finally, to combine them in the so-called multi-scale approaches, in which different length scales are described with different degrees of accuracy and detail. An interesting intermediate stage between DFT calculations, which take into account the full complexity of the materials, and empirical models, which disregard most of the chemistry and structural details of the system, is provided by the tight-binding approaches. Here a minimal basis of atomic orbitals is used to describe the electronic structure of the system. As a consequence, only the valence and lowest lying conduction bands can be accurately treated. Traditionally, the hopping and overlap matrix elements were considered empirical parameters that were adjusted to describe the electronic band structure of the material and its variation with strain. This has proven a quite powerful approach to describe complex system like, for example, quantum dots containing thousands or millions of atoms [34, 35]. A very interesting variation of these methods has been developed in recent years: the so-called DFT-tight-binding. Here the tight-binding parameters (hoppings, overlaps and short-ranged interatomic repulsive potentials) are not obtained by fitting to empirical information but they are obtained from DFT calculations for simple systems (mainly diatomic molecules) [36]. The parameters obtained in this way have proven to be transferable enough to provide a reasonable description of systems like large molecules and even solids.

The ability to treat varying length and time scales, within varying degrees of approximation, leads to the already mentioned requirement for a multi-scale approach to coupled materials/device simulation.

Although a multi-scale approach is more than ever needed at this stage, parameter extraction cannot be performed for a generic material, but must be targeted for the particular device structure being considered, especially for single-molecule transistors.

There has to be a closed loop between the atomistic portion of the simulation and the higher-level parts, guaranteeing a seamless integration. This convergence between material and device studies also implies that a much more interdisciplinary approach than in the past is needed, with close integration between chemistry, physics, engineering, and, in a growing number of cases, biology. To make an example, let us consider the simulation of a silicon nanowire transistor: atomistic calculations are needed to determine the specific electronic structure for the cross-section of the device being investigated, then this information can be used in a full-band solver for transport or parameters can be extracted for a simpler and faster transport analysis neglecting interband tunneling; then the obtained device characteristics can be used for the definition of a higher-level model useful for circuit analysis. It is apparent that, for example, the atomistic simulation is directly dependent on the device geometry, and that, therefore, work on the different parts of the simulation hierarchy has to be performed by the same group or by groups that are in close collaboration. Indeed, the dependence between results at different length scales sometimes requires the combination of different techniques in the same simulation, not just the use of information from more microscopic descriptions to provide parameters for mesoscopic or macroscopic models. Following the previous example, the electronic properties of a silicon nanowire are largely determined by its geometry. However, the geometry of the wire is determined by the strain present in the region where it grows, which in turn is a function of the whole geometry of the device, its temperature and the mechanical constraints applied to it. Thus, a reliable simulation of such device can require, for example, a quantum mechanical description of the nanowire itself, coupled to a larger portion of material described using empirical interatomic potentials, and everything embedded in an even much larger region described using continuum elastic theory. Although still at its infancy, this kind of multi-scale simulations has already been applied very successfully to the study of quite different systems, like biological molecules, crack propagation in mechanical engineering or combustion processes [37, 38]. This is certainly one of the most promising routes towards the simulation of realistic devices.

Another example where multi-scale and multi-physics simulations become essential is represented by the effort to merge electronics with nanophotonics**.** The integration of CMOS circuits and nanophotonic devices on the same chip opens new perspectives for optical interconnections (higher band widths, lower-latency links compare with copper wires) as well as for the possible role of photons in the data processing. These involve the modelling of “standard” passive components, such as waveguides, turning mirrors, splitters and input and output couplers, as well as active elements, such as modulators and optical switches. Modelling of ultra-scaled optoelectronic components involve the design of nanometer scale optical architectures with new properties that may differ considerably from those of their macroscopic counterparts.

This requires the development of new numerical tools able to describe electromagnetic interactions and light propagation at different length scales. They should be able to describe the electromagnetic field from the scale of a few light wavelengths (already of the order of the whole micro-device) down to the nanometer scale elements. These new tools should include a realistic description of the optical properties including electro- and magneto-optical active nanostructures and plasmonic elements which are expected to be key ingredients of a new generation of active optoelectronic components.

A mayor challenge of the “multi-physical” modelling will be to simulate a full nano-device where electronics, mechanics and photonics meet at the nanoscale. For instance, the coupling between mechanical vibrations and quantum conductance of single nanotubes has been recently observed. The interaction of an optical field with a device takes place not only through the electromagnetic properties, but also through the mechanical response (radiation pressure forces). The physical mechanisms and possible applications of optical cooling of mechanical resonators are being explored. Modelling Nano-Electro-Mechano-Optical (NEMO) devices is going to play a key (and fascinating) role in the development and optimization of new transducers and devices.

There are several examples, in the recent history of electron devices, in which physics-based modeling has played an essential role in pointing out new avenues for research or in explaining unexpected phenomena. One interesting example, which has had also important important consequences in terms of applications, is that of the prediction of much improved tunneling magnetoresistance (TMR) of magnetic tunnel junctions. Up to a decade ago, the achieved values of TMR in structures with ferromagnet-dielectric-ferromagnet were at most around 70%, because of the amorphous nature of the dielectric layer. Accurate first-principles calculations [39] made it possible to predict that with crystalline dielectric layers the tunneling process was much more complicated than the previously used simple barrier model, because of the relevance of the symmetry of Bloch states at the Fermi energy and the effect on wave function matching of interfacial resonance states. These results triggered experimental activity aimed at improving the quality of the growth process for the dielectrics and to the actual measurement of the predicted high TMR values [40,41]. The resulting magnetic tunnel junctions have found a very important field of application in the readout heads for hard disks, allowing an unprecedented increase in the information density on a magnetic substrate and represent the building block of magnetic memories, which are likely to be one of the main technologies of the future in the market of non-volatile storage. This further demonstrates the importance of simulation codes that can provide quantitatively reliable estimates of the parameters of interest, instead of approximate models.

6. Carbon-based electronics and spintronics

Amongst the most promising materials for the development of beyond CMOS nanoelectronics, Carbon Nanotubes & Graphene-based materials and devices deserve some particular consideration. Indeed, first, their unusual electronic and structural physical properties promote carbon nanomaterials as promising candidates for a wide range of nanoscience and nanotechnology applications. Carbon is unique in possessing allotropes of each possible dimensionality and, thus, has the potential versatility of materials exhibiting different physical and chemical properties. Diamond (3D), fullerenes (0D), nanotubes (1D-CNTs), 2D graphene and graphene ribbons are selected examples. Because of their remarkable electronic properties, CNTs or graphene-based materials should certainly play a key role in future nanoscale electronics. Not only metallic nanotubes and graphene offer unprecedented ballistic transport ability, but they are also mechanically very stable and strong, suggesting that they would make ideal interconnects in nanosized devices. Further, the intrinsic semiconducting character of either nanotubes or graphene nanoribbons, as controlled by their topology, allows us to build logic devices at the nanometer scale, as already demonstrated in many laboratories. In particular, the combination of 2D graphene for interconnects (charge mobilities in graphene layers as large as 400.000 $cm^2V^{-1}s^{-1}$ have been reported close to the charge neutrality point) together with graphene nanoribbons for active field effect transistor devices could allow the implementation of completely carbon-made nanoelectronics.

Besides the potential of 2D graphene and GNRs for electronic device applications, transport functionalities involving the spin of the carriers have very recently received a particularly strong attention. First, although spin injection through ferromagnetic metal/semiconductor interfaces remains a great challenge, the spectacular advances made in 2007 converting the spin information into large electrical signals using carbon nanotubes [42] has opened a promising avenue for future carbon-based spintronic applications. The further demonstration of spin injection in graphene [43] and the observation of long spin relaxation times and lengths [44] have suggested that graphene could add some novelty to carbon-based spintronics. For instance, taking advantage of the long electronic mean free path and negligible spin-orbit coupling, the concept of a spin field-effect transistor with a 2D graphene channel has been proposed with an expectation of near-ballistic spin transport operation [45]. A gate-tunable spin valve has been experimentally demonstrated [46]. Finally, a ferromagnetic insulator, such as EuO, may be used to induce ferromagnetic properties into graphene, through the proximity effect [47] and also to control the spin polarization of current by a gate voltage [48, 49]. This configuration does not make use of any ferromagnetic metallic contact to inject spin-polarized electrons. Thus, it could be a way to circumvent the problem of "conductivity mismatch" [50-52] which possibly limits the current spin injection efficiency into a conventional semiconductor from a ferromagnetic metal. These phenomena and the corresponding devices need to be investigated using the appropriate models of relativistic-like electron transport in 2D graphene structures. Additionally, the presence of spin states at the edges of zigzag GNRS has also been demonstrated [53-55], and may be exploited for spintronics. Using first-principles calculations, very large values of magnetoresistance have been predicted in GNR-based spin valves [56,57].

Additionally, the potential for 3D based organic spintronics has been recently suggested by experimental studies [58]. Organic spin valves have shown spin relaxation times in the order of the microsecond and spin tunnel junctions with organic barriers have recently shown magnetoresistance values in the same order of magnitude as that of inorganic junctions based on Al_2O_3. However, spin transport in these materials is basically unknown, and many groups are trying to decipher the impressive experimental complexity of such devices. Organic materials, either small molecules or polymers, will definitely allow large scale and low cost production of alternative non volatile memory technologies, with reduced power consumption. These new materials have therefore the potential to create an entirely new generation of spintronics devices, and the diverse forms of carbon-based materials open novel horizons for further hybridization strategies and all-carbon spintronics circuits, including logic and memory devices.

The performance of these spintronic devices relies heavily on the efficient transfer of spin polarization across different layers and interfaces. This complex transfer process depends on individual material properties and also, most importantly, on the structural and electronic properties of the interfaces between the different materials and defects that are common in real devices. Knowledge of these factors is especially important for the relatively new field of carbon based spintronics, which is affected by a severe lack of suitable experimental techniques capable of yielding depth-resolved information about the spin polarization of charge carriers within buried layers of real devices.

In that perspective, it is noteworthy to remark that the fantastic development of first principles non-equilibrium transport methods is progressively allowing for more and more realistic assessment and anticipation on the true spintronics potential of carbon-based structures. This aspect also stands as an essential point for providing guidance and interpretation schemes to experimental groups. As a matter of illustration, a few years ago it has been theoretically shown that organic spin valves, obtained by sandwiching an organic molecule between magnetic contacts, could manifest large bias-dependent magnetoresistance, provided a suited choice of molecules and anchoring groups was made, which is now confirmed by experiments [59].

Finally one also notes that in addition to the potential for GMR in carbon-based materials, the spin manipulation and the realization of spin Qubits deserves a genuine consideration. Recent theoretical proposals have shown that spin Qubits in graphene could be coupled over very long distances, as a direct consequence of the so-called Klein paradox inherent to the description of charge excitations in terms of massless Dirac fermions. The related challenges for device fabrication need to be observed from different perspectives. Indeed, recent experiments in ^{13}C nanotubes reveal surprisingly strong nuclear spin effects that, if properly harnessed, could provide a mechanism for manipulation and storage of quantum information.

This may help to overcome the performance limitations of conventional materials and of the conventional technology for spin valve devices. The real potential of graphene-based materials for FET and related spintronics applications thus requires advanced modelling methods, including *ab initio* techniques, and a precise description of spin degree of freedom.

To date, the development of nanotubes and graphene science have been strongly driven by theory and quantum simulation [60,61]. The great advantage of carbon-based materials and devices is that, in contrast to their silicon-based counterparts, their quantum simulation can be handled up to a very high level of accuracy for realistic device structures. The complete understanding and further versatile monitoring of novel forms of chemically-modified nanotubes and graphene will however lead to an increasing demand for more sophisticated computational approaches, combining first principles results with advanced order N schemes to tackle material complexity and device features, as developed in some recent literature [62].

7. The molecular scale and the end of the road

Molecular electronics research continues to explore the use of single molecules as electron devices or for even more complex functions such as logic gates [63]. Experimentally and theoretically the majority of research work focuses on single molecules between two metallic electrodes or on molecular tunnel junctions.

Reproducibility of the measurements and accurate predictions for currents across single molecule tunnel junctions remains a challenging task, although the results of theory and experiment are converging [64]. To achieve the goal of using molecular components for computing or storage, or indeed for novel functions, requires refinement of the theoretical techniques to better mimic the conditions under which most experiments are performed and to more accurately describe the electronic structure of the molecules connected to the leads.

Most simulations of transport in molecular junctions to date are based on the combination of the non-equilibrium Green's functions techniques with DFT calculations [65,66]. Although this approach has proven quite powerful, it also presents important shortcomings. In particular, the transport calculation is based on the Kohn-Sham spectrum as calculated using standard local or semi-local exchange-correlation functionals. These functionals usually give a reasonable description of the electronic spectrum for the normal metals that constitute the leads. However, they are known to be much less reliable to predict the energy spectrum of small molecules. This is extremely important, since the relative position of the molecular levels and the Fermi energy of the leads is crucial to determine the transport characteristic. Some of the deficiencies of DFT to describe localized levels can be corrected by including the so-called self-interaction corrections [67]. Still, the position of the molecular levels is also strongly influenced by the dynamical screening induced by the metallic leads [68,69]. An accurate description of all these effects requires more elaborate theoretical treatments, beyond standard DFT calculations. Fortunately, part of the effects of screening can be included using a simple non-local self-energy model that basically contains image charge interactions that affect differently the HOMO and LUMO levels [70].

Another interesting issue is that of the coupling of the electrons with structural deformations and vibrational modes. Within the framework of NEGF+DFT calculations inelastic effects associated with the excitation of localized vibration within the contact region have been successfully included in recent years. Most of the approaches rely on different perturbative expansions or on the so-called self-consistent Born approximation [71]. This allows for accurate simulations of the inelastic signal in molecular junctions and, therefore, the characterization of the path followed by the electrons by identifying which vibrations are excited during the conduction process. Unfortunately, the self-consistent Born approximation does not allow accounting for polaronic effects that are crucial to understand the electronic transport in flexible organic molecules [72]. In these cases more sophisticated methods are necessary, the coupling of which to ab initio DFT simulations is still an open question.

Hence much of the work to date has focused on the underlying physical mechanisms of charge transport across molecules, whereas very little is understood in terms of the use of molecular components in complex, or even simple, circuits. This research area could also be categorized as in its infancy in that very little is known about time-dependent or AC responses of molecules in tunnel junctions or other circuit environments. To exploit molecules in information processing, the use of multi-scale tools [73] as described previously are needed to embed molecular scale components between what are essentially classical objects: leads, drivers, and circuits. Further development of the simulations is needed to accurately describe the transport processes in molecular junctions and its coupling to structural degrees of freedom and, in particular, to molecular vibrations, also the time-dependent response of the molecules to external voltages and their interaction with light needs to be studied.

In single-molecule transport treatment of the leads is not well-established and difference of orders of magnitude in the current can be found among different methods. Full Configuration-Interaction is often considered to be the reference, but its application to practical devices is not currently possible, due to the almost combinatorial growth of the size of the problem with the number of particles present in the system.

In order to achieve reliable models all quantities of interest should be computed in a single consistent framework, otherwise there is a risk of having quite different physical descriptions of the various regions of a device.

Also assuming to be able to treat each domain with an appropriate model, a significant problem is represented by the description of the interface between different domains and proper treatment of the coupling. The real difficulty is about boundaries and about how to handle them fast.

Furthermore, there are several fundamental problems that are still open: for example, the integration between approaches such as DFT (which is a ground state, equilibrium theory) with non-equilibrium Green's functions.

Finally, to position a single molecule at the right place, experimental equipment has to be developed with accurate manipulation capabilities, as well as precision electrical probes for four-terminal measurements [74].

Further development of the simulation techniques is needed to describe the time-dependent response of molecules to external voltages and their interaction with light. As the size of molecules considered as a component remains quite large, adapted methods using a scattering approach seem to be more relevant than high-level NEGF or other sophisticated methods [75,76]. The concept of a molecular logic gate has emerged recently and specific approaches including quantum Hamiltonian computing [77] will be used for a numerical integration.

8. Nano-bio-electronics

A further fundamental research line which emerged in parallel to the development of molecular electronics is bio-electronics. It mainly aims at (i) mimicking of biological and biophysical processes via molecular electronic circuits, and (ii) the exploitation of self-assembling and self-recognition properties of many biomolecules as scaffolds in the integration of nano- and sub-nanoscale devices, and (iii) exploring the potential of arrays of biomolecules (like DNA and its artificial modifications) to serve as molecular wires interconnecting different parts of molecular electronic devices. Obviously, great challenges from both the experimental and from the theoretical side exist on the road to achieve such goals. The theoretical understanding of the bio/inorganic interface is in its infancy, due to the large complexity of the systems and the variety of different physical interactions playing a dominant role. Further, state of the art simulation techniques for large biomolecular systems are to a large degree still based on classical physics approaches (classical molecular dynamics, classical statistical physics); while this can still provide valuable insight into many thermodynamical and dynamical properties of biomolecular systems, a crucial point is nevertheless missing: the possibility to obtain information about the electronic structure of the biomolecules, an issue which is essential in order to explore the efficiency of such systems to provide charge migration pathways. Moreover, due to the highly dynamical character of biomolecular systems -seen e.g. in the presence of multiple time scales in the atomic dynamics- the electronic structure is strongly entangled with structural fluctuations. We are thus confronting the problem of dealing with the interaction of strongly fluctuating complex molecules with inorganic systems (substrates, etc). As a result, multi-scale simulation techniques are urgently required, which should be able to combine quantum-mechanical approaches to the electronic structure with molecular dynamical simulation methodologies dealing with the complex conformational dynamics of biological objects. Conventional simulation tools of semiconducting microdevices can obviously not deal with such situations.

9. Simulation of wide-bandgap semiconductors

The market for wide-bandgap materials is not as large as that for silicon, but they are becoming important in the growing LED market, as demonstrated by the significant interest expressed by Applied Materials, as well as in high-power, high-frequency applications.

Simulation of wide-bandgap semiconductors is a task characterized by challenges of its own, which are often quite different from those typical of modeling silicon, due to the different crystal structure, the possibility of engineering the bandgap, the variability of material properties with orientation. It is also difficult to validate the results of the simulations because such materials are often characterized by a high defectivity, which makes comparison with results for ideal materials difficult.

Furthermore large energy ranges are involved, for the particular applications of these materials, which makes calculation of many parameters difficult: for example, it is quite hard to evaluate electron-phonon scattering at 10 eV. In addition, a semiclassical model is not easily applicable, due to the complexity of the electronic structure: this is similar to problems that are becoming relevant also in silicon, in the study of nanowires. Because of the type of crystal, the phonon model is much more complex than in silicon. Also the application of standard approaches to quantum transport is rather challenging.

The typical concentration of dislocations is of 10^8 per cm^2 (a value that can in principle be reduced, but most probably not below 10^6 per cm^2) which makes it look like a miracle that devices based on such materials actually work. It is important to understand the role of extended defects in term of the optical properties and, since the defects cannot be eliminated, it is necessary to design around them, somehow including their effect into simulation tools.

In terms of the development of devices, one of the unsolved issues is to understand why p-type GaN is so hard to achieve. There is a concrete opportunity to introduce much of what the ab-initio community has been developing, in particular in terms of large-scale atomistic models.

Another relevant problem is the power density: GaN HFETs exhibit a power density that is much larger than that of conventional devices, therefore cooling techniques are an important field of research.

10. Thermoelectric energy conversion

The importance of research on thermoelectric energy conversion is growing in parallel with the need for alternative sources of energy. With the recent developments in the field, thermoelectric energy generators have become a commercial product in the market and their efficiencies are improving constantly, but the commercially available products did not take the advantage of nano-technology yet. In fact, thermoelectricity is one of the areas in which nano-scale fabrication techniques offer a breakthrough in device performances.

It was predicted theoretically that, lowering the device dimensions, it is possible to overcome the Wiedemann-Franz Law and enhance the device performances significantly [78].

Quasi one-dimensional quantum wires [79], engineered molecular junctions [80,81], superlattices of quantum dots [82] are the other possible routes proposed for achieving a high thermoelectric figure of merit, *ZT.*

The thermoelectric figure of merit includes three properties of the material, namely the electrical conductivity σ, Seebeck coefficient *S*, the thermal conductivity $\kappa = \kappa_{el} + \kappa_{ph}$ with electronic and phononic contributions as well as the temperature *T*, $ZT = \sigma S^2 T / \kappa$.

In order to optimize *ZT*, an electron-crystal together with a phonon-glass behavior is required [83].

Indeed, it has recently been shown that Si nano-wires with rough surfaces can serve as high performance thermoelectric materials, since the edge roughness suppresses phonon transport by a few orders of magnitude whereas the electronic transport is weakly affected from surface roughness in these wires. Similar behavior is also reported for graphene nanoribbons where edge disorder reduces lattice thermal conductivity while electrons in the first conduction plateau stay almost intact [84].

At the sub-band edges, however, the electronic mean free path is discontinuous which yields a large increase of the Seebeck coefficient and *ZT*. Another criteria for high *ZT* is to have a narrow distribution of the energy of the electrons participating in the transport process [85].

In molecular junctions, it is shown that the Seebeck coefficient is maximized when the electrode-molecule coupling is weak and the HOMO level is close to the Fermi energy, these fulfill Mahan's criterion in the zero-dimensional case [86]. The weak coupling condition is also in favor of the need of reduced vibrational thermal conduction. Therefore self-assembled layers of molecules between semiconducting surfaces are supposed to yield high *ZT* values.

These developments offer new challenges for increasing device performances and also for the modelling of new devices. An accurate modelling of the disordered structures or of the layered structures of self-assembled molecules between surfaces requires a lot of improvements both from the methodological and from the computational point of view. Simulation of these systems entails consideration of very large number of atoms, of the order of 10^6 to 10^8. Therefore fully parallelized order-*N* methods for both electronic and phononic computations are needed. Though important progress has been achieved in order-*N* electronic calculations, such methods are still lacking a proper description for the phonons. Adoption of the methods already developed for electrons to phonons is a first goal to be achieved.

11. Multifunctional oxides

Multifunctional oxides, ranging from piezoelectrics to magnetoelectric multiferroics, offer a wide range of physical effects that can be used to our advantage in the design of novel nanodevices. For example, these materials make it possible to implement a variety of tunable and/or switchable field effect devices at the nanoscale. Thus, a magnetoelectric multiferroic can be used to control the spin polarization of the current through a magnetic tunnel junction by merely applying a voltage; or a piezoelectric layer can be used to exert very well controlled epitaxial-like pressures on the adjacent layers of a multilayered heterostructure, which e.g. can in turn trigger a magnetostructural response. These are just two examples of many novel applications that add up to the more traditional ones - as sensors, actuators, memories, highly-tunable dielectrics, etc. - that can now be scaled down to nanometric sizes by means of modern deposition techniques. In fact, nanostructuring of different types, ranging from the construction of oxide nanotubes to the more traditional multi-layered systems, is opening the door to endless possibilities for the engineering/combination of the properties of this type of compounds, which are strongly dependent on the system's size and (electrical, mechanical) boundary conditions.

The current challenges in the field are plenty, from the more technical to the more fundamental. At the level of the applications, the outstanding problems include the integration of these materials with silicon or the identification of efficient and scalable growth techniques for complex oxide heterostructures. At a more fundamental level, there is a pressing need to identify new systems and/or physical mechanisms that can materialize some of the most promising concepts for the design of devices; for example, we still lack a robust room-temperature magnetoelectric multiferroic system that can be integrated in real devices, we still have to understand the main factors controlling the performance of a ferroelectric tunnel junction, etc. Finally, it should be stressed that the field is rich in opportunities for the emergence of novel effects and concepts that go beyond the current prospects in the general area of electronics, the recent discovery of high electronic mobilities in all-oxide heterostructures (i.e., at the interfaces between $LaAlO_3$ and $SrTiO_3$) being a remarkable example.

Quantum-mechanical simulation is playing a key role in the progress in multifunctional oxides. This has been historically the case, with many key contributions from the first-principles community to the understanding of ferroelectric, magnetic and magnetoelectric bulk oxides [87,88]. This trend is just getting stronger in this era of nanomaterias, for two reasons: (i) there is greater need for theory to explain the novel physical mechanisms at work in systems that are usually very difficult to characterize experimentally, and (ii) modern deposition techniques offer the unique chance to realize in the laboratory the most promising theoretical predictions for new materials. Thus, the importance of first-principles simulation for fundamental research in functional oxides is beyond doubt, and very recent developments, e.g. for the first-principles study of the basic physics of magnetoelectrics [89], ferroelectric tunnel junctions [90] or novel oxide superlattices [91], clearly prove it. The contribution from simulations to resolve more applied problems (e.g, that of the integration with silicon) is, on the other hand, just starting, and its progress will critically depend on our ability to develop novel multi-scale simulation methods that can tackle the kinetics of specific growth processes (from pulse-laser deposition to sputtering methods under various oxygen atmospheres) directly. This is a major challenge that will certainly generate a lot of activity in the coming couple of decades.

12. Simulation of the time-dependent behavior

Although most of the present quantum simulators provide very accurate information about the DC behavior, they are unable to reliably predict the transient, AC or noise properties of quantum devices in most practical operating conditions. There are mainly two reasons that explain why such predictions are so difficult. First, at high-frequency, one has to deal with the role of the "displacement current" that requires a reasonable approximation for the (time-dependent or frequency-dependent) Coulomb interaction among electrons [92,93]. Second, in order to compute correlations (the second or higher moments of the electrical current for instance) one has to measure at least at two different times. One has to take into account that a first measurement "collapses" the evolution of the quantum system and, consequently, it will affect the outcome of a second (or further) measurement [94].

There are some elegant theoretical proposals in the literature that show the path to include time-dependence and correlations into practical quantum simulators. Among others, we cite the work of Büttiker and coworkers, who generalized the successful (DC) Landauer [95,96] model towards current fluctuations and AC conductances [97,98,99]. The work of Levitov, Lesovik and others in the application of Full Counting Statistics in mesoscopic devices for the computation of higher moments of the electrical current [92,93,100]. Recently, a novel proposal that treats quantum transport with quantum (Bohmian) trajectories has also demonstrated its ability to provide accurate approximations for the many body problem and the computation of higher moments in time-dependent scenarios [101,102,103]. Unfortunately, because of their computational burden, these proposals have been only used to predict noise and time-dependent behavior of very simple and idealized quantum devices.

As happened for the microelectronic industry some time ago, in the next future, the nanoelectronic industry will ask for realistic predictions about the time-dependent and noise behavior of these novel quantum devices. Thus, an important effort must be done by the scientific community to develop accurate and versatile quantum simulators providing information beyond the DC predictions that are interesting enough for the nanoelectronic industry, in terms of accuracy, versatility and computational resources.

In this respect, multiscale modeling will be essential, because the time-dependent behavior of a device or circuit involves the interaction of a large number of particles (charge carriers), but at the same time is influenced by detailed quantum interactions. Therefore it requires a treatment based on a hierarchy of models, with a proper microscropic description of particle correlations, a semiclassical transport model within the potential landscape of the device, and a higher-level description for a circuit made up of more than one device.

13. New computational approaches

Although the number of transistors per unit area still follows Moore's law, i.e. it doubles every 18 months, and individual transistor dimensions are scaled down accordingly, thereby decreasing the switching delays, it is not any more possible to make classical general-purpose processors with clock frequency scaling in proportion, due to the limitations in power dissipation and heat removal.

This has halted the progressive improvement in single-CPU performance that was typical of the 1980's and 1990's, leading to a change of paradigm in the quest for ever increasing computational power, with the introduction of multi-core chips.

This type of parallelism reaches its most extreme expression Graphic Processor Units (GPUs), which are special purpose processors, originally designed for performing graphic tasks. Typically, GPUs offer a peak performance that is an order of magnitude larger than that of general purpose processors. However, not all algorithms can use efficiently this additional performance, because GPUs are designed for massive parallel vector operations.

Indeed GPUs offer large-scale parallelism at the low cost afforded by mass production; their processing units are specifically designed to perform dense matrix operations (fundamental for 3D graphic rendering), which do represent a very significant portion within many modelling codes. This means that large speedups are to be expected, and some initial tests have demonstrated factors up to 40-50.

Modern Graphic Processing Units (GPU) approach a peak performance of a Teraflop (10^{12}) floating point operations per second) thanks to a highly parallel structure and to an architecture focusing specifically on data processing rather than on caching or flow control. This is the reason why GPUs excel in applications for which floating point performance is paramount while memory bandwidth in not a primary issue.

Initially the main disadvantage was represented by the availability, in hardware, only of single-precision operations, but more recent generations of GPUs, such as the FireStream 9170 by AMD, can handle double precision in hardware, although at a somewhat reduced rate (possibly by a factor of 5). Another impressive feature of GPU computation is the extremely high energy efficiency, of the order of 5 Gigaflops/W in single precision or 1 Gigaflop/W in double precision, an aspect of growing importance considering the costs for supplying power and air conditioning to computing installations.

The latest GPU hardware opens really new perspectives for simulation of nanodevices, also in "production environments," because GPU based systems could be easily standardized and provided to end-users along with the simulation software.

The latest supercomputers are based on a well-balanced mix of GPUs and CPUs, as in the case of the new Cray hybrid supercomputer, the XK6, which will be based on a combination of multi-core AMD CPUs and NVIDIA GPUs, scalable up to 500,000 cores. OPENACC, which is being implemented into several compilers, will be operable on multiple platforms and should allow a very straightforward acceleration of legacy codes.

14. Major current deficiencies of TCAD

A clear gap, which has in part been addressed in the previous sections, has formed in the last few years between what is available in the TCAD market and what would actually be needed by those working on the development of advanced nanoscale devices. As already mentioned, classical TCAD tools have not been upgraded with realistic quantum transport models yet, suitable for the current 22 nm node in CMOS technology or for emerging technologies, and, in addition, there are some fields of increasing strategic importance, such as the design of photovoltaic cells, for which no well-established TCAD platforms exist.

Bottom-up approaches, which, if successful, could provide a solution to one of the major bottlenecks on the horizon, i.e. skyrocketing fabrication costs, are not supported by any type of TCAD tools as of now. This may be due to the fact that bottom-up approaches are still in their infancy and have not been demonstrated in any large-scale application, but the existence of suitable process simulation tools could, nevertheless, facilitate their development into actual production techniques. Sophisticated tools that have been developed within research projects are available on the web, mainly on academic sites, but they are usually focused on specific problems and with a complex and non-standardized user interface.

Atomistic simulations are becoming a relevant part of device modelling, but there exists a discrepancy between what the industry actually needs and what is being provided by the academia. The industry would like to have fast models, that quickly provide answers, while the academia has developed very advanced models, which are on the average slower than previous, less sophisticated, tools, and require much more CPU power. A partial solution to this specific problem is represented by the new hardware which has become available, such as that based on GPUs, which in the near future could make advanced models practically usable on desktop machines.

An effort would be needed to coordinate the research groups working on the development of the most advanced simulation approaches, the TCAD companies and the final users, in order to define a common platform and create the basis for multi-scale tools suitable to support the development of nanoelectronics in the next decade.

15. Overview of networking for modelling in Europe and the United States

In the United States, the network for computational nanotechnology (NCN) is a six-university initiative established in 2002 to connect those who develop simulation tools with the potential users, including those in academia, and in industries. The NCN has received a funding of several million dollars for 5 years of activity. One of the main tasks of NCN is the consolidation of the nanoHUB.org simulation gateway, which is currently providing access to computational codes and resources to the academic community. According to an NCN survey, the total number of users of nanoHUB.org reached almost 70,000 in March 2008, with more than 6,000 users having taken advantage of the online simulation materials. The growth of the NCN is likely to attract increasing attention to the US computational nanotechnology platform from all over the world, from students, as well as from academic and, more recently, industrials researchers. In Europe an initiative similar to the nanoHUB, but on a much smaller scale, was started within the Phantoms network of excellence (http://vonbiber.iet.unipi.it) and has been active for several years; it is currently being revived with some funding within the NanoICT coordinated action.

In a context in which the role of simulation might become strategically relevant for the development of nanotechnologies, molecular nanosciences, nanoelectronics, nanomaterial science and nanobiotechnologies, it seems urgent for Europe to set up a computational platform infrastructure similar to NCN, in order to ensure its positioning within the international competition. The needs are manifold. First, a detailed identification of

European initiatives and networks must be performed, and de-fragmentation of such activities undertaken. A pioneer initiative has been developed in Spain through the M4NANO database (www.m4nano.com) gathering all nanotechnology-related research activities in modelling at the national level. This Spanish initiative could serve as a starting point to extend the database to the European level. Second, clear incentives need to be launched within the European Framework programmes to encourage and sustain networking and excellence in the field of computational nanotechnology and nanosciences. To date, no structure such as a Network of Excellence exists within the ICT programme, although the programme NMP supported a NANOQUANTA NoE in FP6, and infrastructural funding has been provided to the newly established ETSF (European Theoretical Spectroscopy Facility, www.etsf.eu). This network mainly addresses optical characterization of nanomaterials, and provides an open platform for European users, that can benefit from the gathered excellence and expertise, as well as standardized computational tools. There is also a coordinated initiative focused on the specific topic of electronic structure calculations, the Psi-k network (www.psi-k.org).

An initiative similar to the American NCN would be needed in Europe, within the ICT programme that encompasses the broad fields of devices and applications or, better, in conjunction between the ICT and the NMP programme, since the full scope from materials to devices and circuits should be addressed.

16. Past, present and future European advances in computational approaches

This novel initiative should be able to bridge advanced ab-initio/atomistic computational approaches to ultimate high-level simulation tools such as TCAD models that are of crucial importance in software companies. Many fields such as organic electronics, spintronics, beyond CMOS nanoelectronics, nanoelectromechanical devices, nanosensors, nanophotonics devices definitely lack standardized and enabling tools that are however mandatory to assess the potential of new concepts, or to adapt processes and architectures to achieve the desire functionalities. The European excellence in these fields is well known and in many aspects overcomes that of the US or of Asian countries. Within the framework of a new initiative, specific targets should be addressed in relation with the modelling needs reported by small and medium sized software companies active in the development of commercial simulation tools, such as QUANTUM WISE (www.quantumwise.com), SYNOPSYS (www.synopsys.com), NANOTIMES (www.nanotimes-corp.com), SILVACO (www.silvaco.com), NEXTNANO3 (www.nextnano.de), TIBERCAD (www.tibercad.org).

Similarly, larger companies such as STMicroelectronics, Philips, THALES, IBM, INTEL make extensive usage of commercial simulation tools to design their technological processes, devices and packaging. The sustainable development of the computational simulation software industry, including innovative materials (carbon nanotubes, graphene, semiconducting nanowires, molecular assemblies, organics, magnetic material) and novel applications (spintronics, nanophotonics, beyond CMOS nanoelectronics), could therefore be crucial to foster industrial innovation in the next decade.

17. Conclusions

Recent advances in nanoscale device technology have made traditional simulation approaches obsolete from several points of view, requiring the urgent development of a new multiscale modelling hierarchy, to support the design of nanodevices and nanocircuits. This lack of adequate modeling tools is apparent not only for emerging devices, but also for aggressively scaled traditional CMOS technology, in which novel geometries and novel materials are being introduced. New approaches to simulation have been developed at the academic level, but they are usually focused on specific aspects and have a user interface that is not suitable for usage in an industrial environment. There is therefore a need for integration of advanced modelling tools into simulators that can be proficiently used by device and circuit engineers: they will need to include advanced physical models and at the same time be able to cope with variability and fluctuations, which are expected to be among the greatest challenges to further device downscaling.

In addition, as dimensions are scaled down, the distinction between material and device properties becomes increasingly blurred, since bulk behavior is not observed any more, and atomistic treatments are needed. There is therefore a convergence between material and device research, which should be reflected also in the formulation of research projects. Furthermore, new materials, such as carbon, bio-molecules, multifunctional oxides, wide-bandgap semiconductors, are emerging, with an impressive potential for device fabrication and with completely new requirements for simulation.

As devices based on quantum effects approach applications, a capability for the simulation of their time-dependent behavior becomes necessary, and, although the issue has been investigated in depth from the theoretical, fundamental point of view, no commercial-grade software tool exists yet.

A unique opportunity is now surfacing, with powerful new modeling approaches being developed and new low-cost computational platforms (such as GPUs) with an unprecedented floating point performance. The combination of these two factors makes it clear that the time is ripe for a new generation of software tools, whose development is of essential importance for the competitiveness and sustainability of European ICT industry, and which requires a coordinated effort of all the main players.

Acknowledgements

We acknowledge useful contributions, during the WG meetings and via e-mail, by Steve Laux., Thomas Schulthess, Enrico Bellotti, and Karl Rupp.

18. References

[1] Sparta is part of the Synopsys TCAD suite; http://193.204.76.120/ISETCADV8.0/PDFManual/data/Sparta.pdf
[2] Quantum3D is a Silvaco product; www.silvaco.com/products/vwf/atlas/3D/quantum3D
[3] www.nextnano.de
[4] www.tibercad.org
[5] http://public.itrs.net
[6] H. P. Tuinhout, "Impact of parametric mismatch and fluctuations on performance and yield of deep-submicron CMOS technologies," Proc. ESSDERC, pp.95-101, Florence, Italy, 2002.
[7] D. J. Frank and Y. Taur, "Design considerations for CMOS near the limits of scaling," Solid-State Electron. 46, 315 (2002).
[8] K. Takeuchi, R. Koh and T. Mogami, "A study of the threshold voltage variation for ultra-small bulk and SOI CMOS," IEEE Trans. Electron Dev 48, 1995 (2001).

[9] T. Mizuno, J. Okamura and A. Toriumi, "Experimental study of threshold voltage fluctuation due to statistical variation of channel dopant number in MOSFET's," IEEE Trans. Electron Devices 41, 2216 (1994).

[10] A. Asenov, A. R. Brown J. H. Davies, S. Kaya, and G. Slavcheva, "Simulation of Intrinsic Parameter Fluctuations in Decananometre and Nanometre scale MOSFETs," IEEE Trans. Electron Devices 50, 1837 (2003).

[11] P. A. Stolk, F. P. Widdershoven, D. B. M. Klaassen, "Device modeling of statistical dopant fluctuations in MOS transistors", Proc. SISPAD'97, p. 153, 1997.

[12] H. S. Wong and Y. Taur "Three dimensional 'atomistic' simulation of discrete random dopant distribution effects in sub-0.1 mm MOSFETs", Proc. IEDM Dig. Tech. Papers., p. 705, 1993.

[13] D. J. Frank, Y. Taur, M. Ieong and H.-S. P. Wong, "Monte Carlo modeling of threshold variation due to dopant fluctuations," 1999 Symposium on VLSI Technology Dig. Techn. Papers, p, 169, 1999.

[14] D. Vasileska, W. J. Gross and D. K. Ferry, "Modeling of deep-submicrometer MOSFETs: random impurity effects, threshold voltage shifts and gate capacitance attenuation", Extended Abstracts IWEC-6, Osaka 1998, IEEE Cat. No. 98EX116, p. 259.

[15] A. Asenov, S. Kaya and A. R. Brown, "Intrinsic Parameter Fluctuations in Decananometre MOSFETs Introduced by Gate Line Edge Roughness", IEEE Trans. Electron Dev. 50, 1254, (2003).

[16] M. Bescond, N. Cavassilas, K. Nehari, J. L. Autran, M. Lannoo and A. Asenov, "Impact of Point Defect Location and Type in Nanowire Silicon MOSFETs", Proc. 35th European Solid-State Device Research Conference (ESSDERC), 221, Grenoble (France), September 2005.

[17] A. Martinez, M. Bescond, J. R. Barker, A. Svizhenkov, A. Anantram, C. Millar, A. Asenov, "Self-consistent full 3D real-space NEGF simulator for studying of non-perturbative effects in nano-MOSFET", IEEE Trans. Electron Dev. 54, 2213, (2007).

[18] M. Ono at al. "Effect of metal concentration nonuniformity in gate dielectric silicates on propagation delay time of CMIS invertors", Proc. SSDM 2002 Nagoya, Japan, 710 (2002).

[19] J.R. Barker, J.R. Watling, "Non-equilibrium dielectric response of High-k gate stacks in Si MOSFETs: Application to SO interface phonon scattering", J. Phys.: Conference Series 35, 255 (2006).

[20] J.-C. Charlier, X. Blase, and S. Roche, "Electronic and Transport Properties of Nanotubes", Rev. Mod. Phys. 79, 677-732 (2007) [21] A.K. Geim and K. S. Novoselov, "The rise of Graphene", Nature Materials 6, 183 (2007).

[21] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, "The SIESTA method for ab initio order-N materials simulations", Journal of Physics: Condensed Matter 14, 2745(2002).

[22] S. Goedecker, "Linear scaling electronic structure methods", Rev. Mod. Phys. 71, 1085 (1999).

[23] Ordejon P, "Order-N tight-binding methods for electronic-structure and molecular dynamics", Comp. Mat. Sci. 12, 157 (1998).

[24] http://cms.mpi.univie.ac.at/vasp/

[25] www.castep.org

[26] www.crystal.unito.it

[27] http://cp2k.berlios.de/

[28] www.abinit.org

[29] www.icmab.es/siesta

[30] http://cp2k.berlios.de/quickstep.html

[31] M. Brandbyge, J. L. Mozos, P. Ordejon, J. Taylor, K. Stokbro, "Density-functional method for nonequilibrium electron transport", Phys. Rev. B 65 , 165401 (2002).

[32] A. R. Rocha, V. M. Garcia-Suarez, S. W. Bailey, C. J. Lambert, V. Ferrer, S. Sanvito, "Spin and molecular electronics in atomically generated orbital landscapes", Phys. Rev. B 73, 085414 (2006).

[33] www.quantumwise.com

[34] C. M. Goringe, D. R. Bowler, E. Hernandez, "Tight-binding modelling of materials" Reports on Progrss in Physics 60, 1447 (1997).

[35] W. Jaskólski, M. Zielinski, G. W. Bryant and J. Aizpurua,"Strain effects on the electronic structure of strongly coupled self-assembled InAs/GaAs quantum dots: Tight-binding approach", Phys. Rev. B. 74, 195339 (2006).

[36] D. Porezag, Th. Frauenheim, Th. Köhler, G. Seifert, R. Kaschner, Phys. Rev. B 51, 12947 (1995).

[37] G. Lu and E. Kaxiras, “Overview of Multiscale Simulations of Materials, In: M. Rieth and W. Schommers (eds.), *Handbook of Theoretical and Computational Nanotechnology*, vol. X, pp.1-33, American Scientific Publishers (2005).

[38] P. Vashishta, R. Kalia, University A. Nakano, B. Homan, K. L. McNesby, “Multimillion Atom Reactive Simulations of Nanostructured Energetic Materials”, Journal of Propulsion and Power 23,688 (2007).

[39] W. H. Butler, X.-G. Zhang, T. C. Schulthess, J. M. MacLaren, Phys. Rev. B 63, 054416 (2001).

[40] S. S. P. Parkin, C. Kaiser, A. Panchula, P. M. Rice, B. Hughes, M. Samant, and S. Yang, Nature Materials 3, 862 (2004).

[41] S. Yuasa, T. Nagahama, A. Fukushima, Y. Suzuki, and K. Ando, Nature Materials 3, 868 (2004).

[42] L. E. Hueso, J. M. Pruneda, V. Ferrari, G. Burnell, J. P. Valdes-Herrera, B. D. Simons, P.B. Littlewood, E. Artacho, A. Fert & N. D. Mathur, “Transformation of spin information into large electrical signals using carbon nanotube”, Nature 445, 410 (2007).

[43] M. Ohishi, M. Shiraishi, R. Nouchi, T. Nozaki, T. Shinjo, Y. Suzuki, “Spin injection into a graphene thin film at room temperature”, Jpn. J. Appl. Phys. 46, L605-L607 (2007).

[44] N. Tombros, C. Jozsa, M. Popinciuc, H. T. Jonkman, B. J. van Wees, “Electronic spin transport and spin precession in single graphene layers at room temperature”, Nature 448, 571 (2007).

[45] Y. G. Semenov, K. W. Kim, J. M. Zavada, ”Spin field effect transistor with a graphene channel”, Appl. Phys. Lett. 91, 153105 (2007).

[46] S. Cho, Y.F. Chen, M.S. Fuhrer, ”Gate-tunable spin valve”, Appl. Phys. Lett. 91, 123105 (2007).

[47] H. Haugen, D. Huertas, A. Brataas, “Spin transport in proximity-induced ferromagnetic graphene“, Phys. Rev. B 77, 115406 (2008).

[48] T. Yokoyama, “Controllable spin transport in ferromagnetic graphene junctions”, Phys. Rev. B 77, 073413 (2008).

[49] V. Nam Do, V. Hung Nguyen, P. Dollfus, A. Bournel, “Electronic transport and spin-polarized effects of relativistic-like particles in graphene structures”, J. Appl. Phys. 104, 063708 (2008).

[50] G. Schmidt, D. Ferrand, L. W. Molenkamp, A. T. Filip, B. J. van Wees “Fundamental obstacle for electrical spin-injection from a ferromagnetic metal into a diffusive semiconductor”, Phys. Rev. B 62, 4790-4793 (2000).

[51] E. I. Rashba “Theory of electrical spin-injection: tunnel contact as a solution of the conductivity mismatch problem”, Physical Review B 62, 16267-16270 (2000).

[52] A. Fert, H. Jaffrès “Conditions for efficient spin injection from a ferromagnetic metal into a semiconductor”, Phys. Rev. B 64, 184420 (2001).

[53] H. Lee, Y. W. Son, N. Park, S. W. Han, J. J. Yu, “Magnetic ordering at the edges of graphitic fragments: Magnetic tail interactions between the edge-localized states”, Phys. Rev. B 72, 174431 (2005).

[54] L. Pisani, J. A. Chan, B. Montanari, N. M. Harrison, “Electronic structure and magnetic properties of graphitic ribbons”, Phys. Rev. B 75, 064418 (2007).

[55] M. Topsakal, H. Sevinçli, S. Ciraci, “Spin confinement in the superlattices of graphene ribbons”, Appl. Phys. Lett. 92, 173118 (2008).

[56] W. Y. Kim, K. S. Kim, “Prediction of very large values of magnetoresistance in a graphene nanoribbon device”, Nature Nanotechnology 3, 408 (2008).

[57] W. F. Munoz-Rojas, J. Fernandez-Rossier and J. J. Palacios, “Giant Magnetoresistance in Ultrasmall Graphene Based Devices”, Phys. Rev. Lett. 102, 136810 (2009).

[58] V. Dediu, L. Hueso, I. Bergenti and C. Taliani, ”Spin routes in organic semiconductors”, Nature Materials 8, 707 (2009).

[59] G. Szulczewski, S. Sanvito and M. Coey, ”A spin of their own”, Nature Materials 8, 693 (2009).

[60] A.K. Geim and K. S. Novoselov, “The rise of Graphene”, Nature Materials 6, 183 (2007).

[61] A. Lherbier, X. Blase, F. Triozon, Y-M Niquet and S. Roche Charge Transport in Chemically Doped 2D graphene Physical Review Letters 101, 036808 (2008).

[62] M. Lundstrom, G. Klimeck, G.B. Adams, M. McLennan, "HUB is Where the Heart is", IEEE Nanotechnology Magazine 28, March 2008.

[63] C. Joachim, J. K Gimzewski, and A. Aviram, “Electronics using hybrid-molecular and mono-molecular devices”, Nature 408, 541 (2000).
[64] M. Galperin, M. A. Ratner, A. Nitzan, and A. Troisi, "Nuclear Coupling and Polarization in Molecular Transport Junctions: Beyond Tunneling to Function", Science, 319, 1056 (2008).
[65] Brandbyge M, Mozos JL, Ordejon P, Taylor J, Stokbro K, “Density-functional method for nonequilibrium electron transport”, Phys. Rev. B 65 , 165401 (2002).
[66] Rocha AR, Garcia-Suarez VM, Bailey SW, Lambert CJ, Ferrer J, Sanvito S, “Spin and molecular electronics in atomically generated orbital landscapes”, Phys. Rev. B 73, 085414 (2006).
[67] C. Toher and S. Sanvito,“Efficient Atomic Self-Interaction Correction Scheme for Nonequilibrium Quantum Transport“, Phys. Rev. Lett. 99, 056801 (2007).
[68] J. B. Neaton, M. S. Hybertsen, and S. G. Louie, “Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces”, Phys. Rev. Lett. 97, 216405 (2006).
[69] K. S. Thygesen and A. Rubio, “Renormalization of Molecular Quasiparticle Levels at Metal-Molecule Interfaces: Trends across Binding Regimes”, Phys. Rev. Lett. 102, 046802 (2009).
[70] S. Y. Quek, L. Venkataraman, H. J. Choi, S. G. Louie, M. S. Hybertsen, and J. B. Neaton, “Amine−Gold Linked Single-Molecule Circuits: Experiment and Theory”, Nano Lett. 7, 3477 (2007).
[71] T. Frederiksen, M. Brandbyge N. Lorente*and* Antti-Pekka Jauho*,* *“*Inelastic Scattering and Local Heating in Atomic Gold Wires”, Phys. Rev. Lett. 93, 256601 (2004).
[72] H. Ness, S. A. Shevlin, and A. J. Fisher, Phys. Rev. B 63, 125422 (2001).
[73] H. Guo, D. Martrou, T. Martrou, J. Polesel-Maris, A. Piednoir, E. Dujardin, S. Gauthier, M. A. F. van den Boogaart, L. M. Doeswijk, and J. Brügger, Appl. Phys. Lett. 90, 093113 (2007).
[74] J.S. Yang, D. Jie, N. Chandrasekhar, and C. Joachim, “UHV-STM manipulation of single flat gold nano-islands for constructing interconnection nanopads on MoS2”, J. Phys.: Conf. Series 61, 1288 (2007).
[75] S. Ami and C. Joachim, “Intramolecular circuits connected to N electrodes using a scattering matrix approach”, Phys. Rev. B 65, 155419 (2002).
[76] N. Jlidat, M. Hliwa, and C. Joachim, “A molecule OR logic gate with no molecular rectifier”, Chem. Phys. Lett. 470, 275 (2009).
[77] N. Renaud, M. Ito, W. Shangguan, M. Saeys, M. Hliwa, C. Joachim, “A NOR-AND quantum running gate molecule”, Chem. Phys. Lett. 472, 74 (2009).
[78] L. D. Hicks and M. S. Dresselhaus, Phys. Rev. B 47, 16631 (1993).
[79] A. I. Hochbaum, R. Chen, R. D. Delgado, W. Liang, E. C. Garnett, M. Najarian, A. Majumdar and P. Yang, Nature 451, 163 (2008);A. I. Y. Bunimovich, J. Tahir-Kheli, J.-K. Yu, W. A. G. Iii and J. R. Heath, Nature \textbf{451}, 168 (2008).
[80] P. Reddy, S.-Y. Jang, R. A. Segalman and A. Majumdar, Sicence 315, 1568 (2007).
[81] S.-H. Ke, W. Yang, S. Curtarolo and H. U. Baranger, Nano Lett. 9, 1011 (2009).
[82] T. C. Harman, P. J. Taylor, D. L. Spears, and M. P. Walsh, Electron. Mater. 29, L1 (2000); T. C. Harman, M. P. Walsh, B. E. Laforge, and G. W. J. Turner, Electron. Mater. 34, L19 (2005); R. Venkatasubramanian, E. Silvola, T. Colpitts, and B. O’Quinn, Nature 413, 597 (2001).
[83] G. A. Slack "CRC Handbook of Thermoelectrics", ed. D. M. Rowe, Boca Raton, FL: CRC Press (1995).
[84] H. Sevinçli and G. Cuniberti, arXiv:0908.3207.
[85] G. D. Mahan and J. O. Sofo, “The best thermoelectric”, PNAS 93, 7436 (1993).
[86] D. Nozaki, H. Sevinçli, W. Li, R. Gutierrez, G. Cuniberti, arXiv:0908.0438.
[87] K. Rabe, Ch. H. Ahn, and J.-M. Triscone, Eds., "Physics of Ferroelectrics, A Modern Perspective", (Springer-Verlag Berlin Heidelberg 2007).
[88] M. Imada, A. Fujimori, and Y. Tokura, "Metal-insulator transitions", Reviews of Modern Physics 70, 1039 (1998).
[89] N. A. Spaldin and R. Ramesh, "Electric-field control of magnetism in complex oxide thin films", MRS Bulletin 33, 1047 (2008).
[90] J. P. Velev, P. A. Dowben, E. Y. Tsymbal, S. J. Jenkins, and A. N. Caruso, “Interface effects in spin-polarized metal/insulator layered

structures", Surface Science Reports 63, 400 (2008).

[91] E. Bousquet, M. Dawber, N. Stucki, C. Lichtensteiger, P. Hermet, S. Gariglio, Jean-Marc Triscone, and P. Ghosez, "Improper ferroelectricity in perovskite oxide artificial superlattices", Nature 452, 732 (2008).

[92] L. S. Levitov, and G. B. Lesovik, Pis'ma Zh. Eksp. Teor. Fiz, vol. 55, pp. 555–559,1992.

[93] L. S. Levitov, H. Lee, and G. B. Lesovik, J. Math. Phys., vol. 37, pp. 4845–4865, 1996.

[94] M. Di Ventra, Electrical Transport in Nanoscale systems (Cambridge University Press, 2008).

[95] R. Landauer, Philos. Mag. 21, 863 (1970).

[96] R. Landauer, IBM J. Res. Dev. 1, 223 (1957).

[97] Y. M. Blanter and M. Büttiker, Phys. Rep. Rev. 336, 2 (2000).

[98] M. Büttiker, A. Prêtre, and H. Thomas, Phys. Rev. Lett. 70, 4114 (1993).

[99] M. Büttiker, Phys.Rev.Lett. 65, 2901 (1990).

[100] Yu. Bomze, G. Gershon, D. Shovkun, L. S. Levitov, and M. Reznikov, Phys. Rev. Lett., vol. 95, pp. 176601-1–4, 2005.

[101] X. Oriols, Phys. Rev. Lett. 98, 066803 (2007).

[102] G. Albareda, J. Suñé and X. Oriols, Phys. Rev. B 79, 075315 (2009).

[103] G. Albareda, H. López, X. Cartoixà, J. Suñé, and X. Oriols, Phys.

Nanophotonics
Nanophononics

Nanophotonics and Nanophononics are knowledge areas essential for the development of novel technology and products in ICT, energy, nanomanufacturing, environment, transport, health, security and several others. Photonics is recognised as a Key Enabling Technology and nanophotonics is likely to be at the base of the next wave of photonics innovation. Nanophononics is becoming more and more visible as the “energy issue” rears its head virtually in all research and development fields. In particular, heat transfer in the nanoscale is more than just thermal management since it underpins the science of fluctuations and noise, needed to develop knowledge at the system level all the way to quantum processes in biology and at the heart of information generation and transformation. Many discussions on the progress of the science and technology of both nanophotonics and nanophononics have taken and are taking place in a large number of conferences, workshops and schools. This is a first non-exhaustive attempt to condense what researchers think are priorities and hot topics in both nanophotonics and nanophononics. Among the commonly mentioned key issues in nanophotonics research is design for specific applications including a subset of generic architectures and device performance in the nanoscale. Power efficiency, both as in power management and wall plug efficiency, are also shared key issues and both are followed closely by the need of technologies and standards suitable for very large scale manufacturing. An increasing number of groups are working in various fields of nanophononics, covering modelling of phononic crystals and heat transport at macro and atomic scale. It is important to intensify the collaboration and create a more unified value chain ranging from design and modelling to heat transport calculations to experimental verification of the models. The latter requires ad

Position Paper on Nanophotonics and Nanophononics

Clivia M Sotomayor Torres
ICREA, Catalan Institute of Nanotechnology and Universitat Autonoma de Barcelona (Spain)
Jouni Ahopelto
VTT Technical Research Centre of Finland (Finland)

Executive Summary

Nanophotonics and Nanophononics are knowledge areas essential for the development of novel technology and products in ICT, Energy, nanomanufacturing, environment, transport, health, security and several others. Photonics is recognised as a Key Enabling Technology and nanophotonics is likely to be at the base of the next wave of photonics innovation. Nanophononics is becoming more and more visible as the "energy issue" rears its head virtually in all research and development fields. In particular, heat transfer in the nanoscale is more than just thermal management since it underpins the science of fluctuations and noise, needed to develop knowledge at the system level all the way to quantum processes in biology, and is at the heart of information generation and transformation.

This latest NANOICT project position paper complements on the nanophotonics part, those previously published by the MONA and PhOREMOST projects and the recent one by the Nanophotonics Europe Association. It is probably the first one of its kind in the nanophononics field.

Concepts and technologies provide a base for the research topics in this document. In particular, scalable nanofabrication methods are presented, such as III-V semiconductor growth on Si, nanoimprint lithography, roll-to-roll printing and self-assembly, as potential enabling technologies in future value chains.

Cost and thermal management issues in nanophotonics appear as main concerns as far as integration and packaging is concerned. These are recognised as becoming acute problems when going to the nanoscale and much of the heat transport science in the nanoscale is still at the basic research stage. Nevertheless, as progress is being made towards heterogeneous integration using nanoparticles and nanoscale materials, both issues acquire an urgent dimension in time if Europe will remain a main player in the next and (next+1) technology generations in ICT.

As the feature size goes from micrometres to nanometres, variability arising from several factors becomes crucial to reliability. Thus, concepts developed in adaptive integration approaches, would control the impact of

variability even during operation of optical circuits. Likewise, the missing link in Si photonics, namely a Si-based source, is closer than ever to meet the challenge of integration and performance. Special materials and nanostructuring techniques, aided by advanced and computation-intensive design, are seen as paramount to control the distribution of optical energy in nanoscale energy devices, metamaterials and non-linear nanophotonic structures to make photon management a reality.

Nanophononics forms a relative new research field, although related research topics tackling problems at macro scale have been around for some years. With reducing dimensions, understanding of thermal phenomena at microscopic level is becoming more and more important and new approaches are needed for modelling and simulations and for experimental methods. For example, thermal management at packaging level may not be enough for IC's in near future. Instead one has to solve heat dissipation related problems at device level, including fluctuations and non-linear phenomena. Thus, there is a need to amalgamate the currently somewhat fragmented activities and strengthen the research in of nanophononics in Europe.

Recommendations

1) Targeted European-level support for *fundamental research in application-relevant nanophotonics and nanophononics focusing first on common issues*, for example, heat dissipation at component level, using noise in ICT and ways to cope with the fluctuations in key parameters. The latter bound to be a more serious issue in the nanoscale than in the current micrometre scale but crucial for heterogeneous integration.

2) Bring together the experimental and theoretical communities of phonon physics, heat transfer (mechanical) engineering, statistical physics, biology (fluctuations), nanoelectronics, and (solid-state) quantum communications to start with a *focused research programme on heat control in the nanoscale* in the first instance and on, e.g., *harvesting fluctuations* as a follow-on or parallel focus.

3) A research infrastructure for *emerging cost-efficient nanofabrication methods* jointly with a multi-level simulation hub and a comprehensive nanometrology associated laboratory targeting nanophotonics and nanophononics applications, complementing the Si and the III-V photonic foundries. This infrastructure could then evolve into a potential foundry, with industrial participation, covering combinatory lithography, cost-analysis, packaging and training.

4) Targeted European-level support for research on *material sciences* to develop techniques able to achieve material control at the sub-nanometre and, in particular, in 3-dimensions. This includes, e.g., control of multilayer thickness of silicon-rich silicon oxide and of the barrier dielectric at the wafer scale level.

Foreword

This position paper is the result of an informal consultation among the contributing scientists, who acted on their personal capacity. It originates in the activities and discussions of the EU project NANOICT (www.nanoict.org) in the working groups Nanophotonics and Nanophononics.

On the nanophotonics part, discussions stared early in 2002 when it became known that the European Commission would be calling for a new “instrument” in FP6, the Networks of Excellence (NoE). Researchers then working in nanophotonics became members of several related networks, going through expressions of interests, full proposals and then the execution of the project themselves. One of them was the NoE “Nanophotonics to realise molecular scale technologies” (PhOREMOST) (www.phoremost.org). PhOREMOST started its discussion in 2002 preparing its expression of interest. The NoE was active from October 2004 until December 2008, when it evolved into the Nanophotonics Europe Association (www.nanophotonicseurope.org). A similar development took place with the NoE on Metamaterials which evolved into the virtual institute METAMORPHOSE.VI (www.metamorphose-vi.org).

Concerning nanophononics, an informal meeting was held in October 2005 at Commission’s premises with representatives of the NMP and ICT, including ICT FET) priorities and the participation of Jouni Ahopelto (VTT), Clivia M Sotomayor Torres (then UCC Tyndall National Institute) and Bruno Michel (IBM Zuerich). This and other follow up initiatives, such as workshops and stimuli from outside Europe, helped to trigger the ICT FET proactive initiatives Towards Zero-Power ICT and MINECC. Among such contributing events and reports one can highlight the International Workshop on the Future of Information Processing Technology edition 2005 [1], the report of the USA Semiconductor Research Council (SRC) to the MEDEA/ENIAC workshop in Montreux held on 22nd September 2006 [2], which had phonon engineering among the top five most important research priorities for the SRC, and others.

Many discussions on the progress of the science and technology of both nanophotonics and nanophononics have taken and are taking place in a myriad of conferences, workshops and schools. In Europe we count with the series of the School Son et Lumiere [3], the conference series Eurotherm [4], the CA ZEROPOWER [5] and more recently with the workshops on Phonons and Fluctuations [6] among others.

This is a first non-exhaustive attempt to condense what researchers think are priorities and hot topics in both nanophotonics and nanophononics. Nevertheless, the views expressed here have been distilled from those of the contributors and are the sole responsibility of the editors.

We thank our colleagues and hope this paper is one step towards strengthening the European Research Area.

Clivia M Sotomayor Torres (Barcelona)
Jouni Ahopelto (Espoo)
December 2011

1. Introduction

The NANOICT Coordination Action Nr. 216165 [7] has as one of its missions to document the state of the art and trends in research areas related to the overlap between nanoscience and nanotechnology in ICT. It does so by gathering and publishing position papers in several areas, namely, nanowires, MEMS, carbon nanotubes, molecular electronics, theory, graphene and simulation, among other. All of which can be found in the project website.

At the start of NANOICT research areas such as nanophotonics had a smaller profile than, for example, MEMS/NEMS or nanoelectronics. Some even did not even have a name, such as nanophononics. The situation has changed dramatically since then, calling for a position paper on nanophotonics and nanophononics.

This is an attempt to document not so much the precise state of the art, but the scientific questions or key issues and the trends in some areas of both, nanophotonics and nanophononics. In nanophotonics, two examples of scholarly work are recommended: one by S. Gaponenko [8] and the other by Novotny and Hecht [9].

There have been a few recent reports covering areas of nanophotonics. One of these is the EU project MONA, which published a Roadmap on Nanotechnology and Optics [10] published in 2007. This was complemented by the roadmap of the EU Network of Excellence "Nanophotonics to realise molecular-scale technologies" (PhOREMOST) entitled "Emerging Nanophotonics", published in 2008 [11]. Last November, the Nanophotonics Europe Association [12] (NEA) organised a Foresight exercise and the outcome was published as "Nanophotonics a Foresight Report" [13].

Why a position paper of nanophotonics and nanophotonics?

From the perspective of the editors, there is a need to consider some questions: What has been developed in these fields and to what level of maturity? What area has a higher probability of making an impact in the 5 to 15 year scale needing nanostructuring and nanopatterning down to controlled 10 nm feature sizes? Which are the potentially scalable nanophotonic technologies suitable for industrial production? Which will contribute to make a reality the ambition of photonics as a key enabling technology in a measurable time scale?

To date there is no public roadmap in nanophononics and yet a range of issues at the forefront of research in nanoelectronics, photonics, information technology, signal processing, depend heavily on phonon-mediated interactions.

Indeed, nanophotonics and nanophononics are closely related as we will show in the next pages and is the reason for combining these two topics in a single position paper.

To start with, the possibility to control heat transport by light has been demonstrated by Meschke et al. [14] who showed that at low temperatures in solids heat is transferred by photon radiation and the thermal conductance approaches the unique quantum value G_Q of a single channel. They studied heat exchange between two small pieces of normal metal, connected to each other only via superconducting leads, which are ideal insulators against conventional thermal conduction.

Mechanical vibrations have been recently coupled to photons in optomechanical crystals, leading to greatly enhanced light-matter interactions and facilitating new sensing applications and signal processing approaches [15].

Mediated by careful design of band structures and density of states, the possible light-heat interaction points to a challenging and promising approach to handle information in nm-scale heterogeneous integration, where the matching of otherwise different length scales is enabled using, for example, plasmonic antennas.

In the language of ICT, the information is carried by state variables, charge, photons and other quasi-particles called state variables or "tokens" [16]. Tokens are exchanged in information processing operations and they do not have to be the same. They can be fermions or bosons or have mixed-character.

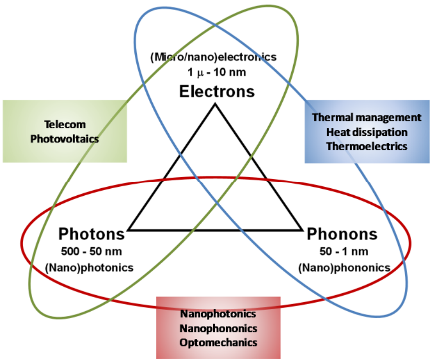


Figure 1. State variables for information processing. The length scales in the diagram also reflect the dimensions needed to manipulate the particles/waves.

It is broadly agreed that photonics cuts across several fields and the same holds for nanophotonics. Photonics is an intrinsic part of More than Moore and Heterogeneous Integration as in the ENIAC Strategic Research Agenda and now the Vision, Mission and Strategy document [17]. In fact, the National Science Foundation workshop series documented in the Nanotechnology 2011-2020 report [18] included nanophotonics in the sections on Nanophotonics and Plasmonics, Metrology, Energy and Nanoelectronics.

Europe enjoys a strong, but not necessarily leading, position in nanophotonics and nanophononics, but the situation is precarious in view of the strong initiatives elsewhere, such as the USA multibillion dollar programs on Centers of Excellence in Basic and in Applied Energy Research. Europe is strong in some research areas including Si photonic integrated circuits (PICs), metamaterials, nanofabrication and nano-scale thermal transport, but the link to the value chain is at best weak since crossing the “valley of death” still has a very low success probability. It is expected that having Photonics labelled as a Key Enabling Technology [19], and the growing number of interaction among interdependent Technology Platforms, will improve the situation. The same is not so obvious in the fragmented academic research.

The academic communities are relatively well established and galvanised around, eg, the European Technology Platform Photonics 21 and the national mirror platforms, several networks of excellence, research infrastructure consortia and associations, eg, METAMORPHOSE VI, NEA; also in professional organisations such as the European Optical Society (EOS), to name but a few. Exciting new developments with a tremendous potential, mainly at conceptual level, eg., in transformation optics [20], need to be tested for the possibility of becoming a technology.

Activities, mainly academic at the moment, in nanophononics include the recently established network on "Thermal Nanosciences and Nanoengineering", led by Sebastian Volz, summer school Son et Lumiere community, Eurotherm meetings and ESF Network on Statistical Physics. Few recent ICT FET projects in FP7 have been addressing nanophononics related issues, including the CA ZeroPower, which focuses on energy harvesting. The integrated Project NANOPACK in FP7 also partially covered nanophononics. Altogether, a fragmented community which, while advanced in its specific areas, does not yet appear as a cohesive community like nanoelectronics and nanophotonics.

We conclude this document with recommendations concerning the research areas included in this report.

2. Concepts and technologies

2.1 Concepts

The main concept in common is the wave picture of photons and phonons in a finite or semi-infinite media. In reality these media can be periodic or semi-periodic and be described in reciprocal space in terms of Brillouin zones and energy bands. The dependence of these bands as a function of wavevector is called dispersion relation of the photon or phonon in that medium. The realisation of artificial nanostructures and or layered material to tailor the dispersion relations is termed dispersion relation engineering. Random nanostructures offer also advantages in novel nanophotonics as will be seen below.

The significance of dispersion relation of electrons and photons in solids as far as device-relevant properties are concerned is associated with the material properties directly related to these dispersion relations, including the effective mass, group velocity, band gaps and ultrarefractive (slow wave) properties.

Dispersion engineering has made major advances including, a significant reduction of optical losses, now down to a few dB/cm, and the understanding of a number of exciting demonstrations of nonlinear effects (see 3.5). The key advantage of the nanophotonic approach is the ability to balance material and structural dispersion in an intelligent way, allowing to control either a very large bandwidth, e.g. for supercontinuum generation [21] or a very small bandwidth for cavity-enhanced nonlinear optics, as in the project LECSIN.

Concepts belonging to solid state physics, optics, mechanics, statistical mechanics, non linear physics, quantum optics and chemical physics, among others, are brought in to use localisation, confinement, cavities or resonators, waveguiding, etc., in most of the applications of photons and, in the future, phonons in practical devices and systems.

2.2 Nanofabrication methods as enabling technologies

In Europe there are consortia which have over the years successfully achieved the setting up of a Silicon photonics platform [22] and a III-V, specifically InP, Components and circuit platform [23] accessible to academic groups, research organisations and SMEs.

It is argued that the key contribution to be made by “nano” is the reduction in switching power. Typical microphotonics achieves pJ/bit, whereas nanophotonics can do fJ/bit. It can be safely argued that power reduction is what drives the entire field.

While the Si and III-V foundries include growth, design, material and device characterisation, processing of devices and sometimes full circuits, there is one gap and that is in packaging. Information on their activities and research activities is in the respective project web pages.

Moving to integrated III-V semiconductors on Si an example is given below on the work at KTH. Since growth methods of Si and III-V separately are well documented and since the top-down nanofabrication as well, in this section we include less well known nanofabrication methods which have been singled out because of their promise and existing demonstrators.

III-V on Si for Si nanophotonics

This is an example of III-V growth on Si based on nanopatterning and selective area growth (SAG). Many electronics providers incorporate photonics to widen applications in several sectors. Hitherto bonding of III-V devices on Si has been successfully demonstrated for integrated silicon photonics. But the industries realize that in the long run heteroepitaxial solutions will be essential. This also would lead to innovative research in the field of generic, nanoscale monolithically integrated photonics-electronics on silicon. It is expected that low cost, scalable manufacturing processes of silicon can be extended to incorporate III-Vs and other related semiconductors. Epitaxial lateral overgrowth of III-Vs on Si using nanopatterns can be one of the approaches to filter defects and obtain high quality layers. Recently, it has been demonstrated that quantum dot templates can be fabricated through SAG on Si.

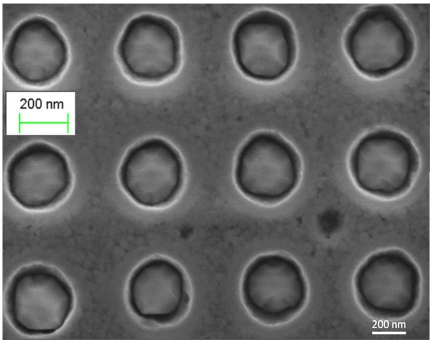


Figure 2*. InP nano-pyramid templates grown on Si at KTH through nanoimprinting and SAG [24].*

Applications: Masks for etching components, direct patterning of passive photonic components based on polymers and metals, microcavities, band edge lasers, waveguides, photonic crystals, polarisers, blue ray devices, memories, metamaterials, optofluidic and lab-on-a-chip devices, organic solar cells, diffractive optical elements, OLEDS and OFETs and anti-counterfeit structures.

Nanoimprint Lithography

Nanoimprint lithography (NIL) is a polymer patterning technique, based on a temperature-pressure cycle (thermal NIL) or a UV exposure-pressure one (UV-NIL). NIL is now used to pattern feature sizes of less than 30 nm in industrial applications for magnetic recording and diffractive optical devices, while structuring polymer films down to the 10 nm level has already been reported [25]. NIL is a radiation-free mask fabrication for pattern transfer and for directly patterning polymer, plain or functionalised, thus functionalising via material choice and patterning. It is a parallel or step-and-print technique which lends itself for volume production. Using appropriate overlay and stacking techniques, multiple layers can be processed. Furthermore, overlay accuracy down to 30 nm has been achieved using Moiré interferometry.

In the context of nanophotonics, patterning 2-dimensional photonic crystals in polymers loaded with light emitting centres close to a patterned metallic layer, has shown enhancement in the light extraction efficiency larger than a factor of 10, compared to unpatterned metal-free polymer films doped with emitting centres. This effect has been explained by a coupling effect of plasmons and excitons [26]. The possibility to realise 3-dimensional patterns is currently undergoing intense investigation. One major achievement has been the printing of 300 mm wafers using UV-NIL with a throughput of 20 wafers per hour, cf. 80 wafers/hr in the semiconductor industry [27].

Applications: Masks for etching components, direct patterning of passive photonic components based on polymers and metals, microcavities, band edge lasers, waveguides, photonic crystals, polarisers, blue ray devices, memories, metamaterials, optofluidic and lab-on-a-chip devices, organic solar cells, diffractive optical elements, OLEDS and OFETs and anti-counterfeit structures.

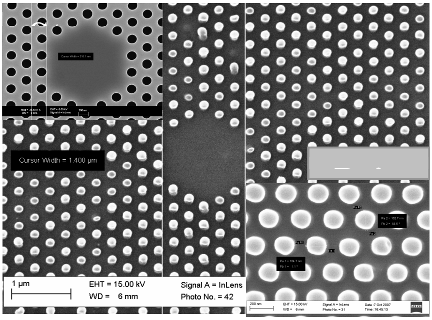


Figure 3. SEM micrographs of stamps and prints of a polymer microcavity. The stamp (top left) is a triangular array of holes with a pitch of 300 nm and hole diameters of 180 nm. The imprints were made on dye doped polymers. © V. Reboud (ICN, CEA LETI), to be published.

Roll-to-Roll nanoimprinting

Recent nano manufacturing technology has advanced to the stage where inexpensive printing of high-performance devices on continuous rolls of polymer-based substrates promises to revolutionize advanced manufacturing. Roll-to-roll (R2R) processes will make it possible to generate high value-added technology products economically, at meters-per-minute rates on plastic film, paper and foil achieving feature sizes as small as 10 – 100 nm over areas containing millions of identical devices. In fact, R2R manufacturing of optical and electronic devices is increasingly progressing from the laboratory to the factory floor. For example, the potential of roll-to-roll nanoimprinting (R2RNIL) has been demonstrated in, e.g., fluidic devices, display illumination devices and printed electronics. A recent development is the production of transparent conducting electrodes using graphene for touch-screen panels by R2R [28] in a web of 30 inches. Feature sizes of 100 nm can easily be reached when a flexible mould is used in continuous R2RNIL as a part of the manufacturing process [29].

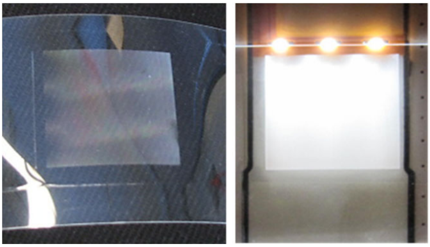


Figure 4. Optical micrographs of roll-to-roll nanoimprinted, transparent 3 cm x 3 cm size backlight device. The device consist more than 60 000 optical binary grating elements. The quality of elements influence directly the light diffraction of the device and therefore excellent edge quality is needed (T. Mäkelä et al, VTT Microsystems and Nanoelectronics, to be published).

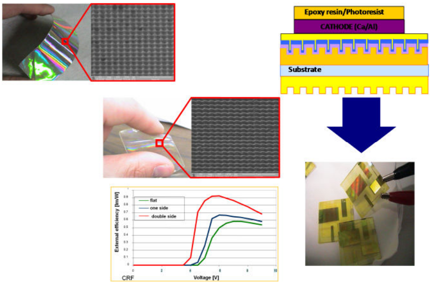


Figure 5. An example of a double-sided printed OLED structure with feature sizes below 1 µm consisting of a high efficiency LED with substrate patterned on both sides by roll-to-roll and NIL The device exhibited 65% external efficiency. (V Lambertini, T Mäkelä and C Gourgon, unpublished data).

Many nano-applications, such as OLED, TFT, nanofluidic device and protein patterning have been proposed [30] and are the target devices for R2R nanomanufacturing, and while low-cost fabrication of anti-reflection films has been demonstrated [31], a high volume manufacturing methods is still needed.

Interest in R2R is also becoming strong in other countries: In the USA, a recent workshop on Roll-to-roll technologies and prospective applications took place last September where bottleneck and applications were discussed among academic, industrialist and government agencies [32].

Applications: Low-cost manufacturing, displays, optical sensors, sensing, fluidics, solar cells, photovoltaics, diffractive and plasmonic nanostructures, touch-panel screens.

Self-assembly

Self-assembly techniques are researched as alternative to electron-beam lithography and interference lithography. They have been identified as a research need in the ENIAC SRA 2007 [33] but were absent in the Multi-annual Plan of the ENIAC Joint Undertaking [34], reflecting that self-assembly is a research area with applications envisaged beyond the five-year time frame.

Scalable self-assembly combined with soft lithography has been shown to produce several cm square of ordered nanoparticles in monolayers as well as in patterns [35]. This has been taken to the limit of nanoparticle printing with single nanoparticle resolution in well specified sites [36].

The use of silicon patterned substrates to engineer the capillary flow has resulted in the self assembly of 3-dimensional photonic crystals in a process which is fully scalable and compatible with silicon fabrication [37]. Efforts towards developing methodology as a measure of quantitative order have been demonstrated [38].

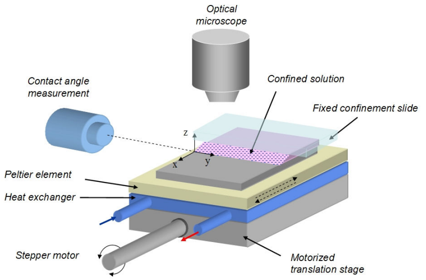


Figure 6*. Illustration of the experimental setup developed for controlled convective and capillary assembly of particles on surfaces. The assembly is performed by dragging the liquid meniscus of a colloidal suspension droplet between a fixed slide and a moving substrate actuated by a stepper motor. The temperature of the substrate is controlled by a Peltier element. (after ref 35 © American Chemical Society 2007).*

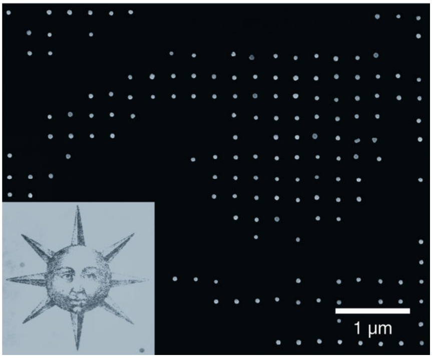


Figure 7*. Optical micrograph (inset) and SEM image of 60 nm Au nanoparticles positioned by capillary assembly and transferred to a silicon wafer (after [40] © Macmillan 2007).*

Recent development in self-assembly include directed self-assembly of di-block copolymers in order to reach the sub 20 nm size regime. The FP7 project LAMAND [39] investigates the use of this nanofabrication approach for scalable high resolution nanopatterning for ICT.

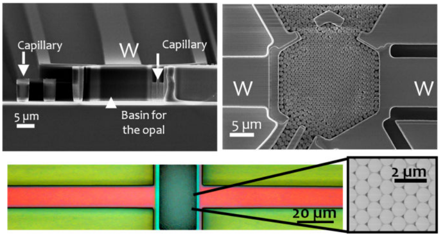


Figure 8. Top left: Cross-sectional view of the capillary channels entry points. Top right: Sub-micrometre spheres deposited using capillary forces in an optimised pattern in a basins and waveguides fabricated in Silicon. Bottom: Waveguide and 3D photonic crystals by self-assembly © S. Arpiainen and J. Ahopelto, VTT. Further details in reference 37 (Arpianen et al).

Applications: heterogeneous integration, opto-biotechnology, environmental sensor, medical sensors, artificial nano-scale materials, bio-circuits, energy harvesting, artificial tissues and organs, high resolution lithography.

2.3 Conclusions

Novel concepts in nanophotonics have been slow to appear as commercial products and probably the main reason is the long and hard way denoted by Photonics21 as the "valley of death". Sophisticated concepts carry with them special terminology which is poorly understood outside a small circle of specialists who, in addition, interact little with the rest of actors in other parts of the value chain. An effort is needed in making as realistic as possible projections of these new concepts so that targeted programs can be set up. An invaluable European asset is the creativity of a large nanophotonics community in Europe working in photonic crystals, nanoplasmonics, non-linear optics and metamaterials, to name but a few.

Concerning nanofabrication technologies, the emphasis in cost is balanced by the improved performace of nanophotonic structures and, in the future, of nanophononic ones.

In general, they all need high resolution lithography, be electron beam or deep UV lithography at some stage. These are already used in the Si and III-V photonics foundries in work to prove and up-scale device and circuit concepts and architectures. They are also needed for stamp (mould) fabrication of masters for UV and thermal NIL, R2R and directed self assembly [41], which offer the versatility needed in heterogeneous integration, among others. One way to lower costs is to improve master replication for these techniques and research in new materials and methods for this are essential. Completing the value chain in Si and III-V nanophotonics must consider the ability to test a set of generic packaging concepts when fabricating devices, an area of research activity which will need serious investment in such platforms, perhaps co-financed by stake holders.

A common research need in nanofabrication for nanophotonics and nanophononics is encompassed under the field of dimensional (nano)metrology. The importance of this cannot be over emphasised: nanometrology [42] is the link to test the validity of simulations and critical dimensions needed for a specific function. Nanometrology is an ubiquitous factor defining the uptake of a new product and or technology. But the dimensional nanometrology methods and tools have to be non-invasive, cost efficient and have the capability of being used in-line, use efficient data file size, since these have to be transferred quickly across a factory platform for measures to be taken in case of unacceptable deviations. Thus dimensional (nano)metrology is a key step in the way to overcome the valley of death. Once we have metrology under control, participation in European Standards bodies, and there are maybe too many, and in the Intelligent Manufacturing Systems (IMS) [43] program discussions on standards, will become an easier task.

Below some of the more specific key issues and research needs are mentioned.

Heteroepitaxy: To be useful it is necessary to achieve defect-free growth of thin III-V on Si to allow the integration of components on Si. This will need not only advanced epitaxial growth but also advanced characterisation and simulation. For advanced heteroepitaxy large area nanopatterned substrates are perceived as a bottleneck but perhaps NIL and interference lithography can meet this need.

Nanoimprint lithography: The bottleneck is the cost of stamps and stamp wear. While the former could in principle be solved by stamp replication, the latter needs chemical treatments and or new materials developments to allow 1000s of prints without changing an anti-adhesive coating on the stamp. Work is still needed in nanorheology and in improving our understanding of demoulding forces for a rich variety of designs [44]. For this time-efficient simulations are needed [45]. One of the most promising research areas if combinatory nanofabrication, for example combining NIL and or flexoprinting and or gravure and self-assembly, which will enable much progress in heterogeneous integration.

Roll-to-Roll printing: Going to sub 20 nm feature size and or alignment accuracy remains a huge challenge, specially the alignment procedures which, as part of quality and yield process control, constitute a go-no go type of milestone. For this, in-line metrology is required with application-defined tolerances to print complete devices on a platform. Furthermore, registration of multiple layers on flexible substrates is another milestone.

Self-assembly: Since this method uses liquids, although not in all its variants, control of convection forces and surface energy is an important issue. Moreover, quantification of order and metrology is required here, in addition to dimensional, chemical and biological metrology, depending on the nature of nanoparticles or moieties being assembled. While some routes are envisaged for dimensional metrology down to 3 nm, biological and chemical metrologies lag significantly behind. Methods to ensure and control ordering by, e.g., use of external fields [46] are likely to help achieving high levels of order in self assembled structures. The control of classical and quantum fluctuations inherent in liquid processes is an area of research which is wide open and has probably the highest return in process know-how. Last but not least, the scalability of self-assembly as a nanofabrication technology remains to be demonstrated.

3. Nanophotonics

While this is a position paper on European research it is helpful to look at other attempts to prioritise research in nanophotonics. One of this was the EU-NSF Workshop on Nanotechnology 2020 (nano2), which took place in Hamburg in June 2010, one of the four global workshops organised by the NSF and the NNI. The conclusions of the Photonics and Plasmonics session came up with the following important applications and goals for 2011-2020:

- The all-optical chip
- Metamaterials operating in the visible
- Single-(bio)molecule detection
- Artificial photosynthetic systems for energy conversion

One point emphasised several times was that progress will depend on key access to state-of-the-art computational tools, optical and structural characterisation tools and 1 nm precision nanofabrication.

In this section we focus on topics which have been left out or treated briefly in other position papers.

3.1 Integration of nanophotonics in Si Photonic circuits

In Europe the integration of photonics into silicon technologies is pursued within European, national and industry-led, projects, by researchers at universities, research organisations and few SMEs. There are several approaches to integrate Si nanophotonics in photonic integrated circuits. Two examples are those of IBM and of the University of Ghent/IMEC. Luxtera, ST Microelectronics and Intel, among others have their own approaches. In the IBM concept, routers based on ring oscillators [47] have been proposed, while the IMEC/Ghent approach is less explicit about the work-horse of the optical layer but contains the key layers of thermal, electronic, photonic and sensing functions.

In what follows examples will be given of research areas which have not been included in the recent NEA report or that here are presented from a different angle. Not all of them are strictly speaking nanophotonics but bring with them opportunities for nanophotonics to be deployed there.

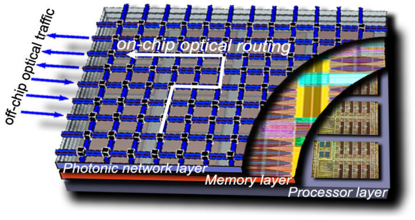
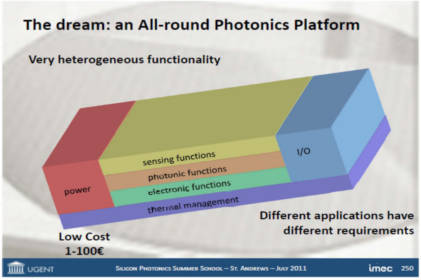


Figure 9. Artist impression of a 3D silicon processor chip with optical IO layer featuring an on-chip nanophotonic network. From: www.research.ibm.com/photonics.


The dream: an All-round Photonics Platform

Very heterogeneous functionality

Different applications have different requirements

Low Cost
1-100€

UGENT Silicon Photonics Summer School – St. Andrews – July 2011 imec 250

Figure 10. One approach to an all-optical circuit (From: W Bogaerts, Photonics Research Group, Ghent Univ - IMEC, Silicon Photonics Summer School July 2011 St Andrews).

3.2 Adaptive Integration Photonics

Heterogeneous integration technologies and miniaturization allow a wider functionality and complexity of circuits, but complexity needs control. Moving from single devices to complex photonics circuits, an overall management of all the building blocks and constitutive parts is mandatory, especially in view of the convergence between photonics, electronics and bioscience. Parameters deviation from ideal values due to fabrication tolerance, functional drifts induced by aging, mutual crosstalk effects (thermal, optical, electrical) must be corrected either in the manufacturing phase or/and during operation, in order to achieve the desired circuit functionality and adapt it to application specific requirements.

Trimmable silicon waveguides with induced stresses or covered with a chalcogenide glass cladding [48] have already been demonstrated an effective tool for post-fabrication manipulation of photonic integrated circuits, with remarkable advantages with respect to classical heathers. Also, feedback control signals extracted through transparent optical probes are an unavoidable requisite to locally inspect the status of a generic PIC, and to drive and control the working points of its functional elements.

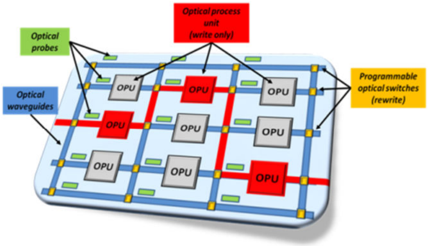


Figure 11. Example of programmable optical circuit. A set of Optical process Units (OPU) interconnected with reconfigurable switches and optical waveguides (Courtesy of Prof. A. Melloni, Politecnico de Milano).

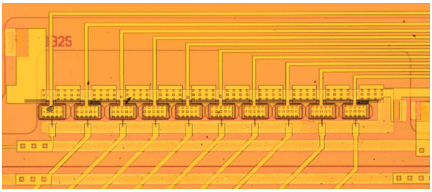


Figure 12. Example of optical process unit combining electronic, photonic and microwave. Coupled ring resonators tunable delay line (Courtesy of Prof. A. Melloni, Politecnico de Milano).

Applications: generic programmable arrays of optical building blocks [49]; tunable, adaptive, reconfigurable and programmable PICs; (re)writable waveguides and circuits [50]; devices robust against nonlinearities, temperature and aging; sensors with locked working point; increase yield by compensating fabrication imperfections and aging effects.

3.3 CMOS-compatible colour filters

An example of integration of a device inspired in nanophotonics is the colour filter which can be integrated with CMOS image sensors. Band pass filtering can be achieved in thin metallic layer drilled with a sub wavelength array of holes. To address several issues related to filtering for optical image sensors, i.e., metal layer thickness with respect to colour filtering, wavelength dependence, incident angle dependence, polarization behaviour, cross talk, process compatibility with CMOS constraints among others, a double-breasted rectangular hole array in aluminium has been chosen due many advantages compared to square, rectangular, circular holes or infinite slits in metallic layers (figure 13).

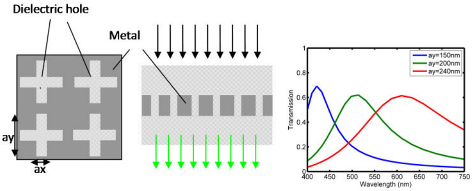


Figure 13. Diagram of symmetric cross holes of sides ax and ay perforated metal film and corresponding FDTD transmission spectra for normal incident plane wave. Parameters are: period = 250 nm, metal: 40 nm thick Aluminium, ax = 60nm. (Courtesy of Stefan Landis (CEA-LETI).

Colour filtering functions, especially in the visible spectrum, are associated with high resolution features and high density pattern etched in a metallic layer. New lithography strategies are often needed to manufacture such stamps for large scale manufacturing up to 200 mm wafers. Figure 14 shows a recently developed pattern shape modification strategy, mainly used in Optical Proximity Correction to manufacture optical mask [51], for electron beam lithography and the corresponding SEM picture of the stamp and the resulting imprint and thin aluminium layer etching.

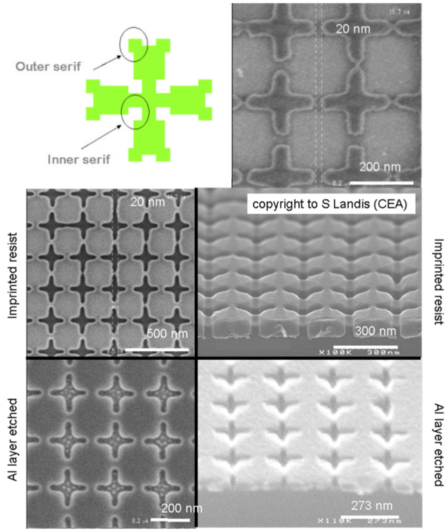


Figure 14. Pattern design and SEM top view stamp picture. SEM cross section pictures of imprinted resist patterns with cross array on silicon substrate and etched aluminium layer. Left images are SEM top view, right images are cross sectional views. © S. Landis CEA, LETI-Minatec Campus.

3.4 Silicon nanoemitters

The still-missing device in silicon photonics [52] is an integrated silicon light source which is efficient and can be easily integrated in CMOS photonics. Few concepts have been proposed, among which there is the use of low dimensional silicon quantum dots formed in a dielectric matrix. Reliable CMOS manufactured devices have been produced which show bright reddish emission when electrically driven. Figure 15 (bottom) shows an example of an orange emitting device. There are still open problems associated with the efficiency of the process (maximum power efficiency is 0.2%). In addition, the emission wavelength can be tuned by using suitable rare earth ions which can be electrically excited. Figure 15 (top) shows a fully processed wafer where electrically driven erbium doped silicon nanocrystals amplifiers have been fabricated. In figure 15 (middle) an image of an active optical resonator is shown.

Figure 15. Top: a silicon photonic integrated circuits with active emitters for electrical driven Er coupled to Si-nc optical amplifiers. Middle: an electrical driven active optical resonators. Bottom: a CMOS LED with emitting silicon nanocrystals. (Courtesy of Pavesi et al, UNITN and LETI unpublished data).

In the project LECSIN [53] surprisingly high efficiency luminescence has been observed from silicon based on Purcell enhancement and mode engineering in photonic crystal cavities. Furthermore, a large effort in nanoparticle-based emission work is conducted in Catania (Matis CNR INFM and ST Microelectronics Catania) mainly on Erbium-doped photonic crystals.

Applications: optical interconnects, silicon photonics, datacom, telecom, integrated biosensors, light emitting device, lighting, photovoltaics.

3.5 Photon Management

Photon management refers to the ability to engineer materials and devices structures at the nanometre scale to control the spatial distribution of optical energy and mould the flow of propagating light. The huge progress in fabrication of nanostructured materials has enabled new strategies for photon management in a range of photovoltaic devices and lighting devices.

The ultimate success of photovoltaic cell technology requires great advancements in both cost reduction and efficiency improvement. Photon management is able to simultaneously face these problems thanks to the great advances made in light trapping schemes in photonic materials. Indeed, light trapping schemes allow the design of devices with a very thin layer of active absorbing materials, reducing the amount of material used and improving cell efficiency.

Photon management is also of fundamental importance to optimize the performances of light emitting diode (LED) for lightning applications. In this case the target is to maximize the out-coupling of light to the external environment.

The optimal technological platform to manage and conceive new trapping mechanism, control far-field patterns, polarization properties, up- and down-conversion of absorbed light, are thin dielectric membranes (planar waveguides), where scattering centres are included in the material, with standard growing/processing technique. Varying the size, the density, the refractive index, which can be also metallic and/or non-linear, of the scatterering centres it is possible to mould and manage the photonic properties at will.

Ordered arrangements of scattering centres (photonic crystals) have been extensively studied in this last decade. On the other hand, quasi-ordered, completely disordered and correlated disordered arrangements have been and are the subject of extensive studies in this last two-three years because they retain many features of the ordered counterpart with the

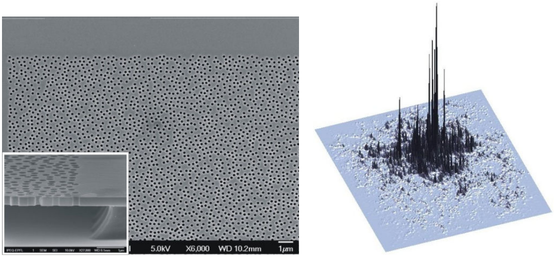


Figure 16. *Example of a new device structure for light trapping in thin dielectric membrane. (left) Scanning Electron Microscopy image of a completely disordered photonic system realized on a thin dielectric membrane of Gallium Arsenide (thickness 300 nm). Air holes (220 nm of diameters, filling fraction of 0.3) are the scatterers. The inset shows a detail of the suspended membrane. (right) Surface Intensity distribution of a typical trapped mode inside the membrane (© LENS Firenze, Italy).*

advantage of not suffering of structural disordered imperfections during the growing process, being the disorder part of the game.

Applications (key words): photon management, photonic crystals, photonic quasi-crystals, disordered photonic materials, correlated disorder, light trapping schemes, thin film photovoltaics, light emitting diode, far field radiation.

3.6 Metamaterials

These are artificial materials with superior and unusual electromagnetic properties not found in nature, currently being fabricated for targeted applications. The materials follow specific designs of electromagnetism and in the visible regime pose a major nanofabrication challenge, however, there are several potential new technologies to manufacture these materials from top-down to bottom up. The tremendous potential impact of the applications should they become a reality make this field uniquely attractive. Comprehensive reviews can be found at www.metamorphose-vi.org.

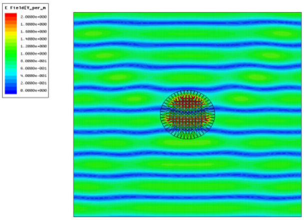


Figure 17. *"Invisible" cylinder (copyright Pekka Alitalo, Aalto University).*

Applications: In ICT: Smart and adaptive integrated electronic and optical circuits and devices, sub-wavelength optical information processing systems, low-cost low power consumption communication and control systems, magnetically and electrically controllable components. In Energy: Low-loss electronic and optical components, advanced solar cells harvesting at all frequencies, materials for thermal flow control, intelligent control of power consumption and generation. In Health: Sensors including biosensors, on-body communication systems, in-body drug delivery and control devices, implanted actuators. In environment: Monitoring and imaging devices. In transport: Car radars, sensors, road safety monitoring systems, road monitoring and vehicle tracking. In Security: Security control devices, sensors, imaging and monitoring devices.

3.7 Nonlinear nanophotonics

The research toward compact and efficient nonlinear photonic devices has greatly improved in the recent years in view of potential application in many areas where the integration is a key issue, including new spectroscopy techniques. Given the general structure of the nonlinear interaction between light and matter, in term of polarization $\vec{P} = \chi(1)\vec{E} + \chi(2):\vec{E}\vec{E} + \chi(3):\vec{E}\vec{E}\vec{E}$, one may act on the susceptibilities χ or on the field enhancement. This translates into a research of new materials and new geometries ranging from the UV to the THz domain.

Novel effects can be obtained when material properties are modulated at the sub-wavelength scale, that is, by exploiting molecular structures or nanostructures.

The tight confinement of the electromagnetic field is achievable in the vicinity of metal dielectric boundary, commonly referred to as surface plasmon polaritons. As a consequence nonlinear effects are greatly enhanced: Raman scattering [54], CARS, optical switches, surface enhanced second harmonic generation, high-harmonic generation by coupling nanoantennas [55] and, recently, two-photon emission has been also demonstrated [56]. The field confinement allows the visibility of nonlinear magneto-optical effects, such as Magnetization-induced Second Harmonic (MSHG), where a nonlinear rotation of the e.m. polarization plane is achieved [57]. The combination of geometry and materials (here metals are referred as nonlinear metamaterials) gives other interesting nonlinear effects at the nanoscale and the promise of new ones. In this last case it is possible to "play" with the conformation of the meta-molecules changes, providing novel mechanism of nonlinearity [58] and improving the nonlinear response related to the chirality of the medium [59].

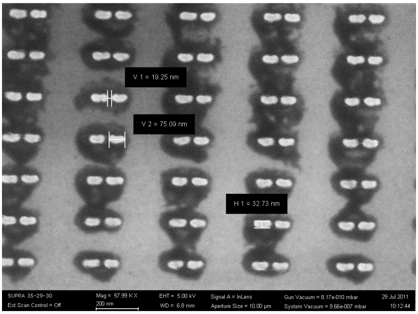


Figure 18. *SEM micrograph of Au nanoantennas/GaN to enhance the second harmonic generation signal in the visible (400 nm). (F. Bovino and A. Passaseo et al, Selex –SI, CNR-Italy, Univ. Roma La Sapienza, to be published).*

Recently, a number of exciting demonstrations of nonlinear effects have been made, especially in terms of third harmonic generation [60] and four wave mixing [61]; efficiencies previously unthinkable have now been demonstrated for mW-level pump powers and miniaturised devices. This is a major advance over the time when nonlinear optical experiments required high power lasers and entire optical benches, and this opens new opportunities in on-chip all-optical signal processing and on-chip quantum circuits.

In this context, research for new materials and combination of them is of great importance.

Applications: Surface and interface nonlinearity for high resolution spectroscopy; bio applications and sensing. Nonlinear magnetism in the optical range for bio sensing. Improved new devices, in space and time, for optical information processing such as modulators and switch. Integrated circuit for quantum optical information, including quantum sensing. New integrated parametric sources (UV –THZ).

3.8 Conclusions

Among the commonly mentioned key issues in nanophotonics research is design for specific applications including a subset of generic architectures and device performance in the nanoscale. Power efficiency, both as in power management and wall plug efficiency, are also shared key issues and both are followed closely by the need of technologies and standards suitable for very large scale manufacturing. More specific research needs and key issues can be found below.

Si photonic circuits: Being one of the areas with a higher Technology Readiness Level, the research needs are seen in technology development, in interconnects and design rules for monolithic and vertical integration.

Silicon nanosources: The key issues include the low power efficiency of silicon nanocrystal emitters, the low areal density of silicon nanocrystals and the low ratio of Er ions directly coupled to silicon nanocrystals, which prevents reaching lasing thresholds. To mitigate these issues research needs are seen in alternate system for light emission monolithically integrated in silicon, in deposition methods able to control the density of silicon nanocrystals independently of their size, e.g., sol-gel deposition and in fabrication techniques which should be able to control at the sub-nanometre level the deposition of dielectrics acting as tunnelling barrier for charge injection into the active centres.

Adaptive Integration Photonics: The research issues identified include hitless monitoring of optical signals to provide feedback, waveguide activation to provide tuning and permanent trimming and programmable and adaptive circuits. As specific research needs the question of light detection without photodiodes and the functionalisation of waveguides through new material combination to obtain electro-photo sensitivity are mentioned.

Colour filters: Two main issues are crucial, namely, omnidirectionality and process compatibility to enable the integration. Simulations of critical dimension fluctuations impact on performance are essential.

Photon management: Key issues include numerical characterizations, characterization of electrical properties of the dielectric membranes with scattering inclusions and the role of the correlations between scatters positions. As specific research needs the partnership with research growing facilities and with original equipment manufacturer (OEM) is seen as crucial.

Metamaterials: The research needs in this field include fundamental research on exotic-property and non-classical optical and microwave materials; theoretical modelling and design of artificial electromagnetic materials; engineered non-linearity of materials; approaches to targeted synthesis and design of electromagnetic materials; material architectures providing design control over material parameters, losses, spatial dispersion, nonlinearity, reconfigurable photonic metamaterials, conceptually novel architectures for electrical, magnetic, and optical control of the properties of engineered materials; develop and implement active optical materials with compensated loss; develop nano-structured light and microwave energy harvesting materials; research on field-transforming metamaterials (cloaks, concentrators, dividers) and in-situ and non-destructive characterisation of artificial electromagnetic materials.

Non linear nanophotonics: Key issues are: the definition of the operational wavelength for specific applications (deep UV for oceanic sensing, which needs an enhancement of the non-linearity, and MID-IR for sensing in general), new materials with high nonlinear coefficients, design of suitable antennas geometry, better time response of the nonlinearity. Furthermore, loss reduction, especially in slow light waveguides in silicon or III-V's to reduce further the pump power for nonlinear interactions. Reduction of nonlinear losses by, eg., working in the mid-IR or by developing novel materials, to increase the efficiency of nonlinear interactions. The research needs include also materials with reconfigurable nonlinearity and nonlinear meta-molecules. For most of the above sources and detectors are needed. A need to improve the local enhancement of the nonlinearity for quantum information processes, for bio sensing in the THZ and optical range is also seen as a priority.

4. Combining nanophotonics and nanophononics

Recent advances in nanofabrication have made it possible to realise structures in which photons and phonons can be coupled. These optomechanical structures open new avenues for very interesting research and, also, to new applications for sensing and signal processing.

4.1 Optomechanics

A single cavity can confine simultaneously both phonons and photons and increase the interaction among them (slow light and sound) and produce well known physical effects like stimulated Raman and Brillouin scattering, supercontinuum generation or light octave spanning at the chip scale [62]. In general, optomechanics addresses the coupling of optical (photons) and mechanical (phonons) vibrations via radiation pressure. Typically, light is in the near infrared regime, usually at wavelengths around 1.55 micrometres, whereas mechanical resonances vary from some MHz to some GHz depending on the structure. A key aspect of cavity optomechanics is the possibility of laser sideband cooling of the cavity down its ground state of motion, which should ultimately lead to the observation of quantum effects and to extremely sensitive mechanical sensors [63]. But the real advantage of the dual confinement of such cavities and waveguides, known as optomechanical crystals [64], lays in the fact that light and sound act as mutual driving forces at the meso and nanoscale through both the back-action effect [65] and the optical gradient force [66]. That means that phonons can be used with an extremely high efficiency (0.7 photons/phonon) to drive photon modes, and the reversal effect has been already proposed for a photon-phonon transducer. The potential applications range from quantum computing and information technology to study of quantum mechanical systems in their ground state. Especially remarkable is the aim of producing a coherent source of phonons, the first building block towards the sound equivalent of a laser, a SASER (Sound Amplification by Stimulated Emission of Radiation) that could be realised on a CMOS compatible platform using optomechanical concepts. Different geometries have already been proposed and experimentally characterised, including ring micro-resonators, slabs and nanobeams. All these structures have good optomechanical coupling, but do not have a complete stop band or band gap for both photons and phonons, which is a crucial point to avoid energy leakage, especially in the mechanical domain.

Experimental demonstrations of optomechanical effects in high-Q optical cavities have made used of large, in terms of optical wavelengths, cavities such as toroids or microspheres. In order to enhance further the optomechanical interaction, cavities with size comparable to the wavelength of photons and phonons have to be used. This has led researchers to implement novel cavities by using photonic-phononic crystal membranes, i.e., periodic structures which possess band gaps for both photons and phonons simultaneously. This has resulted in the concept of “optomechanical crystals” [67], or “phoxonic crystals” [68]. In addition to the possibility of enhancing optomechanical, or acousto-optic, interaction by building smaller cavities, optomechanical crystals possess other important features in comparison with other implementations of optomechanics: i) flexibility in the design of the structures owing to the maturity of the photonic/phononic crystals fields, ii) structures built on planar substrates by conventional top-down lithographic means, ultimately using mainstream CMOS processes, with the possibility to create arrays of devices on a same chip, iii) possibility to create additional optomechanical structures, e.g., waveguides to guide phonons and photons simultaneously and phonon sources [69], iv) possibility of new ways of photon-phonon interaction such as via electrostriction.

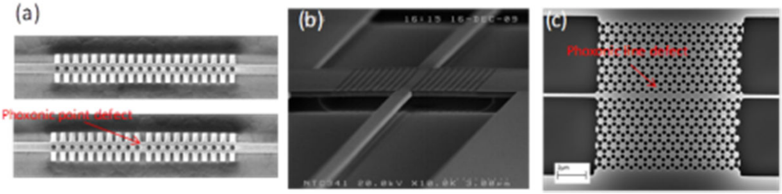


Figure 19. *SEM images of suspended silicon phoxonic crystal membranes. (a) Corrugated waveguide with holes that support a bandgap for TE-polarized photons around 1.55 micrometres and 4 GHz phonons (top panel). The introduction of a λ/4 defect (bottom panel) should lead to the localization of photons and phonons in a nanoscale volume. (b) Removal of the buried oxide leads to a suspended phoxonic crystal that facilitates the excitation and propagation of GHz phonons. (c) Top-view of a line defect created in a honeycomb-lattice. The structure can confine and guide slow photons and phonons simultaneously (Courtesy of A. Martinez, U. Polytechnic Valencia and Vincent Laude, CNRS-FEMTO).*

Applications: optical delay lines, highly sensitive sensors, modulators, optical memories, optical isolators.

4.2 Photothermal effects

Combining thermal waves with photonics gives rise to photothermal modulation. In photothermal techniques a heat pulse propagates through medium and the backscattered photothermal signal is monitored [70]. The method can be used for example to investigate inhomogeneous and layered materials. The problem of the photothermal modulation of optical beams is extremely complex due to the inhomogeneously modulated refractive index combined with multiple optical reflections inside the sample. A treatment for normal-incidence optical probing of photothermally modulated layered thin-film samples with arbitrary optical constants has been given [71].

Applications: Contactless experimental techniques to study thermal transport in inhomogenous media.

4.3 Conclusions

Optomechanics is a relatively new research field which have potential for new sensing applications and signal processing approaches. To capitalise this potential, better understanding of the physics behind photon-phonon coupling at nanoscale is needed, together with well-established fabrication processes for the optomechanical structures. One missing building block is a phonon source that can be integrated with the photonic/phononic crystals.

Photothermal techniques are a good candidate for non-invasive characterisation method for nanomaterials and composites. Here again understanding of coupling between photons and phonons or thermal waves is crucial.

5. Nanophononics

The control and manipulation of acoustic/elastic waves is a fundamental problem with many potential applications especially in ICT. One can mention confinement, guiding and filtering phenomena at the scale of the wavelength (and even below) which are useful for signal processing, advanced nanoscale sensors and acousto-optic on-chip devices, acoustic metamaterials for sound isolation and for focusing and super-resolution.

Phonon engineering can be achieved for example by periodically patterning a Si membrane (phononic crystal, PnC, membrane) [72], which is a strategy that is being exploited to provide a means for a controlled influence on phonon transport properties including functions like generation, propagation, storage, manipulation and detection. Optomechanical crystals for simultaneous control of both phonons and photons and cavities for enhanced phonon-photon coupling expand the prospect for novel applications of nanopatterned membranes [73,74,75].

5.1 Phononic crystals

Phononic crystals, which are artificial materials constituted by a periodic repetition of inclusions in a matrix, can be used to achieve these objectives via the possibility of engineering their band structures. Due to the contrast between the elastic properties of the matrix and the inclusions, the phononic crystals can exhibit absolute band gaps where the propagation of acoustic waves is prohibited in any direction of space and for any polarization, see Fig 20 [76]. The structure behaves like a perfect mirror in the frequency range of the band gap. Then, it is possible to create waveguides, for example by removing or changing a row of inclusions, that are able to produce localized modes inside the band gaps and therefore confine, propagate and bend waves at the scale of the wavelength [77]. Confinement inside cavities (point defects) and coupling between waveguides and cavities can also be used for filtering and multiplexing operations [78]. Another possibility of opening a gap, especially at low frequency as compared to the Bragg gap, is to use inclusions exhibiting local resonances, the so-called locally resonant sonic materials useful for the purpose of sound isolation and/or absorption.

Phononic crystals of finite thickness, such as a periodic array of holes in a plate or a periodic array of dots on a membrane, have only been studied recently, since it was demonstrated that they can also exhibit absolute band gaps and thus provide the possibility of the above functionalities in small size integrated structures working at high, GHz to THz telecommunication frequencies.

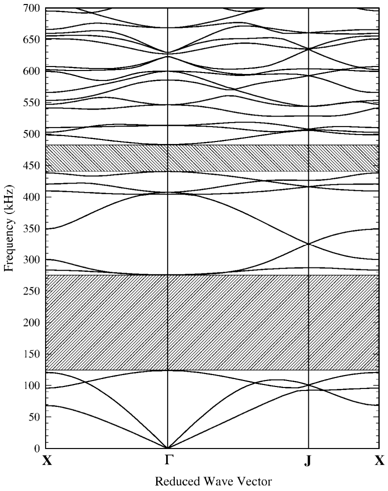


Figure 20. Plane wave expansion calculation results for the band structure of the two dimensional XY modes of vibration in the periodic triangular array of steel cylinders in an epoxy resin matrix for a filling fraction f=0.4. The reduced wave vector **k**(k_X, k_Y) *is defined as* **K***a/2p where* **K** *is a two-dimensional wave vector. Absolute band gaps are represented as hatched areas. (Reprinted with permission from J. O. Vasseur et al., Phys. Rev. Lett. 86 (2001) 3012, © 2001 American Physical Society).*

The progress in the field of phononic crystals goes in parallel with their photonic counterpart, although they involve a larger variety of materials that have the possibility of high contrast among the elastic properties, large acoustic absorption and the solid or fluid nature of the constituents. Since the band structure is scalable with the dimensions of the structure, a great deal of work has been devoted to macroscopic structures in the range of sonic (kHz) and ultrasonic (MHz) frequencies where the proof of concepts of band gaps and manipulation of sound (such as waveguiding, confinement, sharp bending) have been established with simple demonstrators. Yet, there are a continuous interest in the engineering of bands with new structures and materials.

With the advancements of nanotechnologies as well as self-assembling techniques, the interest on nanophononics is increasing. Phononic circuits, including waveguides and cavities, inside sub micrometre phononic membranes and working at a few GHz are started to be studied but still remain mostly at the level of demonstrations. The band structure of these so-called hypersonic crystals can be studied by light (Raman and Brillouin) scattering techniques, in particular to investigate tunable systems in which the properties can be changed drastically with external stimuli such as stress or temperature (for example the phase transitions of a polymer infiltrating the holes of a phononic crystal).

The configuration being normally considered is the insertion of periodic holes in silicon plates, where the opening of band gaps is the consequence of the coherent destruction of phonon modes by Bragg scattering, but also geometries based on the periodical arrangement of cylindrical cavities on top of a membrane (see Figure 21). The latter allows for a superior control of the phonon dispersion, and almost dispersionless phonon branches, which are not related to the opening of band gaps, exist on large wavevector domains. While coherent scattering phenomena in phononic crystals have been shown to affect the low frequency phonons, recent reports address the possibility of extending these effects to the high frequency THz phonons that dominate heat transfer process [79,80]. Thus, future functionalities of PnC membranes related to heat management need the development of cutting-edge nanofabrication techniques allowing to downscale the characteristic sizes to a few nanometer scale.

Besides the topics related to the existence of absolute band gaps, there is growing interest on refractive properties of phononic crystals, in particular: negative refraction phenomena and their applications in imaging and sub-wavelength focusing in phononic crystals, self-collimation and beam-splitting in relation with the shape of the equifrequency surfaces, controlling the propagation of sound with metamaterials with emphasis on cloaking and hyperlens phenomena.

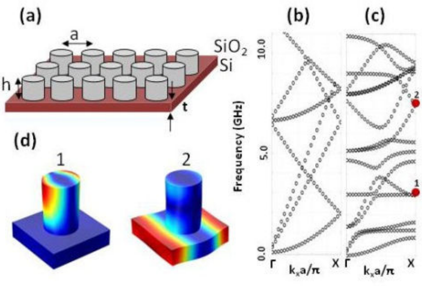


Figure 21. *Schematic of the proposed structure with periodic pillars on a Si membrane (a). (b): Calculated phonon dispersion curves of 100nm thick Si membrane (b), and of the phononic structure with* SiO_2 *pillars (c). (d) Displacement field of the modes at the points marked with red dots in (c) (J. Gomis et al., unpublished).*

Thermal transport in nonmetallic nanostructured materials can be strongly affected by the specific phonon dispersions as well as by different scattering mechanisms. The existence of band gaps and flat dispersion curves can reduce the thermal transport and be useful for thermoelectric applications. On the other hand, channels for propagation of heat can be envisaged either inside the phononic crystal or by avoiding the escape of heat outside a thin film surrounded by a phononic crystal. Different frequency domains of phonons can be involved depending on the temperature and on the wavelength dependent mean free paths. Some insights into the latter can be derived from molecular dynamic calculations.

In conclusion, the field of phononic crystals should acknowledge a continuous growth in relation with the fundamental understanding of the wave phenomena in these heterogeneous materials and with their numerous expected technological applications. The latter cover a broad range of frequencies from the sonic regime for sound isolation and metamaterial behaviors, to GHz regime for telecommunications and to THz regime for phonon-photon interaction and thermal transport phenomena.

5.2 Heat transport through interfaces and in nanoscale structures

An important field where nanophononics will a have striking impact is the heat transfer area, as much better thermal insulators and much better thermal conductors are required if one wants to meet the energy challenges of the 21st century. The electronic conductivity σ spans over more than 30 orders of magnitude ($[10^{-22}\text{-}10^{8}]\ \Omega\,\mathrm{m}^{-1}$), something which has led to the development of electronics, whereas the thermal one κ spans barely over 5 orders of magnitude ($[10^{-2}\text{-}10^{3}]\ \mathrm{Wm^{-1}K^{-1}}$) [81]. The typical phonon wavelengths have a broad distribution around 2 nm at room temperature, and wavelengths are much longer at liquid helium temperature. The phonon mean free paths are known to be longer than 100 nm, even at room temperature.

At the Fourier scale, in addition to the 'volume' transport represented by the conductivities, the interface effects known as 'boundary resistances' R_b, also sometimes called Kapitza resistances, can be dominant in the effective transport coefficients $\kappa_{eff}=\kappa+R_b/d$ at small scale ($d\rightarrow 0$). The impact of the boundaries at the nanoscale has been studied since the beginning of the 2000's, especially for the purpose to develop more efficient thermoelectric materials, as lower thermal conductivity imply higher thermoelectric figure-of-merit ZT [82]. The partial phonon diffuse reflection at the surfaces implies loss of coherence, which integrated over all frequencies, is represented by a so-called 'specular coefficient' p. As the roughness is not always easy to analyse, it is often a fit parameter that allows to reproduce numerically the experimental data. An additional significant challenge is the control of the surface states.

The confinement of phonons leads to discretisation of the phononic density of states. Similar to concepts developed for photonics, such as periodic structures, superlattices, etc, one can consider manipulating phonons or thermal energy, including storage, conversion, emission, absorption and rectification. So far the confinement induced effects have hardly been treated for simple geometries. The extension to more complex geometries will provide a grand challenge.

In addition to continuum models, phonon behaviour has been analysed also using atomic-based simulation methods, such as molecular dynamics, Green's function and ab-initio methods. These methods are not suitable for structures with intermediate sizes in the range of 10-100nm due to computational restrictions. To bridge the acoustic scale, continuum elasticity based methods and the atomic scale more extensive use of the Boltzmann transport equation (BTE) will be required.

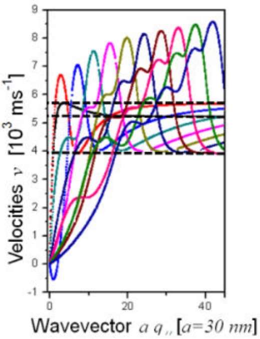


Figure 22. *Calculated thermal phonon group velocities (heat propagation velocity) due to confinement in a 30 nm-thick Si membrane. Dotted black lines: planar bulk reference (E. Chavez et al, to be published).*

One main property that distinguishes phonons from other bosons such as photons is that they interact between themselves [83] and, consequently, their lifetimes, or relaxation times, are strongly correlated to their distribution. Recent numerical calculations [84] have shown that the bulk phonon mean free paths might be much larger than previously expected, so that nanoscale models might already be needed at the 1 µm scale.

The calculation of the phonon lifetimes relies on formalisms based on the Fermi's golden rule that were developed in the 1950s mainly for bulk phonons [85,86]. Some of the main results are obtained in the framework of isotropic approximation, whereas others require anisotropy to be explicitly taken into account as the main cause of damping, as in the Herring mechanism [87]. The impact of non-resistive phonon interaction, called normal processes, is not well understood, and although atomic simulations allow extracting some of these lifetimes, the simulations do not provide means to control them. The extension of the formalism to the phonons existing in nanostructures appears to be of highest importance if one wants to understand how to modify phonon conductivity by dimensions and geometry. In particular, phonon momenta conservation rules ($q_1=q_2+q_3$) relax at small scales. The current deterministic approach is therefore incomplete and more statistics-based ones are required.

It is very difficult experimentally to correlate the thermal macroscopic effective conductivity coefficients, e.g., conductivity and specific heat, to the phonon spectra. One can measure thermal conductivity relevant for bulk or thin films samples with various methods such as the 3-omega method or photothermal spectroscopy. The thermal diffusivity, i.e., the ratio of the thermal conductivity to the specific heat, can be measured by various time-domain methods probing the dynamics of the studied systems [88]. These include the laser flash method, the more-recently developed thermal transient grating technique and time-domain thermoreflectance. All these techniques give access to macroscopic effective coefficients. If the medium is strongly out of equilibrium, as in many times is the case with graphene or carbon nanotubes, and no local temperature can be defined, as in ballistic regime, such parameters are not meaningful and the transport should be represented for instance by conductances.

Regarding spatial resolution, scanning thermal microscopy has been proven to possess the highest one. Raman spectroscopy or fluorescence-based methods can reach sub-

10 µm resolution. Dispersion relations can be measured using neutron diffraction, or using inelastic light scattering, i.e., Brillouin and Raman spectroscopy. The latter gives a limited part of the room temperature momenta range. Ultrafast phonon spectroscopy has been used up to ~ 2 THz, the very beginning of the room-temperature spectrum. One approach is to use passive detection, i.e., to measure thermal THz radiation using microbolometers. This technology has been used, for example, to realise real-time THz cameras for security screening [89].

Applications: Thermal management for ICs and heterogeneous integration applications, THz cameras for security and medical applications.

5.3 Issues relevant to micro and nanoelectronics

Heat dissipation has become one of the most important limiting factors toward increasing density, performance and reliability of modern electronic devices, including: microprocessors, high-power radio frequency transmitters, photovoltaic cells and power electronic modules; and it is particularly critical in 3D chip stacks of integrated circuits, where the inherent difficulty of supplying power to and removing heat from individual dies has become a crucial factor for the future growth of the semiconductor industry that could potentially reduce the design window of 3D products.

In these devices, heat generated during their normal operation is dissipated through dissimilar interfaces comprising metals, semiconductors, oxides, thermal interface materials (TIMs) and fluids (air or water); and from small areas which are continuously reduced to lower manufacturing cost. The reduction of the spatial characteristic dimensions not only allows faster switching and better electrical performance, but also changes the thermal properties of the constituent materials from their bulk values. It is well known, that at scales comparable to or below the mean free path of phonons (as in current and future transistor designs), the scattering of phonon with boundaries is one of the main sources of thermal resistance leading to a significant reduction in the thermal conductivity of semiconductors. Phonons are subject to complex scattering mechanisms, i.e., phonon-phonon, phonon-impurities, phonon-boundaries and phonon-defects, which play a crucial role in describing how the heat is transported in the material. Furthermore, the difference between the thermal properties of bounding materials translates to a significant mismatch in their thermal impedances and in low phonon transmission rates, which also promotes high thermal interface resistances. The latter, not only reduce the efficiency of cooling systems, leading to larger carbon dioxide emissions, but also hinder the reuse of the thermal energy.

While in some situations the reduction of the thermal conductivity can be beneficial, such as for thermoelectric devices using, for example, silicon nanowires; this reduction significantly deteriorates the thermal performance and reliability of other devices, such as: SOI, UTB FD-SIO, III-V, FinFET and nanowire transistors. It is estimated that future III-V and nanowire-based transistors will be subject of serious heat dissipation problems. In particular, since: i) III-V semiconductors have thermal conductivities which are 5 to 30 times lower than that of silicon (e.g. $In_{50}Ga_{50}As$ or $In_{50}Al_{50}As$), ii) additional insulating layers with very low thermal conductivity will be used to control current leakage and iii) the inherent low dimensionally of the involved structures will promote phonon-boundary scattering; restricting in this way heat dissipation and inducing large thermal stresses. Note that most of the failure mechanisms in transistors are temperature-dependent.

Despite the design of current transistors relying almost exclusively on charge transport models, the ITRS 2009 has defined that future nanoscale device simulators, coupling electronic band and phonon spectra interactions, are necessary to enable future transistor architectures. In particular, to predict the limit of CMOS-based transistors, to design and evaluate devices beyond traditional planar CMOS, to assess the performance new devices subject to electrical and thermal fluctuations, and to propose physical models for the evaluation of novel materials (e.g. high-k stacks, III-V channels, etc.) in these new architectures.

From the thermal point of view, to model the thermal behavior of these devices considering all scales involved is a complex task. The complexity lies: in the large variation of the participating spatial (from nanometers to centimeters) and temporal scales (from picoseconds to hours), in their intricate operation and in the physical behavior and nature of each scale. Even though the formulation of the thermal transport at the sub-continuum level has long been established, no mathematical method is able to fully resolve the thermal response of electronic devices from nano to macro scales and hierarchical models are required for this purpose [90]. Traditionally, different numerical tools have been used: to characterize the thermal properties of materials and interfaces, to estimate phonon properties (i.e. relaxation times), to describe the transient transport of phonon in 2D and 3D domains, to conduct thermal device simulations at macroscopic scales, etc. These include molecular dynamics (MD), lattice dynamics (LD), phonon Monte Carlo (MC), phonon Boltzmann transport (BTE), Cattaneo equation and Fourier law, among others. Quantum based approaches, other than LD, have been typically neglected due to the computational time involved, the requirement of large computational facilities, i.e., thousands of processors, and the difficulty to model large molecular systems.

5.4 Molecular dynamics modelling of interfaces and heat transport

Molecular dynamics (MD) is one of the few methods used to characterize the thermal properties of materials and interfaces, partially due to a positive balance between the accuracy of results and the computational time involved. The method, which has a classical nature, solves the Newton's second law to describe the dynamics of atoms subject to one or more interacting potentials. MD has been used extensively to estimate a broad range of thermal properties of the materials. For thermal characterization purposes, the method offers many advantages at the expense of no quantum effects since: i) it does not require previous assumptions about the nature of the thermal transport, ii) it captures the anharmonic interaction between atoms, iii) it does not require simplification on the underlying molecular structure, iv) well documented inter-atomic potentials for common semiconductors are available, v) it can be applied to relatively complex geometries and vi) can be used to model solid, liquid and gas phases.

MD has been particularly valuable and useful: i) to estimate the thermal conductivity of semiconductors [91], ii) to calculate the phonon transmission and reflection probabilities at smooth and rough semiconductor interfaces [92], iii) to determine the phonon relaxation times of silicon and germanium [93], iv) as part of hierarchical modeling approaches, v) to determine the thermal conductivity of silicon-germanium core shell nanowires [94], vi) to study molecular mechanisms to enhance heat dissipation and thermal rectification at solid-liquid interfaces [95], vii) to determine the metal-nonmetal thermal interfaces resistance subject to phonon and electron interactions [96], viii) to determine thermal properties of carbon nanotubes and graphene sheets [97], and ix) to thermally characterize the matrix-filler thermal interface resistance in TIMs [98]. An example of a calculated thermal profile in a solid-liquid interface is shown in Fig. 23.

Despite all these advantages and progress towards the characterization of materials and interfaces, the lack of quantum effects [99] and the difficulty to include realistic electron-phonon interactions limit the application of MD and its results. Novel approaches for the incorporation of these two phenomena in MD are currently in progress [100]. However, larger efforts in this area are mandatory to facilitate the design of future transistors.

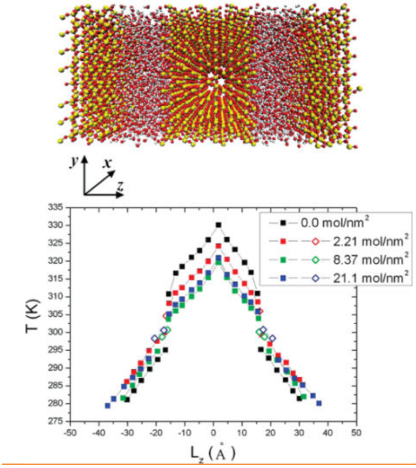


Figure 23. *Top panel: a snapshot of quartz-confined water model structure. The quartz slabs are in the middle and on two sides. Water is confined between quartz slabs. Bottom panel: steady-state temperature profiles for heat flux of 6400 MW/m^2 for four selected fully hydrophilic cases at 300 K. The solid squares are for quartz and the open diamonds are for water. Reprinted with permission from M. Hu et. al., Nano Lett. 2010, 10, 279-285. Copyright 2010 American Chemical Society.*

5.5 Heat transport between particles

Nanofabrication provides means to control thermal properties of nanomaterials and nanosystems, with impacts on, for example thermoelectric materials and thermal interface materials [101]. The physical mechanisms are mostly related to heat carrier scattering between two bodies through interfaces or gaps or at surfaces. Developing tools to quantify and design the corresponding thermal resistance remains a crucial task. Recent work has proposed a general derivation of the inter-body thermal resistance based on fluctuation-dissipation theorem [102]. It has provided relevant predictions of the near-field radiation based thermal resistance between two nanoparticles. For example, the heat transfer between two silica nanoparticles is enhanced by orders of magnitude at distances less than twice the diameter of the particles. This near-field interaction was then experimentally proven for microscopic objects [103]. Further studies have then extended the derivation proving that the inter-body thermal resistance is identical to the energy carrier mean relaxation time [104]. This analysis not only provides a simple and direct means to study and design the thermal resistance of nanostructures, it might also indicate a new degree of freedom to control heat transfer in nanostructures through the tuning of the carrier relaxation.

Moreover, larger solid bodies separated by a small vacuum gap can exchange energy and momentum (and information) by various mechanisms [105,106,107]. It has been considered that the most significant exchange channel is formed by inter-body photon coupling. Surface excitations involving optical phonons and plasmons can also play an important role. These polariton effects can enhance the coupling close to the maximal fundamental limit. When the different bodies represent thermal baths the heat exchange is via near-field heat transfer effects and considerable efforts have been devoted to understand the heat transfer via photon and polariton channels. Advances in experimental techniques have also enabled near-field heat transfer measurements from µm down to nm body distance [108].

Acoustic phonons are the major heat carriers in dielectrics, but their effect on heat transfer through a vacuum gap has been considered to be negligible, because they couple weakly to photons. Recently, it was theoretically demonstrated [109] that significant energy transmission and heat flux is possible if the acoustic phonons can induce an electric field, which then can leak into the vacuum [see Fig. 24]. Such mechanism is provided, for example, by the density response of free carriers due to phonons, by the piezo-electric effect or by response of built-in fields. The built-in field refers to fields that occur, for example, due to work function differences. The solid-vacuum-solid acoustic phonon transmission phenomenon can be thought of as an acoustic phonon tunneling through vacuum.

Altfeder et al. [110] explained the outcome of their near-field heat transport experiment (between Au and Pt/Ir STM tip) by lattice vibration induced temporal changes in the built-in fields. They observed an extremely large heat flux, which is significantly larger, ~ 6 orders of magnitude, than the flux suggested by the photon based near-field heat transport theories, where the heat is essentially transmitted due to electron density fluctuation induced photons and/or polaritons. Such magnitude led them to interpret that their experiment actually involves phonon tunneling. Detailed theory of this experiment is lacking and this leaves room for speculations.

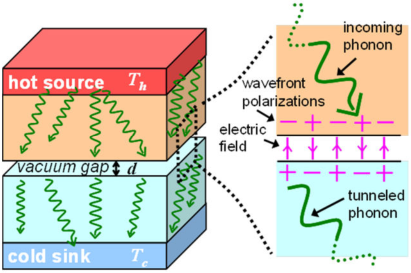


Figure 24. Illustration of the phonon transmission/tunneling effect through a vacuum gap. Hot source radiates phonons towards cold sink and vice versa. Single phonon carries an electric field, illustrated by + or - signs of wavefront polarization. The polarization induces an electric field into the vacuum gap. The field enables finite transmission over the gap (M. Prunnila et. al., VTT).

5.6 Phonon dispersion in ultra-thin membranes

Phonon confinement is an important component of phonon engineering as the density of states of confined phonons, their frequency and symmetry depend on the geometrical shape of the cavity, as well on the acoustic characteristics of the cavity constituents. Thus, confined phonons are particular to a specific acoustic cavity and depend on the configuration of the structure. In this context, free-standing ultrathin Si films, which can be building blocks for many future applications and, especially, for nano-electrical mechanical devices, represent an excellent example to study experimentally the effect of the reduction of the characteristic size on the phonon dispersion relation (see Fig. 25). This knowledge is crucial in order to identify the role of confined phonons in device performance, for example, phonon-limited electron mobility and thermal transport. In addition, cavity design already represents a means to tailor the phonon dispersion relation for phonon manipulation, given that an effect of confinement in membranes is the manifestation of phonon modes presenting zero and negative group velocity [111].

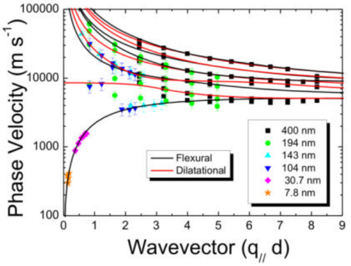


Figure 25. *Phonon dispersion relation of Si membranes (with thicknesses, d, from 400 nm down to ~8 nm) measured by inelastic light scattering and plotted on one curve by representing the phase velocity as a function of the dimensionless* $q_{//}\cdot d$*. The ultra-thin nature of the membranes results in a slow phase velocity for the fundamental flexural modes, with a phase velocity dowsn to 300 m* s^{-1} *recorded for the ~ 8 nm membrane. This is 15 times smaller than the comparable Rayleigh Wave (J. Cuffe et al. to be published).*

5.7 Low temperature effects

In the low temperature limit several new issue emerge.

Thermalization of electronic nanodevices at low temperatures is an interplay between electrons, phonons and photons. Ultimately, the performance of the electronic device is determined by the level of coupling to the low temperature bath by phonons and photons, and by decoupling the electronic system from the high T thermal photons, e.g., microwaves travelling via the wiring [112,113]. Noise of heat current is showing interesting behavior at low temperature. The curious property is that the noise, at least for certain mesoscopic realizations, is non-vanishing in the T -> 0 limit. This observation, so far only theoretical, puts in doubt the validity of the fluctuation-dissipation theorem (FDT) of heat current in the quantum regime. Mesoscopic phonon heat transport is one of the examples where this non-vanishing noise might be observable experimentally another system is electron-phonon heat transport. The second interesting topic in terms of noise of heat current is testing the validity of the Jarzynski equality and fluctuation-dissipation relations (FDR) for small systems and conversion of information to energy. The realizations using the combined electron-phonon –systems seem feasible. Statistical physics of both electron and phonon systems in nanostructures looks like an interesting avenue for future research [114]. The thermal wavelength of phonons, exceeding tens of micrometres at practical low temperature conditions, exceeds in many cases (some of) the dimensions of the heat conductor. This has both fundamental and practical interest in engineering of thermal detectors and on-chip refrigerators [115]. It has been shown, for example, that the phonon thermal conductance can be reduced drastically at low sub-5 K temperatures by geometrical design, i.e., introducing serpentine structures in nanowires to block the propagation of ballistic phonons [116].

Applications: Micro-coolers, detectors, quantum computing.

5.8 Improving the efficiency of thermoelectric materials

One application of nanophononics is to improve the performance of thermoelectric materials. The figure of merit

$$ZT = \frac{\sigma}{\kappa_{ph} + \kappa_{el}} S^2 T$$

can be enhanced by reducing the thermal conductivity κ_{ph} by increasing the scattering of phonons. This can be done by alloy scattering, by introducing superlattices or, very efficiently, using nanoparticles [117]. In Fig. 26 is shown a Si/SiGe nanodot multilayer with which the minimum room temperature thermal conductivity achieved was below 1 W/mK [118]. The materials are fully compatible with CMOS fabrication process and the approach potentially provides a mean to integrate TE energy harvesters with ICs.

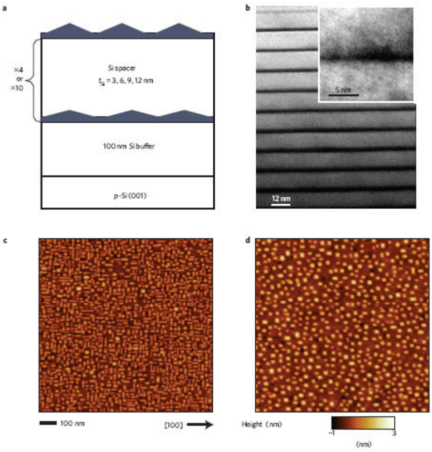


Figure 26. *a Schematic of the self-assembled nanodot multilayers fabricated by molecular beam epitaxy. **b** Bright-field TEM image of a sample with t_{Si}=12 nm. The dark areas correspond to the Ge layers. The inset shows a high-resolution TEM of a nanodot. **c** AFM image of a single Ge/Si(001) dot layer before overgrowth with Si. **d** AFM image of the topmost layer of a sample with t_{Si}=3 nm. Reprinted with permission from G. Pernot et. al., Nature Materials 9 (2010) 491. Copyright © 2010 Macmillan Publishers Limited.*

Applications: Energy harvesting, cooling, heat blocking layers for thermal insulation

5.9 Conclusions

An increasing number of groups are working in various fields of nanophononics, covering, e.g., modelling of phononic crystals and heat transport at macro and atomic scale. It is important to intensify the collaboration between the various activities and create a more unified value chain for nanophononics ranging from design and modelling to heat transport calculations to experimental verification of the models. The latter requires advanced nanofabrication techniques sometimes well beyond the state of the art. An interesting nuance here is that the THz frequency range covered by nanophononics is the only unoccupied frequency band available due to the lack of practical THz sources and detectors.

A large effort is being put into solving thermal management related issues in microelectronics at package level. It has become clear that the next step should be to go inside the transistors and try to find ways to control heat dissipation at micrometre and nanometre level. Here, new models for heat transport are needed to close the gap between continuum models and molecular dynamics modelling. Extensive experimental work is needed to support and qualify the new approaches, meaning also development of improved experimental techniques. Finally, it is obvious that phonons and vibrations have an important role in biological processes. This area remains still unexplored and would potentially open new avenues to understand the interplay of phonons, photons and electrons in environments where functions have been refined and optimised through evolution in millions or billions of years.

Phononic crystals: There are several groups working on band structure calculations of phononic crystals. The calculations should be extended to cover phonon propagation to understand and predict heat transport in these structures. Fabrication of phononic crystals is rather demanding due to small dimensions and well controlled surfaces, and various nanofabrication approaches have to be tested and, in the longer term, up-scaled to wafer level.

Heat transport at nanoscale: There is a clear need to develop modelling and simulation tools for heat transport for mesoscopic structures, i.e., tools for structures with dimensions from a few nm up to a few hundred nm, a range that is difficult for continuum models and, due to huge computational power needed, impractical for atomistic models. Also, there is a need to develop experimental methods for investigation of thermal properties of nanoscale structures, methods that are commensurable and can be compared with physical models. At low temperatures the demands are more relaxed and low temperature measurements can provide a first route to experimentally test the models.

6. Conclusions and recommendations

Nanophotonics and nanophononics underpin basic science to develop know-how and methods to overcome scientific and engineering challenges in nanoscience and nanotechnology, impacting specially ICT. This is supported by the numerous applications mentioned throughout this position paper spanning not only communications but also energy, health, transport and the environment.

Nevertheless, the increasing complexity in the science of light-matter and phonon-(electron, spin) interactions in the nanoscale is resisting a reductionist approach. There are several sub-communities using highly specialised terminology and approaches which need to become more accessible to each other to enable qualitative progress in nanophotonics and nanophononics in their quest to become relevant ICTs.

Sustainable progress requires a strong synergy with new materials, instrumentation, modelling methods and nanofabrication. However, a much stronger interaction with components, nanomanufacture, design and architecture consortia is needed to make serious inroads into completing the value chain.

Although this paper does not include bio-photonics nor bio-phononics, we have much to learn from fluctuations in biology where there are ample opportunities to develop, e.g., optical, methods to study them.

Recommendations

a. Targeted European-level support for *fundamental research in application-relevant nanophotonics and nanophononics focusing first on common issues*, for example, heat dissipation at component level, using noise in ICT and ways to cope with the fluctuations in key parameters. The latter bound to be a more serious issue in the nanoscale than in the current micrometre scale but crucial for heterogeneous integration.

b. Bring together the experimental and theoretical communities of phonon physics, heat transfer (mechanical) engineering, statistical physics, biology (fluctuations), nanoelectronics, and (solid-state) quantum communications to start with a *focused research programme on heat control in the nanoscale* in the first instance and on, e.g., *harvesting fluctuations* as a follow-on or parallel focus.

c. A research infrastructure for *emerging cost-efficient nanofabrication methods* jointly with a multi-level simulation hub and a comprehensive nanometrology associated laboratory targeting nanophotonics and nanophononics applications, complementing the Si and the III-V photonic foundries. This infrastructure could then evolve into a potential foundry, with industrial participation, covering combinatory lithography, cost-analysis, packaging and training.

d. Targeted European-level support for research on *material sciences* to develop techniques able to achieve material control at the sub-nanometre and, in particular, in 3-dimensions. This includes, e.g., control of multilayer thickness of silicon-rich silicon oxide and of the barrier dielectric at the wafer scale level.

Acknowledgements

This report has been made possible with the support of the EU ICT FET Coordination Action NANOICT. Contributors acknowledge the support of the EU and national projects: ACPHIN, GOSPEL, HELIOS, LECSIN, LIMA, NANOPACK, Nanophotonics4Energy, NANOPOWER, NaPa, NaPANIL, POSITIVE, SPLASH, TAILPHOX, among others.

7. References

[1] ftp://cordis.europa.eu/pub/ist/docs/fet/enano-5.pdf (panel 2 on Phonon engineering for themal management).

[2] Talk by S Hillenius at the joint MEDEA+/ENIAC Workshop, Montreux, CH, September 22, 2006 www.eniac.eu/web/downloads/events/Agenda220906.pdf

[3] www.ioffe.ru/sonetlumiere/previous.htm

[4] http://eurotherm91.conference.univ-poitiers.fr/ (Micro Scale Heat Transfer III).

[5] www.zero-power.eu

[6] www.em2c.ecp.fr/Members/volz/phonons-and-fluctuations/folder_contents

[7] www.nanoict.org

[8] S. Gaponenko, Introduction to Nanophotonics, Cambridge University Press, Cambridge UK, 2009.

[9] L. Novotny and B. Hechts, Principles of Nano-optics, Cambridge University Press, New York, 2006.

[10] "A European Roadmap for Photonics and Nanotechnologies", EU project MONA, 2007. www.ist-mona.org/pdf/MONA_v15_190308.pdf

[11] "Emerging Nanophotonics", EU project PhOREMOST, 2008. www.icn.cat/~p2n/wp-content/uploads/PhOREMOST_Roadmap_Final_Version.pdf

[12] www.nanophotonicseurope.org

[13] "Nanophotonics Foresight Report", Nanophotonics Association Europe, 2011. www.nanophotonicseurope.org/nanophotonics-news/52-nanophotonics-foresight-report.html

[14] M. Meschke, WW Guichard and J. P. Pekola, Single-mode heat conduction by photons, Nature 444 (2006) 187.

[15] M. Eichenfield, J. Chan, R. M. Camacho, K. J. Vahala, and O. Painter, Nature 462, 78 (2009).

[16] K. Bernstein, R. Calvin III, W. Porod, A. Seabaugh and J. Welser, Device and Architecture Outlook for Beyond CMOS Switches, Proc. IEEE, 98, 2169 (2010).

[17] "Vision, Mission and Strategy", AENEAS and CATRENE, 2011, www.aeneas-office.eu/web/documents/VMS_MASP.php

[18] "Nanotechnology Research Directions for Societal Needs by 2020", Eds. M.C. Roco, C. Mirkin and M. Hersam, Springer and NSF/WTEC (Berlin and Boston), 2010.

[19] "Photonics-Our vision for a Key Enabling Technology of Europe", Photonics21, 2011. www.photonics21.org/download/FinalEditionPhotonics21VisionDocument_InternetVersion.pdf

[20] See, for example, H. Chen, C. T. Chan and P. Sheng, Nature Materials 9, 387 (2010).

[21] M. Foster, J. S. Levy, O. Kusucu, K. Saha, M. Lipson and A. L. Gaeta, Opt. Express 19, 14233 (2011).

[22] www.epixfab.eu

[23] www.jeppix.eu

[24] W. Metaferia, et al., Phys. Stat. Sol (c), in press.

[25] For a recent review see, eg., H. Schift, J. Vac. Sci. Technol. B, 26, 458 (2008).

[26] V. Reboud et al, Microelectronic Eng. 87, 1367 (2010).

[27] R. Hershey et al, SPIE, 6337-20 (2006).

[28] S. Bae et al. Nature Nanotechnology 5, 574 (2010).

[29] B. Lucas, J. Kim, C. Chin and J. Guo, Adv. Funct. Mats. 20, 1129 (2008); S. H. Ahn, J. Kim and J. Guo, J. Vac. Sci. Technol. B 25, 2388 (2007); A. L. Vig, T. Mäkelä, P. Majander, V. Lambertini, J. Ahopelto and A. Kristensen, J. Micromechanics and Microengineering, 21, 035006 (2011).

[30] See, for example, L. J Cao, J. Phys. D: Appl.Phys 37, R123 (2004).

[31] See, for example, C-J, Ting et al., Nanotechnology 19, 205301 (2008).

[32] Nanofabrication Technologies for Roll-to-roll processing, An academic-industry workshop on Technologies for American Manufacturing Competitiveness, Boston, MA, 27-28 September 2011. www.internano.org/content/view/34/223

[33] ENIAC Strategic Research Agenda 2007, p. 42. www.eniac.eu/web/downloads/SRA2007.pdf

[34] www.eniac.eu/web/downloads/documents/ masp2010.pdf

[35] L. Malaquin, T. Kraus, H. Schmid, E. Delamarche and H. Wolf, Langmuir 23, 11513 (2007).

[36] T. Kraus, et al, Nature Nanotechnology, 2, 570 (2007).

[37] S. Arpiainen et al, Adv. Funct. Mat. 19, 1247 (2009). Patent FI/02.03.07 FIA 20075153 and US-2008-8220-0220159-A1.

[38] W. Khunsin et al, Adv. Funct. Mat. Accepted manuscript adfm.201102605 (2012).

[39] www.lamand.eu

[40] T. Kraus, et al., “Nanoparticle printing with single-particle resolution” Nature Nanotechnology, 2, 570-576 (2007).

[41] For an overview of emerging nanoabrication methods, see, for example, C M Sotomayor Torres (Ed), Alternative Lithography: unleashing the potential of Nanotechnology, in the series on "Nanostructures: Science and Technology", series editor: D J Lockwood, New York, Kluwer Academic/Plenum Publishers, 2003.

[42] See, for example, the European Metrology Research Program. www.emrponline.eu

[43] www.ims.org

[44] J. Ahopelto and H. Schift, Eds. “NaPa Library of Processes”, www.NAPANIL.org, (2008).

[45] D. Mendels, software “NS Suite”, www.cognoscence.com

[46] W. Khunsin, G. Kocher, S. G. Romanov and C. M. Sotomayor Torres, Adv. Funct. Mat. 18 2471 (2008).

[47] A. Biberman and K. Bergman, Int. Conf. Solid State Devices & Materials, Tokyo, 2010. http://lightwave.ee.columbia.edu/?s=publications

[48] A. Canciamilla et al., Opt. Lett. 36, 4002 (2011).

[49] E. J. Norberg, R. S. Guzzon, S. C. Nicholes, J. S. Parker and L.A. Coldren, IEEE Phot. Techn. Lett., 22, no. 2, Jan 2010.

[50] Y. Ikuma et al., Electron. Lett. , 46, 368 (2010).

[51] Work in the NaPANIL project www.NAPANIL.org

[52] See, for example, Silicon Photonics, Eds. L. Pavesi and D. J. Lockwood, Springer (2004); Silicon Photonics II: Components and Integration, Eds. D. J. Lockwood and L. Pavesi, Heidelber-Dordrecht-London-New York, Springer 2011; and Silicon Photonics III: Systems and Applications, Eds. D. J. Lockwood and L. Pavesi, Springer (2012).

[53] http://fisicavolta.unipv.it/nanophotonics/ Projects/lecsin/index.htm

[54] A. Zayats et al., Phys. Report ,408 131 (2005).

[55] S. Kim, *Nature* 453, 757 (2008).

[56] A. Nevet, et al., Nanoletters 10, 1848 (2010).

[57] V. Valev, ACS Nano 5, 91, (2011).

[58] M. Lapine et al., Scientific Reports, 1,138 (2011).

[59] A. Belardini et al., Phys. Rev. Lett., (2011) DOI: 10.1103/PhysRevLett.107.257401.

[60] www.st-andrews.ac.uk/physics/splash

[61] www.gospel-project.eu/Web/index.php

[62] V. Laude et al., Opt. Express, 19, 9690 (2011).

[63] J. Chan et al., Nature 478, 89 (2011).

[64] M. Eichenfield, J. Chan, R. Camacho, K. J. Vahala and O. Painter, Nature 462, 78 (2009).

[65] T.J. Kippenberg and K.J. Vahala, Science 321, 1172 (2008).

[66] D. Van Thourhout and J. Roels, Nature Photonics 4, 211 (2010).

[67] M. Eichenfield et al., Nature 462, 78 (2009); M. Eichenfield at al., Nature 459, 550 (2009).

[68] Y. Pennec, at al., Opt. Express 18, 14301 (2010); V. Laude et al., Opt. Express, 19 9690 (2011).

[69] D.A. Fuhrmann et al., Nature Photonics 5, 605 (2011).

[70] R. Li Voti, C. Sibilia and M. Bertolotti, International Journal of Thermophysics, 26 1833 (2005).

[71] O. B. Wright et al., J. Appl,. Phys. 91 5002 (2002).

[72] Yan Pennec et al. Surface Science Reports 65, 229 (2010).

[73] Yan Pennec et al. Opt. Express 18, 14301 (2010).

[74] J. Cuffe et al. Microelectronic Engineering 88, 2233 (2011).

[75] M. Eichenfield et al. Nature 459, 550 (2009).

[76] J. O. Vasseur et al., Phys. Rev. Lett. 86, 3012 (2001).

[77] A. Khelif et al., Phys. Rev. B 68 214301 (2003); A. Khelif et al., Appl. Phys. Lett. 84 4400 (2004).

[78] A. Khelif et al., J. Appl. Phys. 94 1308 (2003).

[79] J. Tang et al., Nano Letters 10, 4279 (2010).

[80] Yu, J.-K et al., Nat.Nanotechnol. 5, 718 (2010).

[81] W. Kim, R. Wang, A. Majumdar*,* Nano Today *2,* 40 (2007).

[82] D. Li et al, Applied Physics Letters 83, 2934 (2003); A.I. Hochbaum et al, Nature 451, 163 (2008).

[83] G.P. Srivastava, The Physics of Phonons, Taylor & Francis, New York (USA) and Milton Park (UK) (1990).

[84] A. Henry and G. Chen, J. Computational and Theoretical Nanoscience 5, 141 (2008).

[85] P.G. Klemens, Proc. Royal Society (London) A208, 108 (1951).

[86] J. Callaway, Physical Review 113, 1046 (1959); M. G. Holland, Physical Review 132, 2461 (1963).

[87] C. Herring, Physical Review 95, 954 (1954).

[88] A. Huynh, N. D. Lanzillotti-Kimura, B. Jusserand, B. Perrin, A. Fainstein, M. F. Pascual-Winter, E. Peronne, and A. Lemaıtre. Phys. Rev. Lett. 97, 115502 (2006).

[89] E. Grossman et al., Applied Optics 49 E106 (2010).

[90] J.V. Goicochea, M. Madrid and C. H. Amon, ASME Journal of Heat Transfer, 132, 102401 (2010).

[91] C. Gomes, M. Madrid, J.V. Goicochea. and C. H. Amon, C.H., ASME Journal of Heat Transfer, 128, 1114 (2006).

[92] J.V. Goicochea. and B. Michel, THETA3 Conference 2010, Cairo, Egypt.

[93] J.V. Goicochea, W. Escher, X. Tang, and B. Michel, SEMITHERM 2010, Santa Clara, CA, USA.

[94] M. Hu, K. P. Giapis, J.V. Goicochea, X. Zhang, B. Michel and D. Poulikakos, Nano Lett. 11, 618 (2011).

[95] J.V. Goicochea, M. Hu, B. Michel and D. Poulikakos, ASME Journal of Heat Transfer, 2011 (in press); M. Hu, J.V. Goicochea, B. Michel and D. Poulikakos, Nano Letters 10 279 (2010); M. Hu, J.V. Goicochea, B. Michel and D. Poulikakos, Applied Physics Letters, 95, 151903 (2009).

[96] J.V. Goicochea and B. Michel, SEMITHERM 2011, San Jose, CA., USA.

[97] S. Maruyama, Y. Igarashi, Y. Taniguchi and J. Shiomi, J.Thermal Science and Technology, 1 138 (2006); X. Ruan and Y. Chen, Nano Letters, 9, 2730 (2009).

[98] C. F. Carlborg, J. Shiomi and S. Maruyama, Phys. Rev. B, 78, 205406 (2008); J.V. Goicochea, W. Escher, X. Tang and B. Michel, THERMINIC 16th, 2010, Barcelona, Spain.

[99] J.V. Goicochea, M. Madrid, C. H. Amon, THERMINIC 15th, 2009, Brussels, Belgium.

[100] H. Dammak, Y. Chalopin, M. Laroche, M. Hayoun and J.-J. Greffet, Phys. Rev. Lett., 103, 190601 (2009); J.-S. Wang, Phys. Rev. Lett., 99, 160601 (2007); D. Duffy and A. Rutherford, J. Physics: Condensed Matter, 19, 016207 (2007).

[101] Thermal Nanosystems and Nanomaterials, S. Volz ed. Springer, Topics in Applied Physics 118 (2010).

[102] G. Domingues, S. Volz, K. Joulain and J.-J. Greffet, Phys. Rev. Lett., 94, 085901 (2005).

[103] E. Rousseau, A. Siria, G. Jourdan, S.Volz, F. Comin, J. Chevrier and J.-J. Greffet, Nature Photonics, 3, 514 (2009).

[104] A. Rajabpour and S. Volz, J. Appl. Phys., 108, 94324 (2010).

[105] J. B. Pendry, J. Phys.: Condens. Matter 11 6621 (1999).

[106] K. Joulain et al., Surf. Sci. Rep. 57, 59 (2005).

[107] A. I. Volokitin and B. N. J. Persson, Rev. Mod. Phys. 79, 1291 (2007).

[108] See, for example, E. Rousseau et al., Nature Photonics 3, 514 (2009).

[109] M. Prunnila and J. Meltaus, Phys. Rev. Lett. 105, 125501 (2010).

[110] I. Altfeder, A. A. Voevodin, and A. K. Roy, Phys. Rev. Lett. 105, 166101, (2010).

[111] S. Bramhavar et al. Phys. Rev B 83, 014106 (2011).

[112] F. Giazotto, T.T. Heikkilä, A. Luukanen, A.M. Savin and J.P. Pekola, Rev. Mod. Phys. 78, 217 (2006).

[113] A.V. Timofeev, M. Helle, M. Meschke, M. Möttönen, and J.P. Pekola, Phys. Rev. Lett. 102, 200801 (2009); M. Meschke, W. Guichard and J. P. Pekola, Nature 444, 187 (2006). J. P. Pekola et al., Phys. Rev. Lett. 105, 026803 (2010).

[114] D. V. Averin and J. P. Pekola, Phys. Rev. Lett. 104, 220601 (2010).

[115] J.T. Muhonen, A.O. Niskanen, M. Meschke, Yu.A. Pashkin, J.S. Tsai, L. Sainiemi, S. Franssila, and J.P. Pekola, Appl. Phys. Lett. 94, 073101 (2009).

[116] J.-S. Heron, C. Bera, T. Fournier, N. Mingo and O. Bourgeois, Phys. Rev. B 82, 155458 (2010).

[117] N. Mingo, D. Hauser, N. P. Kobayashi, M. Plissonnier and A. Shakouri, Nano Letts 9 711 (2009).

[118] G. Pernot et al., Nature Materials 9 491 (2010).

List of contributors

- Prof. Jouni Ahopelto (VTT Technical Research Centre of Finland, Finland).
- Dr. Francesc Alsina (Catalan Institute of Nanotechnology, Barcelona, Spain).
- Dr P.-Olivier Chapuis (Center for Thermal Sciences of Lyon (CETHIL), INSA Lyon - Université Claude-Bernard Lyon 1 - CNRS, France).
- Prof. Bahram Djafari-Rouhani (IEMN, CNRS, France).
- Dr. Javier Goicochea (IBM Zurich Research Laboratories, Switzerland).
- Dr. Jordi Gomis-Bresco (Catalan Institute of Nanotechnology, Barcelona, Spain).
- Dr. Nikolaos Kehagias (Nanofabrication Division, Catalan Institute of Nanotechnology, Barcelona, Spain).
- Prof. Thomas F Kraus (University of Saint Andrews, Scotland, UK).
- Dr. Stefan Landis (CEA-LETI, Grenoble, France).
- Prof. Vincent Laude (Institut FEMTO-ST, Université de Franche-Comté, CNRS, Besançon, France).
- Dr. Roberto Li Voti (Universita’ di Roma La Sapienza – Dept. of Basic and Applied Science, Italy).
- Prof. Sebastian Lourdudoss (KTH, Sweden).
- Dr. Tapio Mäkelä (VTT Technical Research Centre of Finland, Finland).
- Dr. Alejandro Martinez (Nanophotonics Technology Center, Universidad Politécnica de Valencia, Spain).
- Prof. Andrea Melloni (Dipartimento di Elettronica e Informazione, Politecnico di Milano, Italy).
- Dr. Natalio Mingo (CEA-LITEN, Grenoble, France).
- Prof. Lorenzo Pavesi (Nanoscience Laboratory, University of Trento, Italy).
- Prof. Jukka Pekola (Low Temperature Laboratory, Aalto University, Finland).
- Dr. Mika Prunnila (VTT Technical Research Centre of Finland, Finland).
- Dr. Vincent Reboud (CEA-LETI, France).
- Dr. Francesco Riboli (LENS, Florence, Italy).
- Prof. Concita Sibilia (Universita’ di Roma La Sapienza – Dept. of Basic and Applied Science, Italy).
- Prof. Clivia M Sotomayor Torres (ICREA, Catalan Institute of Nanotechnology and Univ. Autonoma de Barcelona, Spain).
- Prof. Sergei Tretyakov and Partners of the European Virtual Institute *Metamorphose* (Aalto University, Finland; Virtual Institute Metamorphose www.metamorphose-vi.org).
- Prof. Sebastian Volz (EM2C, UPR CNRS, France).
- Prof. Diederik Sybolt Wiersma (LENS, Florence, Italy).
- Dr. Heiko Wolf (IBM Zurich Research Laboratories, Switzerland).

BioInspired Nanotechnologies

There is no doubt that bioinspired nanotechnology bears approaches dealing with Information, communication, and data treatment. It is even worth considering that the increase of our understanding of life systems will be of great use to conceive new methods in the domain of information. However while being a very reasonable proposal, it remains of great difficulty trying to define what could be information in a life system, in turn to use this to develop new dynamical networks creating and processing information. One usual, and old working hypothesis was that it does exist a genetic code, constructed with the same basis that of sequences of bit information, that determines the whole machinery and replication. This naïve and simple picture suggests that the development of life systems is based on an alphabet, from which it is enough to understand the organization of the letters for to understand the words that are constructed. Following this aim, we should be able to read DNA sequences that would be equivalent to sentences and, ultimately a book. If such a picture is correct, the road map is simple: as soon as you have grasp the whole alphabet with its grammatical rules, not only you can read any book but you may write yours. Based on this analogy, metabolic and anabolic activities can be seen as sophisticated books derived from the genetic code alphabet and its companion grammatical rules running the protein synthesis. Therefore, it should be just a question of time to question and solve any processes belonging to life systems or else, using the analogy with computing science, to produce appropriate algorithm that help to understand or produce life systems. However, we know that restricting the behaviour of life system to a computing process, whatever the level of complexity of the computer architecture, is by far too much a reductionist approach and strictly does not hold as the appropriate picture. Nevertheless, it is safe and of some use

Position Paper on BioInspired Nanotechnologies

DNA sequences: the building bit unit to simulate information processing in life systems?

Jean-Pierre Aimé
CNRS_CBMN UMR 5248, University of Bordeaux (France)
Chair Nanosciences Nanotechnologies network C'nano GSO
Chair COST TD 1003 «Bioinspired nanotechnologies»

1. Bioinspired nanotechnology and information

There is no doubt that bioinspired nanotechnology bears approaches dealing with Information, communication, and data treatment. It is even worth considering that the increase of our understanding of life systems will be of great use to conceive new methods in the domain of information. However while being a very reasonable proposal, it remains of great difficulty trying to define what could be information in a life system, in turn to use this to develop new dynamical networks creating and processing information. One usual, and old working hypothesis was that it does exist a genetic code, constructed with the same basis that of sequences of bit information, that determines the whole machinery and replication. This naïve and simple picture suggests that the development of life systems is based on an alphabet, from which it is enough to understand the organization of the letters for to understand the words that are constructed. Following this aim, we should be able to read DNA sequences that would be equivalent to sentences and, ultimately a book. If such a picture is correct, the road map is simple: as soon as you have grasp the whole alphabet with its grammatical rules, not only you can read any book but you may write yours. Based on this analogy, metabolic and anabolic activities can be seen as sophisticated books derived from the genetic code alphabet and its companion grammatical rules running the protein synthesis. Therefore, it should be just a question of time to question and solve any processes belonging to life systems or else, using the analogy with computing science, to produce appropriate algorithm that help to understand or produce life systems. However, we know that restricting the behaviour of life system to a computing process, whatever the level of complexity of the computer architecture, is by far too much a reductionist approach and strictly does not hold as the appropriate picture.

Nevertheless, it is safe and of some use to start from the viewpoint that nature replicates, manipulates & creates Information, a route that many scientists use to better understand what could be the «origin of life». In other words, to design new systems of information one needs to investigate and understand how nature processes, although to have a good definition of what information is for life systems still remains challenging.

On the other hand, thanks to the emergence of nanoscience-nanotechnologies, we are able to access all the scale at which the life systems create and process information. In particular, the nanometer scale is of primary importance, as it happens to be the ultimate, smallest size, to bear functions still managing a good interaction with its neighbourhood. This kind of size optimization to create and transfer information is typical of what is observed with membrane proteins. Nanometer scale appears to be the right size: - large enough to afford sophisticated functions, see for instance the rodopsin proteins that converts photons to electrochemical potential across the membrane; - small enough to be easily insert in a given phospholipids environment with a surface area providing the ability to transfer the information to the surrounding medium.

2. Freeman Dyson conjecture and Self assembled-self organized systems

Gene code is in many instance a concept that have been discussed for long without leading to consensus, in many circumstance we are not able to identify specific genetic sequences with proteins synthesis so that an exact definition of what a gene is has still to be done. Many sequences appear to be involved in several proteins synthesis while splicing processes that involve several steps play an important role to select the transcribed RNA sequences governing the protein synthesis. Therefore, it is not straightforward to establish any robust causal rules between genetic code and protein products. One known example is the case of multiplication of prions showing that a structure with a specific shape and function can be replicated without the help of any gene coding, e.g. memory structure. There are many debates discussing the relationship between genotype and phenotype, among which a consequence is that the concept of mutation is far to be so clearly understood. There are no clear frontier allowing to decipher between coding sequences and well defined mutations that exhibit unambiguous consequence on the state of the targeted products.

In an attempt to present the aim of the present report ICT bioinspired final document, one wishes to cite a conjecture Freeman Dyson suggested 30 years ago in a small book titled “Origin of Life”. Following an analysis of the different attempts to reproduce experimental conditions from which spontaneous synthesis of amino acids and nucleotides sequences may emerge, F. Dyson were convinced that there was the need to set a new type of experiments. The book was a strong pleading for new experiments that mimic homeostasis condition that is suggesting which is now called with the generic expression “Synthetic Biology”. However, the main flaw of the various attempts to determine experimental conditions mimicking the evolution from the prebiotic period suggested him that DNA sequences were the parasitic products of ATP molecules that supplies the energy in many biochemical reactions. With a soap of AA where only thermodynamic rules were at work to synthesise more or less complex molecules, the rate of errors was large, about 10^{-3}, so that no reproducible synthesis of identical molecules can be expected. The situation was very much different with what happens with DNA replication thanks to regulatory gene network and competitive reaction rate leading to a error factor of 10^{-9}. The clever F. Dyson's idea was thus that, sequences of DNA were built as degraded products from ATP building a code acting as a memory of the type of molecules synthesised. In other words, information was created at the heart of a set of biochemical reactions. However, because there is no reason that code sequences were perfectly constructed for any kind of proteins products, neither do we expect that the sequences of synthesized DNA were of all of use, see for instance the viral DNA and RNA that can be considered as junk DNA of no use for metabolic activities. Therefore, the F. Dyson conjecture did ask many questions in the domain of information in life systems.

Based on these many questions and of the interest of synthetic biology, from a fundamental point of view, as well as a practical one, it is of importance to be able to design experiments that are close, as much as possible, from those in which complex chemical machineries are able to fabricate and control selected molecules with dedicated functions.

The interest of using DNA as a tool presents several advantages as for instance the simplicity and robustness of the WC pairing rules and the use of DNA tweezers and DNA origami platforms. These results make DNA sequences an attractive basic unit to build complex logical operations distributing information at different scales.

3. DNA the alphabet?

A natural way to analyse complex set of biochemical reactions can be readily address with the ability to represent the chemical reaction as sequences, in parallel or not, of logical gates, from which a hierarchy of Boolean operations can be design in place of the set of competitive chemical reactions. Simple logical abstraction can be conducted with the combination and control of chemical reaction networks made of DNA strands that behave as a succession of logical gate operations. With those approaches, it becomes possible to build truth tables of different level of complexities.

Following these remarks, it is of interest to focus the attention on the numerous works done in the domain of DNA nanotechnology, works that have been done over the last 3 decades. DNA nanotechnology gives the opportunities to build new approaches and tools that can both provide new insights on fundamental questions of how the life systems process information. DNA nanotechnology can also be able to bring efficient solutions for synthetic biology and to simulate adaptive neuronal networks. DNA nanotechnology has led to a wealth of objects and functions at many different scales. There is now a palette of numerous platforms from nanometer to micrometer scale. Also many strategies provide dynamical constructions, the dynamic of which being driven with DNA strand displacements and enzyme. Therefore, not only DNA is a unique self-assembled structure that provides a cheap platform with 5 nm resolution, it also gives the possibility to involve DNA molecular motors and prescribed pathways from which programmable motion and sequence of logical operations can be conceived and fabricated.

Below we select a few results of innovative and creative works to illustrate the main orientation of the bioinspired ICT.

3.1 DNA Molecular motors: DNA tweezers [1]

The creation of DNA tweezers as controllable molecular motors has had a great influence on the conception of many self-assembled and dynamical structures. DNA tweezers are

DNA molecular actuators that can act as catalytic DNA system and, since the beginning of its fabrication, were designed with the aim to fabricate self-guided self-assembly using molecular recognition that will allow construction of VLSI structures with molecular scale features.

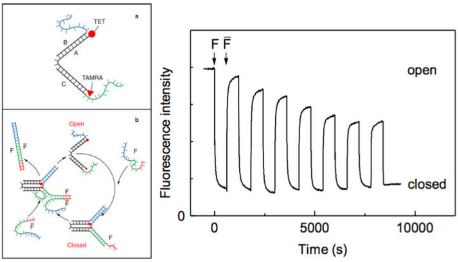


Figure 1. *Scheme of DNA tweezers with fuel and anti fuel strands and the use of FRET experiments with the fluorescent tags TET and TAMRA[1].*

3.2 DNA Origami [2,3]

The creation and fabrication of DNA origami is the kind of breakthrough that had a great influence on the development of the DNA nanotechnology and, probably, has been the key achievement that exemplifies the domain of DNA nanotechnology as a very efficient and powerful approach, may be similar to that of the silicon technology. The Origami nanometer platform presents several advantages that all support the use of DNA sequence as a basic technological tool:

- It is a simple, one pot, fabrication method.
- The yield can be as high as 90% without the need to obey severe constraints requiring expensive control steps. It is a robust fabrication method that should be able to produce billions of platforms without inducing many ill formed structures.
- DNA origami is a versatile platform able to integrate different developments, that is not only restricted to the DNA technology domain. Hybrid structures can easily be fabricated opening several possibilities to conceive input/output functions.
- DNA origami open new area of multi scale platforms still keeping the 5 nm resolution.
- DNA origami open new area of active platforms with the capability to change its topology and function under appropriate stimuli.

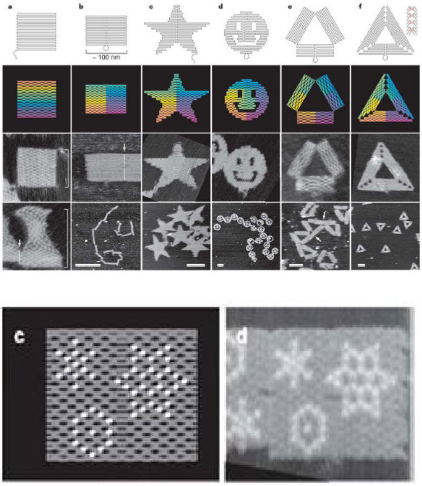


Figure 2. *Example of different structures of DNA origami and of the possibility to decorate the platform with desired functions with 5 nm spatial resolution [2]*

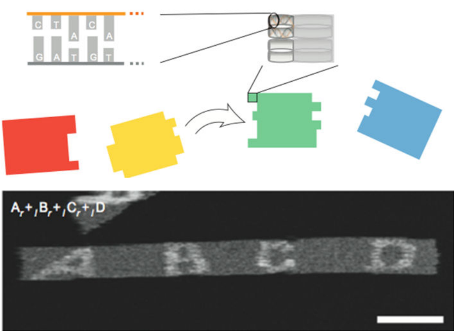


Figure 3. Combination of origami platforms providing controlled self-assembly up to the micrometer scale [3].

3.3 DNA Computing & Chemical reaction networks [4,5]

Since the Adelman' proposal, DNA contribution to computer science has led to numerous attempts. Recent developments showed that the concept of DNA computing can be used to simulate complex sets of biochemical reactions. As a result, DNA computing is switching towards new applications, in which DNA strand sequences act as inputs and outputs of series of logical operations. Recently, solutions involving more than hundred different DNA strands were prepared affording the possibility to run an already sophisticated chemical reaction network DNA, which can be usefully translated as combination of logical Boolean operation. These recent achievement allow the use of chemical reactions as logical operators providing a powerful approach to investigate structure and function of various complex systems. Several applications can be envisioned in the domain of neuroscience or health providing alternative to develop the theranostic objective (Figure 4).

3.4 DNA molecular motor: programmable motion and logical gate operation [6,7]

The strand displacement reactions that were successfully used with DNA tweezers, were then used in DNA computing but also by setting motion of molecular motors especially on biased pathways design with origami platforms.

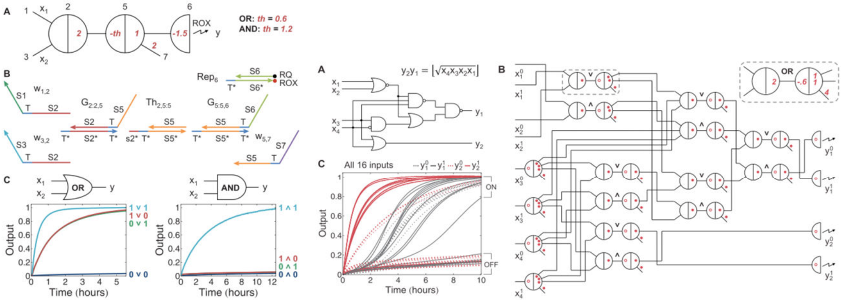


Figure 4. Example of OR and AND logical gates using the seesaw method based on the strand displacement technique and using the DNA strand input as a catalytic species. On the right, an example of already complex combination of logical gates to perform elaborate Boolean operations [4,5].

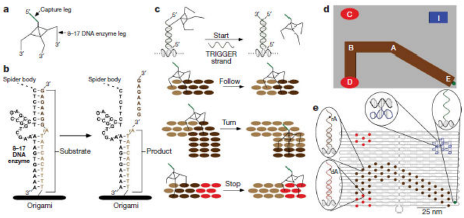


Figure 5. *Example of DNA molecular motors used as spider legs to migrate the spider along a biased pathways designed on a origami [6].*

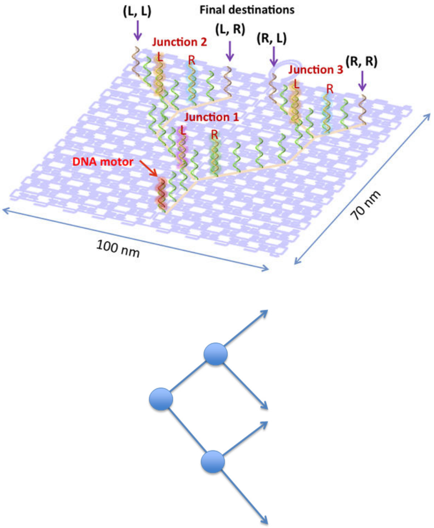


Figure 6. *Base on the work that show molecular robots guided by prescriptive landscapes, a step forward was to design a logical circuitry on an origami in which a molecular moves either to the left or the right at the node as a function of the information received [7]. On the top a scheme of the logical network (from the Sugiyama Lab, Kyoto University), on the bottom a simple diagram of the logical operations performed.*

In many cases, a unique molecule has only few conformational shapes available, thus a low capability to store a complex level of information. Therefore, the above strategy clearly shows that using a programmable motion on a track can overcome such a limitation. The second example shown below is a very good one of what can be achieved using both the motion of molecular motors and logical gate operations, the later acting as a signalization process.

3.5 Dynamical change of shape and topology

An interesting result was the demonstration that one may trigger topological transformation at hundredth nanometer scale by using fuel strands, e.g. the strand displacement technique. Hao Yan group designed a Moëbius stripe that can be converted in different structures by using fuel strands as a scissor. These finding affords a multi scale conception of topological transformation of network with creation and destruction of connections.

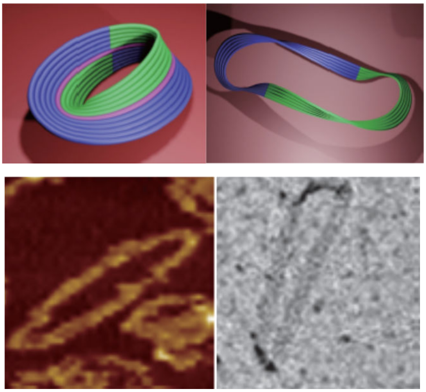


Figure 7. *Moëbius origami, which under the action of fuel strands, a molecular scissor, is converted on a simple stripe [8].*

4. References

[1] "A DNA-fuelled molecular machine made of DNA" ; Yurke, B., Turberfield, A. J., Mills, A. P., Simmel, F. C. & Neumann, J. L. et al Nature 406, 605 (2000).

[2] "Folding DNA to create nanoscale shapes and patterns"; P.W.K. Rothemund: Nature 440, 297 (2006).

[3] S. Woo, P.W. Rothemund Nature Chemistry |2011 | DOI: 10.1038/NCHEM.1070.

[4] "Scaling Up Digital Circuit Computation with DNA Strand Displacement Cascades"; L. Qian, E. Winfree: Science 332, 1196 (2011).

[5] "Neural network computation with DNA strand displacement cascades"; L. Qian, E. Winfree, J. Bruck: Nature 475, 368 (2011).

[6] "Molecular robots guided by prescriptive landscapes";K. Lund, A. J. Manzo, N. Dabby, N. Michelotti, A. Johnson-Buck, J. Nangreave, S. Taylor, R. Pei, M.N. Stojanovic, N.G. Walter, E. Winfree, H Yan: Nature 465, 206 (2010).

[7] “A DNA-based molecular motor that can navigate a network of tracks”. Shelley F. J. Wickham, Jonathan Bath, Yousuke Katsuda, Masayuki Endo Kumi Hidaka, Hiroshi Sugiyama and Andrew J. Turberfield. Nature Nanotechnology, V 7, p 170 (2012).

[8] Dongran Han, Suchetan Pal Yan Liu and Hao Yan; Nature Nanotechnology, vol 5, October 2010, p 712.

NEMS

he vibrant activities in the nano-scale research for producing finer nanostructures of various novel 1D and 2D materials, as well as advanced in on-chip integration and signal transduction supply strongly the development of NEMS. Several years of a highly interdisciplinary NEMS community at this stage yields extensive and important findings. This paper offers an update of activities in the research and development of NEMS over the last years. The following sections will describe the achievements and highlights the work done on fundamental studies using NEMS, their transduction and nonlinear behaviour, NEMS fabrication and incorporation of novel materials, including carbon-based 1D and 2D structures. NEMS fundamental and characteristic properties, e.g. high surface-to-volume ratios, extremely small masses and small onsets of nonlinearity, make of them an outstanding scientific tool to study different physical phenomena that would otherwise be not accessible. In particular, over the years NEMS have extensively been used as tools to probe quantum physics. Originally aimed to detect individual quanta of electrical [1] and thermal conductance [2-5], we have experienced in the last few years an exciting race to cool down systems to their mechanical ground state. Even though this was finally attained by using micron-sized devices [6-7], smaller devices, in the sub-micron range and even below 100 nm, are still of the greatest interest because they are more susceptible to be affected by back-action of the surroundings, like detection or actuation techniques. Interaction with a superconducting qubit [8] or coupling to electronic conduction are some of the examples that have been recently proved [9-10]. NEMS small mass makes them ideal for mass sensing experiments. Usually, mass detection experiments seek the detection of mass landing on to the device [11]. But they can also be used to study adsorption-desorption and diff

Position Paper on Nanoelectromechanical systems (NEMS)

V.Auzelyte[1], L. G. Villanueva[2], N. Barniol[3], F. Perez-Murano[4], W.J. Venstra[5], Herre S. J. van der Zant[5], G. Abadal[3], L. Nicu[6], V. Savu[1], M. Muoth[7], C. Hierold[7], J. Brugger[1]

[1] Microsystem Laboratory, Ecole Polytechnique Federal de Lausanne (EPFL), 1015 Lausanne, Switzerland
[2] California Institute of Technology, 1200 E California Blvd., MC 149-33, Pasadena, CA, USA
[3] Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona (UAB), E-08193 Bellaterra, Spain
[4] Insititut de Microelectrònica de Barcelona (IMB-CNM, CSIC). Campus de la UAB. E-08193 Bellaterra. Spain
[5] Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands
[6] CNRS-LAAS, 7 avenue du Colonel Roche, F-31077 Toulouse, France

[7] Micro and Nanosystems, Department of Mechanical and Process Engineering, ETH Zurich, Tannenstrasse 3, 8092 Zurich, Switzerland

1. Introduction

The vibrant activities in the nano-scale research for producing finer nanostructures of various novel 1D and 2D materials, as well as advanced in on-chip integration and signal transduction supply strongly the development of NEMS. Several years of a highly interdisciplinary NEMS community at this stage yields extensive and important findings. This paper offers an update of activities in the research and development of NEMS over the last years. The following sections will describe the achievements and highlights the work done on fundamental studies using NEMS, their transduction and nonlinear behaviour, NEMS fabrication and incorporation of novel materials, including carbon-based 1D and 2D structures. Applications in the fields of electronics using linear and non-linear NEMS, bio-NEMS as well as energy scavenging will be covered. The following text is an update of the position paper published in 2008 in E-Nano Newsletter nº 14 (www.phantomsnet.net/Foundation/Enano_newnewslet14.php).

2. Fundamental studies

NEMS fundamental and characteristic properties, e.g. high surface-to-volume ratios, extremely small masses and small onsets of nonlinearity, make of them an outstanding scientific tool to study different physical phenomena that would otherwise be not accessible. In particular, over the years NEMS have extensively been used as tools to probe quantum physics. Originally aimed to detect individual quanta of electrical [1] and thermal conductance [2-5], we have experienced in the last few years an exciting race to cool down systems to their mechanical ground state. Even though this was finally attained by using micron-sized devices [6-7], smaller devices, in the sub-micron range and even below 100 nm, are still of the greatest interest because they are more susceptible to be affected by back-action of the surroundings, like detection or actuation techniques. Interaction with a superconducting qubit [8] or coupling to electronic conduction are some of the examples that have been recently proved [9-10].

NEMS small mass makes them ideal for mass sensing experiments. Usually, mass detection experiments seek the detection of mass landing on to the device [11]. But they can also be used to study adsorption-desorption and diffusion of particles on the device surface [12], leading to deeper understanding of the microscopic dynamics of deposited materials, together with understanding of the limitations of mass sensing with NEMS [13]. In [12], the authors used a system to perform mass spectroscopy measurements in order to monitor the landing of Xe atoms on top of the NEMS. The landing of atoms can be switched on/off via a shutter (Figure 1a). By continuously running a phase locked loop, the frequency is monitored over time for different temperatures of the device. The frequency stability can be therefore plotted as a function of temperature and different models for adsorption desorption can be checked. The data indicates that diffusion along the beam, an effect neglected up to date, is the dominant effect at lower temperatures (Figure 1b).

An additional topic of interest is the study of nonlinear and complex dynamics with NEMS. Their reduced dimensions make their onset of nonlinearity to be quite small, readily accessible, and easily predicted theoretically. In addition, their high quality factors and even higher frequencies make them easy to analyze quasi Hamiltonian systems and also to experimentally measure stationary states reached in very short times, i.e. few milliseconds. Finally, their small size facilitates array fabrication, which increases the complexity and the interest of the systems to be studied [14]. Numerous theoretical studies have been undertaken and published in recent years dealing with nonlinear behavior and its implications for certain applications. Euler instability in clamped-clamped beams [15] and diffusion induced bistability [16] are some of those examples.

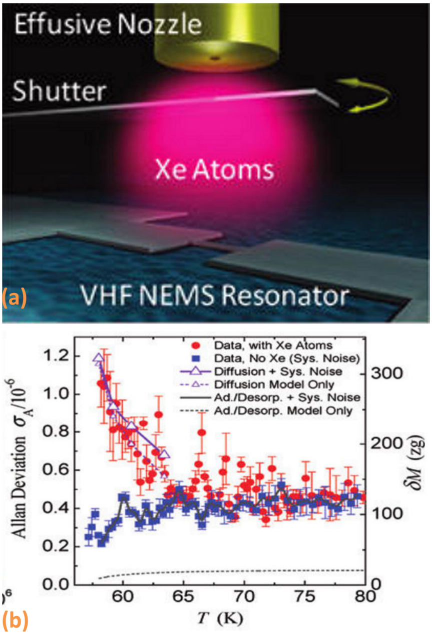


Figure 1. Experimental determination of the nature of frequency noise in NEMS [12] (a) Schematic showing the system utilized for the experiment with a clamped-clamped silicon carbide beam in a cryostat with a nozzle that ejects Xe atoms on the sample. (b) Frequency stability as a function of temperature with and without Xe atoms landing on the device. The noise cannot be interpreted as being caused by only adsorption/desorption of particles, but by the inclusion of diffusion of particles.

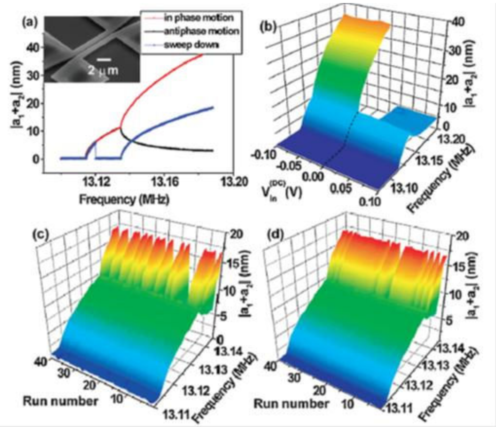


Figure 2. Bifurcation Topology Amplifier [18] (a) Experimental measurement of the parametric response of two uncoupled NEMS beams, confirming the predicted pitchfork bifurcation. Inset: pair of coupled clamped-clamped beams to perform the experiment. (b-d) Amplitude response of the coupled system as a function of frequency. When the voltage difference between the beams is zero (b) the system presents a perfectly symmetric behaviour and the upper branch is chosen 50% of the time. If the voltage is slightly negative (c) or positive (d) (±3 mV) the symmetry gets broken, as predicted by theory. This symmetry breaking can be interpreted as a very effective signal amplifying sensor.

Experimentally, the verification of the predicted behavior of a system of two coupled resonators has been shown screening rich nonlinear dynamics and even chaos [17]. A novel detection system has been proposed, based on symmetry breaking close to a Hopf bifurcation (Figure 2) [18]. But it has also been proven that it is not necessary to have arrays of individual beams to observe such behavior. Due to the nature of the nonlinearity in NEMS, it is also possible to observe such effects on one single beam using the existing coupling between several vibrational modes, which is of great importance when considering frequency-based sensing or similar applications [19]. Finally, NEMS have also been used to observe nonlinear damping in mechanical resonators, something that had not been observed before and which origin is not understood, predicted or modeled [20].

3. Transduction at nanoscale

The reduced size is what makes NEMS appealing from a fundamental and applications point of view. But everything comes at a cost, and the trade-off we need to pay in order to have such outstanding, e.g., sensing capabilities is very low transduction efficiencies.

In order to use a NEMS, it is necessary to make it move (actuation) and to detect such motion (detection). The combination of actuation and detection is what is usually referred as transduction. Finding an optimal transduction technique that works universally for a wide variety of NEMS has been pursued by many different research groups.

We can divide transduction mechanisms in two big groups, those based (or using) optics and those based (or using) electronics. The first group had been traditionally overlooked for NEMS, as diffraction effects were assumed to be detrimental when going deep into the sub-micron regime. However, recent experiments have shown that it is possible to not only detect motion [21-23], but also to actuate NEMS devices using optics (Figure 3) [24-26]. Another point against optical transduction methods was that they could not be integrated on-chip, which limited the future applicability of such methods. However, this has also been disproved, and integrated solutions for optical transduction have been proposed [24, 27].

But even though optics seems to be catching up, electronic transduction is usually preferred, mainly due to on-chip integration possibilities. A plethora of methods have been used over the years: magnetomotive [28], thermoelastic [29], piezoelectric [30-31], capacitive [32], ferromagnetic [33], Kelvin polarization force [34], etc. A common problem for any of these methods is the fact that the motional signal produced by the NEMS is minute when compared to the parasitic cross-talk coming from the actuation signal. This is mainly caused by the great size difference between the NEMS and the necessary elements to connect it to the macroscopic world like metal pads, wire bonds, etc. This undesired effect creates a background on the response of the device that hides the actual mechanical signal and makes it very difficult to be distinguished, which in turn affects the stability of the closed-loop systems, used for frequency-based sensing. A number of solutions have been proposed to solve this issue, most of them based on the use of some mixing mechanism that moves the frequency of the detected signal away from the frequency of the actuating signal. Down-mixing [35], amplitude modulation [36-37], frequency modulation [20, 38], use of superior harmonics actuation [39], parametric actuation [40] are some of the mentioned techniques used to cancel the effect of the background and have given much more stability and superior performance than more traditional approaches as direct bridging of the signal [41-42].

However, even though these techniques have proven very useful from a research point of view, the most promising option for future integration and with wider applicability is the use of an on-chip amplifier located very close to the NEMS [43], or even within the mechanical device itself [44-47]. The amplifier boosts the motional signal, making it bigger and less susceptible to the parasitic effect mentioned before. At this point the problem then stops being the NEMS and becomes electronic (how to lay-out best a series of transistors to obtain the biggest gain with the smallest noise) and/or technological (how to integrate on-chip the mechanical device with the adjacent electronic circuitry).

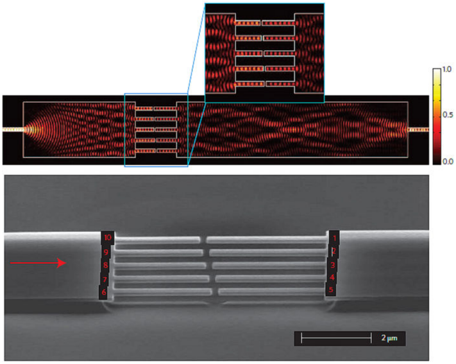


Figure 3. Novel transduction mechanisms for the nanoscale- photonic circuit. Simulation of the light propagation through an array of NEMS, shown in SEM image below, when no motion is present. As soon as the cantilevers start moving, misalignment occurs, and therefore the output intensity gets modulated [24].

4. Materials, Fabrication & System integration

Most of the fabrication methods used for investigating the ultimate performance of NEMS devices still rely on silicon based technology. The reason is the combination of good mechanical properties and well-established processing methods. Mechanical resonators require materials that provide high quality factors and high resonance frequency. For this reason, the most relevant progress in the exploitation of the functional properties of NEMS devices has been obtained with devices made of silicon [48-49], silicon nitride [50-51], silicon carbide [52-55] or related materials like SiCN [56], addressing a range of diverse aspects like ultra-high frequency operation [49], information processing [48], parametric amplification [51-52] or sensing [53, 57]. Remarkably, silicon is also present in the promising approach of building-up devices based on bottom-up fabrication methods. For example, a silicon NEMS resonator made of a single silicon nanowire grown by CVD methods combines good mechanical properties, ultra high mass sensitivity and additional functionality given by the possibility of exciting flexural modes in two dimensions [58] (Figure 4).

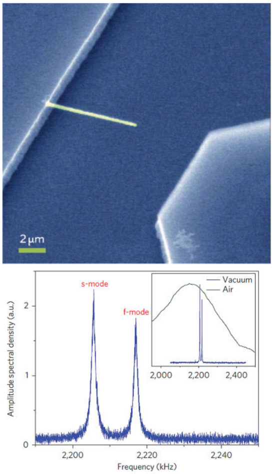


Figure 4. *NEMS resonator made of a single crystalline silicon nanowire provides good mechanical properties, high resonance frequency and high quality factor, that can be exploited to build-up ultra-high sensitivity mass sensors, including extra functionality due to the existence of several resonance modes. The frequency response of the nanowire can be detected by optical methods [58].*

In parallel to this majority use of silicon based technology, an increasing attention is being paid to piezoelectric materials due to the possibility of easy implementation of self-transduction (sensing and actuation) [31, 44, 59-60]. Realization of SiN/AlN piezoelectric cantilevers was made (Figure 5). 50 nm thick AlN films presents high piezoelectric coefficient that enables electrical transduction with excellent frequency stability, while SiN provides the good mechanical behaviour, demonstrating an achievable limit of detection of 53 zg/μm^2.

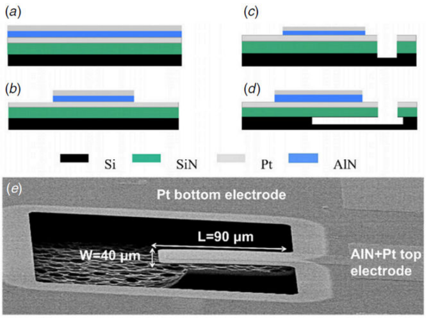


Figure 5. *Fabrication process and SEM picture of cantilevers with 50 nm thick AlN films that provide ultra-high sensitivity mass sensing with electrical transduction [59].*

Electron beam lithography is still the most used method to define NEMS devices from an experimental point of view, as it is a simple and proven method, although not convenient for massive fabrication and future industrial application. New prototyping approaches have been recently reported, including the use of focused ion beams [61-65]. However, little progress has been made in finding processes that would allow scaling up the fabrication of NEMS. Some activities include the technology being developed by the so-called *Nanosystems alliance* between Leti and

Caltech [66], optical based technologies for fabricating single carbon-nanotube devices [67], and the extension of CMOS technology to integrated NEMS resonators in microelectronic circuits taking advantage of the high resolution provided by DUV optical lithography [68-72] (Figure 6).

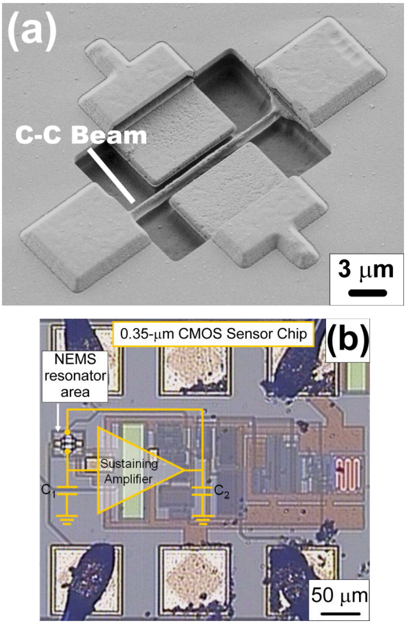


Figure 6. Integration of NEMS into CMOS using conventional DUV optical lithography. (a) Shows an SEM image of clamped-clamped metallic beam: the closely located electrodes serve for electrostatic actuation and capacitive detection. The resonator is monolithically integrated into the CMOS circuit shown in (b) for building-up a self-oscillator system [69]

Besides the top-down fabrication, new approaches have been explored for parallel integration of 1D nanostructures (carbon nanotubes (CNTs), Si NW, ZnO NW) into functional devices. Usually a bottom-up technique is necessary for growing from small amounts of catalysts wire-like nanostructures in a specific chemical and thermal environment. Blank or micrometer-size "forests" of such 1D nanostructures can be easily grown from lithography-defined catalysts. But reaching a position-controlled, single-digit number of wires using parallel fabrication techniques is still a worth-while goal. The localized synthesis can be done by having control either over the thermal environment or over the catalyst position. Blank deposition of the catalyst material combined with localized heating during the growth has been demonstrated [73-81]. Both methods are consistent with horizontal growth on vertical sidewalls, enabling the nanostructures to be positioned between two electrodes.

An alternative method is the localized deposition of the catalyst via parallel techniques such as stencil lithography. The advantage here is the possibility of reaching the single nanostructure limit with high-resolution positioning accuracy [82-83]. Self-limiting deposition of carbon nanotubes from suspension gains control on the number and simultaneously on the orientation of nanostructures positioned between electrodes, allowing for piezoresistive pressure sensors based on single-walled CNTs [84].

The fabrication of suspended nanotube devices was also demonstrated by on-chip stencil lithography that allowed resistless fabrication of electrical contacts to as-grown single-walled CNTs (Figure 7). Contamination issues of wet chemistry are avoided and hysteresis-free CNT FET operation was achieved. Furthermore, shadow masking is compatible with a wide range of contact materials and the contacts are self-aligned to the suspended section of the nanotube [85]. To fully benefit from the tapered contact geometry and the material compatibility, large-scale processes have to substitute the manual movement of the shadow masks. The reduction of charge traps by metallising all oxide surfaces may contribute to drift-stability in the electronic readout of NEMS and cleanliness might help to minimize damping.

In graphene-based NEMS, lithographically fabricated graphene edges are typically nanometre-rough, which can affect the uniformity of characteristics in a set of devices. Cai et al. [86] achieved ultimate dimensional precision by a synthesis technique based on covalent interlinking of precursor monomers. This chemical route provides atomically precise edges and uniform widths of graphene nanoribbons. So far, the surface-assisted synthesis requires metallic substrates hindering device fabrication. Transfer to technologically relevant non-conducting substrates, dedicated etching processes or alternative synthesis surfaces will be needed for NEMS fabrication. The demonstration of junction monomers encourages further investigations to engineer covalently bonded electrical contacts to atomically precise graphene nanoribbons.

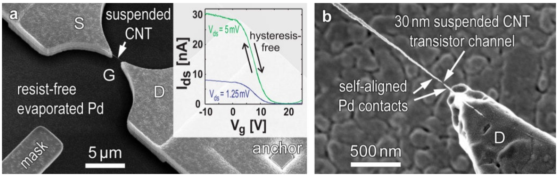


Figure 7. Hysteresis-free transistor response of a suspended carbon nanotube contacted by contamination-free shadow masking [85]. (a) SEM image of a nanotube transistor and electrical transfer characteristics. The shadow mask is retracted. (b) Close-up view of the same 30 nm long transistor channel with self-aligned Pd contacts.

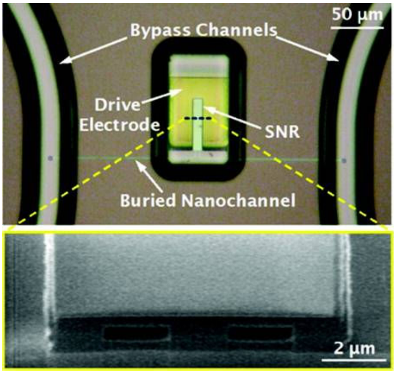


Figure 8. Suspended nanochannels used for the realization of NEMS mass sensors, providing a mass resolution below 30 ag [94].

Combination of NEMS devices with CMOS circuits provides also a route towards system integration, as it incorporates on-chip the functionalities of signal read-out and amplification. Alternative directions to integration have been proposed in order to reduce the parasitic signals in capacitive detection [87-88]. In addition, many efforts are directed towards combination with diverse devices and structures: integration of field effect transistor for electrical read-out [89-90], integration of a Schotky diode for optical detection [91], integration of waveguides [92-93] and integration of nanofluidic channels [94]. In this latter approach, the degradation of the performance that experience mechanical resonators when operated in solution due to the viscose drag is overcome by defining a suspended nanochannel (Figure 8). Using this approach, the best mass resolution in solution using NEMS sensing 27 ag has been demonstrated. A step further in the use of NEMS for system integration is the proposal of using piezoelectric NEMS resonators for extracting signals from biosensors [95].

5. Electronics

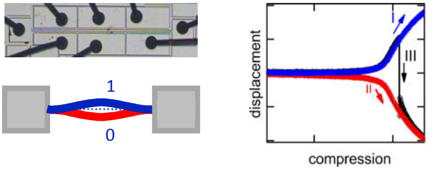
NEMS devices may play a role in future electronics both in the analogue and digital areas. For several years they have been proposed as basic building blocks for telecommunication systems by replacing components that cannot be integrated using conventional technologies. More recently, application of NEMS in information processing is gaining more attention, mainly because their lower power consumption and harder resistance to harsh environments compared to pure electronic processing in miniaturized systems. Application of NEMS for developing high efficiency telecommunication systems is being addressed by several groups [43, 67-68, 70-71, 96-104]. NEMS resonators are called to replace quartz crystals in the field of the RF communications due to their capability to be fabricated with standard IC process, the higher frequencies they can achieve and the small area they require.

The primary building blocks for any telecommunication system are oscillators. Self-sustaining oscillator with feedback can be implemented by employing a NEMS resonator as the frequency determining element for the feedback oscillator. Such NEMS oscillators are active systems that are self-regenerative; thus are distinct from the more readily available NEMS resonators, which are passive devices and require external signal sources to provide periodic stimuli and driving forces to sustain the desirable stable oscillations. Therefore the NEMS oscillators clearly could have important potential for a number of emerging applications. An important drawback when reducing the dimensions of NEMS is the resulting increase of the motional resistance, especially for the use of capacitive detection. In this case, piezoresistive sensing is viewed as a promising alternative [104]. Some other relevant examples of the use of NEMS for telecommunications are the mechanical implementation of filters [70] and frequency convertors [96].

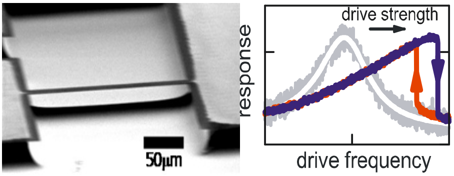
NEMS switches also present great potential for application in other areas, like logic computation [105] and memories [48, 106]. Main advantages are not only the expected lower power consumption [107], but also the possibility for operation at high temperatures [54]. The feasibility of building-up several computational and memory blocks by using only passive components and mechanical switches has been recently demonstrated [108]. Although NEMS-based switches cannot compete with MOSFETs in terms of switching speed, they can provide alternative paths for reduction power consumption of electronic circuits, with possibilities for high density integration [109]. A paradigmatic example is the realization of the analogous of a semiconductor transistor by means of a three-terminal NEMS switch [110]. NEMS switches provide zero leakage current, almost infinite sharp on/off transitions and a square hysteresis window.

6. Nonlinear MEMS/NEMS applications

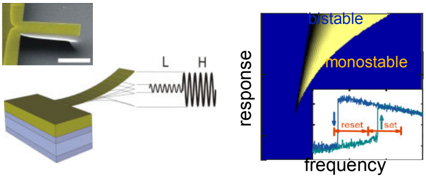
Mechanical sensors and actuators usually act as linear transducers. It is worthwhile having a look at the behaviour of mechanical resonators several 10s of microns in size to learn and adapt to sub-micron scale, where possible. At large amplitudes nonlinear effects dominate the response and reduce the range over which mechanical resonators can be applied as linear transducers. Nonlinear effects can be balanced in order to restore a linear response [88, 111-113]. On the other hand, there is a growing interest in MEMS/NEMS operating in the nonlinear regime. Characteristic phenomena were observed in the nonlinear regime, including multi-stability, hysteresis, and chaotic motion [14, 19, 114-115]. Several new applications based upon nonlinear MEMS/NEMS have been demonstrated. This is an important range in sensor applications, and to enhance it several concepts have been proposed.



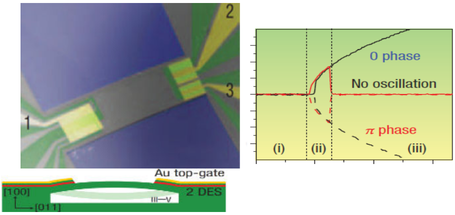
(a) Euler buckling: A doubly-clamped beam buckles when the compressive stress exceeds a critical limit. The post-buckled state, up(1) or down(0), represents one bit of information [106, 116-118].



(b) Duffing nonlinearity: In doubly-clamped beams and strings, the displacement-induced tension results in bistability. At the same drive conditions, vibrations with a high and a low amplitude are stable [19, 133].



c) Geometric nonlinearity: In cantilever beams vibrating at large amplitudes, by the geometric nonlinearity the resonance frequency becomes dependent on the amplitude. The amplitude of a strongly driven cantilever is bistable [88, 120-121].



(d) Parametric instability: A parametric oscillator is driven by modulating the spring constant at twice the resonance frequency [122-123]. Information can be encoded in the oscillator phase: Φ=0 (0) or Φ=π (1) are stable.

***Figure 9**. Nonlinearities in microresonators: the designs and responses of doubly-clamped beams, wires and singly-clamped cantilevers.*

Figure 9 summarizes four nonlinearities in doubly clamped beams or wires and singly clamped cantilevers that are 10s of micrometer in size. Euler buckling, Duffing nonlinearity, geometric nonlinearity and parametric instability. Perhaps the best-known instability in mechanics is Euler buckling (Figure 9 a) and makes use of a buckled bistable beam that does not require energy to remain in a bistable state. This enables applications in micromechanical relays, switches and non-volatile memory [106, 116-118]. Other nonlinearity in doubly clamped resonators is due to the displacement-induced tension, Duffing nonlinearity (Figure 9 b). Here two vibration amplitudes can be stable at the same driving conditions and fast transitions between the states can be induced by applying short excitation pulse. The distinct jumps in this bistable response can be used to resolve closely spaced resonators in arrays [113, 119-120]. Strongly driven cantilevers exhibit a similar response, a geometric nonlinearity, as is shown in Figure 9 c. Since the cantilever is singly-clamped, it can move without extending leading to parametric instability [19, 88, 121]. Besides driving a resonator with a force, it can also be driven by periodically changing one of its parameters, for example the spring constant.

When this parametric drive exceeds a threshold, oscillations occur and two phases of the resonator are stable [122], see Figure 9 d. A small change in the driving signal alters the symmetry of the system, and can be detected very accurately by measuring the probability of the resonator being in either phase [123]. Small signals can also be detected by dynamically changing the coupling between two parametric oscillators [18].

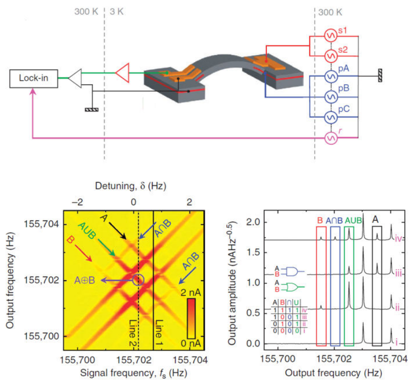


Figure 10. Multi-bit logic in a doubly-clamped resonator. (a) Setup and resonator with integrated piezoelectric transducers for direct and parametric driving and on-chip motion detection. The response is measured close to the resonance frequency f_0 by directly driving the resonator at $f_s+\delta$, while parametrically exciting it at $f_{pA}=2f_0+\Delta$ and $f_{pB}=2f_0-\Delta$. (b) Mixing between the parametric and direct drive results in splitting of the mode, where higher order mixing frequencies occur when $\Delta\neq0$. When the parametric driving signals are considered as logic inputs, where A (B) denotes the presence of the parametric excitation at f_{pA} (f_{pB}), logic functions can be implemented. Depending on the drive frequency (horizontal axis) and the detection frequency (vertical axis), the resonator functions as an AND (∩), OR (∪), and XOR (⊕) gate. (c) shows cross-sections of (b), to demonstrate the resonator logic response when the parametric signals are switched on and off. In these experiments Δ=0.5 Hz. More complex logic functions are possible by generating more mixing frequencies by driving the resonator at multiple frequencies.

A bistable mechanical resonator can be used to represent digital information and several groups have demonstrated mechanical memory elements. Elementary mechanical computing algorithms have been implemented by coupling resonators in a tuneable way [30, 124]. The coupling can also be formed by properties intrinsic to the resonator. In this case, no connections are needed as the algorithm is executed in a single resonator. This concept was demonstrated by exciting a parametric resonator at multiple frequencies, where each excitation signal represents a logic input, and the resulting motion is the output (Figure 10) [125].

The high Q-factor of mechanical systems compared to electronic circuits, and the low 'on' / high 'off' resistance of MEMS/NEMS switches could provide a key to low-dissipation signal processors, and it is believed that mechanics holds a promise of low-power computing in the distant future [126-127]. Mechanical computing is also applicable in harsh conditions where electronics fail, e.g. at high-temperatures or in high-radiation environments (oil industry, space and defence).

In a bistable MEMS/NEMS, otherwise detrimental noise can be employed to amplify the response to weak signals. This counter-intuitive process where noise enables the detection of weak signals is called stochastic resonance, and has been demonstrated in doubly-clamped beams at high noise levels [128-131]. Noise-induced switching between stable states of a nonlinear oscillator can also improve the figure of merit in energy harvesting applications [132]. By matching the energy barrier to the noise intensity, the noisy displacements of a bistable piezoelectric power generator are amplified and this results in an increased output voltage, when compared to energy harvesting with a linear transducer. Implementing this scheme in nonlinear MEMS/NEMS could lead to efficient power generators for stand-alone devices.

7. Carbon based NEMS

Despite most NEMS devices being based on silicon technology, during the last years carbon-based NEMS devices have been gaining more and more interest, mostly because of their high Young modulus and small diameter. The carbon-based mechanical resonators have large tunable frequencies and exhibit large amplitudes. Due to their low mass, they operate in a different regime from their silicon-based counterparts, as evidenced by the very strong nonlinear response. Moreover, they generally exhibit an extremely high sensitivity to external stimuli, making them interesting candidates for various sensing applications for fundamental studies as well as applications. As discussed above, fabrication processes for carbon nanotube based and graphene based NEMS resonators are now well established for prototyping and demonstration activities. From an applied point of view, the challenge is to fabricate devices suitable for large-scale applications that operate at room temperature. Future research is still necessary to elucidate which of the two carbon forms, carbon nanotubes or (few layer) graphene, due to its larger area, is easier to contact and to fabricate on an industry-scale [134].

An example of a suspended carbon nanotube device is shown in Figure 11. These bottom-up devices are expected not to suffer from excessive damping, as their surface can be defect-free at the atomic scale. Combined with their low mass the expected low damping makes them ideal building blocks. Moreover, because of their small sizes carbon-based resonators typically have frequencies in the MHz to GHz range. All these properties (low mass, high Q, large frequencies) are advantageous for sensing applications and the study of quantum properties of resonating objects [135]. For example, when cooled to dilution refrigerator temperatures, carbon-based resonators can be in the quantum mechanical ground-state while exhibiting relatively large amplitude zero-point fluctuations.

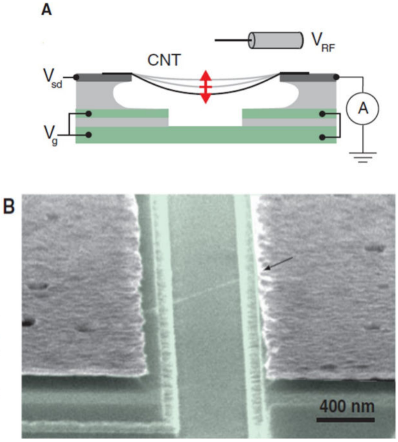


Figure 11. a) A high Q mechanical resonator layout with suspended carbon nanotube; A suspended carbon nanotube is excited into mechanical motion by applying an ac voltage to a nearby antenna b) SEM image of a suspended carbon nanotube clamped between two metal electrodes. A bottom gate can be used to tune the frequency of the resonator, b) [10, 145].

Position detectors of carbon-based bottom-up NEMS, however, are not yet as sophisticated as those for the larger top-down silicon-based counterparts. Consequently, neither non-driven motion at cryogenic temperatures (either Brownian or zero-point motion), nor active cooling have been reported for carbon-based NEMS. Nevertheless impressive progress in understanding the electromechanical properties of bottom-up resonators has been made in recent years using so-called self-detecting schemes. In these schemes, the nanotube or graphene resonator both acts as the actuator and detector of its own motion.

Various device geometries with carbon-based materials exist. The motion of singly-clamped carbon nanotubes has been visualized in scanning [136] and transmission electron microscopes [137]. Another method to detect motion of singly-clamped carbon resonators is based on field emission of electrons from a vibrating tip [138]. When a large voltage is applied between a multi-walled carbon nanotube and an observation screen, it lights up at the position where electrons accelerated by the electric field are impinging. The vibration amplitude is enlarged by applying a RF driving signal, and the spot blurring becomes even more pronounced on resonance. Furthermore, the electric field also pulls on the nanotube, thereby increasing the resonance frequency. The method has also been used to build a nanotube radio [139] and a mass sensor approaching and achieving atomic resolution [140].

For doubly-clamped resonator geometries, it is also advantageous to use the suspended device *itself* as a detector of motion. Using current rectification and frequency mixing, information about the driven motion of the suspended nanotube and graphene has been obtained. Sazonova *et al.* [36] were the first to apply frequency mixing to suspended carbon nanotube resonators. They observed multiple gate-tunable resonances with Q-factors on the order of 100 at room temperature. Subsequently the bending mode vibrations of a carbon nanotube were also identified [141]. Nowadays the technique has been employed by many groups, not only restricted to carbon nanotubes, but also to suspended doubly-clamped graphene sheets [37]. Furthermore, several variations to the original mixing scheme have been implemented, including frequency [142] and amplitude modulations [143].

At low temperatures, Coulomb blockade can be used to drastically enhance the displacement sensitivity. For example, the change in equilibrium position of a suspended nanotube quantum dot after adding a single electron easily surpasses the zero-point motion. A strong coupling results between mechanical motion and the charge on the nanotube, leading to frequency shifts and changes in damping as a function of gate voltage [10, 144]. The readout using current rectification is employed instead of frequency mixing [10, 145]. While the nanotube motion is actuated by a RF signal on a nearby antenna, the detected signal is at DC (Figure 11). The key to understand this is the notion that nanotube motion effectively translates into an oscillating gate voltage, leading to changes in the DC current, which are the largest on resonance.

The technique is of special interest as it allows for the motion detection with small currents, enabling the observation of ultra-high Q-factors, exceeding 100,000 at mK temperatures [145]. Furthermore, the experiments show that the dynamic range is small, i.e., carbon-based resonators are easily driven into the nonlinear regime as illustrated in Figure 12. This can be understood from the small tube diameters or the extremely thin membrane-like shape of the graphene flakes: with increasing driving power the amplitude of flexural motion rapidly grows to their characteristic sizes inducing sizable tension in the resonator. In addition, nonlinear damping effects have recently been reported using mixing techniques in nanotube and graphene resonators [146]. Finally, electron tunneling and mechanical motion are found to be strongly coupled [144-145] resulting in single-electron tuning oscillations of the mechanical frequency and in energy transfer to the electrons causing additional mechanical damping.

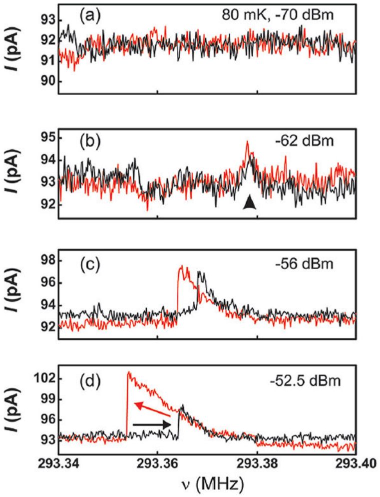


Figure 12. Evolution of the resonance peak with increasing driving power (a-d) at a temperature of 80 mK [10]. Black (red) traces are upward (downward) frequency sweeps. At low powers, the peak is not visible, but upon increasing power, a resonance peak with Q=128627 appears. As the power is increased further, the line shape of the resonance resembles the one of a Duffing oscillator exhibiting hysteresis between the upward and downward sweep [145].

8. Towards functional bio-NEMS

High-frequency NEMS are attracting more and more interest as a new class of sensors and actuators for potential applications to single (bio)molecule sensing [53, 147]. For NEMS to be considered as a viable alternative to their actual biosensing macro counterparts, they have to simultaneously meet three major requirements: high mass responsivity (MR), low minimum detectable mass (MDM) and low response time (RT).

Without any doubt, as emphasized by theoretical studies [148-149], the two first specifications (MR and MDM) can be successfully addressed by NEMS devices. Such predictions have been already validated in case of virus sensing [150], enumeration of DNA molecules [151] or even single molecule nano-mechanical mass spectrometry [53]. Hopelessly, nanometer scale sensors have been proved, still in theory [152-153], to be inadequate to practical RT scales which, if confirmed as such, could definitely impede the NEMS' route towards realistic biosensing applications. To prevent this from happening, one possible trade-off strategy would consist in taking advantage from considering a single NEMS device not alone, but as part of a functional array of similar devices [154]. This paradigm allows, while preserving the benefits of high MR and low MDM of a single device, to use the considerably higher capture area of the NEMS array, because the RT reaches practical relevance. However, in that case, the non-reactive areas of the chip containing multiple sensors functionalized with a single type of probe molecule must be adequately coated with an anti-fouling film in order to lower the probability of adsorption of target molecules anywhere else than on sensitive areas and hence to permit ultra-low concentration detection.

To address the production of massively parallel arrays of NEMS for bio-recognition applications, one has to be able to perform uniform, reliable bio-functionalisation of nanoscale devices at a large scale (the array's level), while being able to obtain an anti-fouling surface everywhere else. For this to become reality, a major challenge is the functionalisation of closely packed nanostructures in such a way that biological receptors are precisely located solely onto the active biosensing areas, thus preventing the waste of biological matter and enabling the subsequent biological blocking of the passive parts of the chip. So far, the issue of the freestanding nanostructures functionalisation has been seldom addressed because of the absence of generic tools or techniques allowing large-scale molecular delivery at the nanoscale. One way to circumvent this difficulty would be to perform the functionalisation step before completing the fabrication of the NEMS. This strategy can typically be used in a top-down NEMS fabrication process by protecting the biological layer during the subsequent NEMS fabrication steps, that consists in placing the functionalized nanostructures at specific locations on a substrate and releasing them [155] The main limitation of this strategy is the trade-off between the choice of the post-functionalisation processing steps and the resilience of the chosen biological receptors to such technological constraints, which for most of them are biologically unfriendly.

9. Energy harvesting

The impact of NEMS technology in the energy harvesting field, i.e. a discipline aiming at converting wasted ambient energy into useful electrical energy to power ultralow consumption ICT devices, is still incipient. A notable level of maturity has been achieved in this field by MEMS applications, where energy is extracted from ambient vibrations. Several mechanical to electrical transduction methods have been applied so far, but piezoelectric has demonstrated to be the preferred solution because of the increasing integrability of piezomaterials and, especially, due to the simplicity of the associated power management circuitry. Although most of the technologies and concepts that have been demonstrated to be feasible at the micro-scale using MEMS are not improved when dimensions are reduced at NEMS scale, the combination of piezoelectric and nanowire technologies becomes relevant. A very recent study [156] theoretically demonstrated the giant piezoelectricity of ZnO and GaN nanowires, which is due to the effect that charge redistribution on the free surfaces produce the local polarization. This effect, which has been theoretically reported previously [157], demonstrates that it is more efficient to fill a certain volume with a compact array of nanowires than to use a bulk thin film piezoelectric substrate, a clear enhancement produced by nanometre scale downscaling. An exhaustive study of the potential performance of piezoelectric nanostructures for mechanical energy harvesting is provided by C. Sun et al. [158]. In this paper, the authors compare rectangular and hexagonal nanowires and 2-D vertical thin films (nanofins), as well as different piezomaterials such as ZnO, $BaTiO_3$, and conclude that the power density ideally obtainable by filling the whole volume is in the range of 10^3-10^4 W/cm^3.

This previous concept is in fact experimentally exploited in many different ways to implement energy nanoconverters or energy nanoharvesters based on arrays of piezoelectric nanowires. One specific nano piezotronic technology is based on combining the piezoelectric properties of ZnO nanowires or fine-wires (its micro scale version) with the rectifying characteristics of the Schottky barrier, formed between the ZnO (semiconductor) and a metal. Most recent work demonstrate biomechanical to electrical conversion using a single wire generator, which is able to produce output voltages around 0.1 V from human finger tapping or from the body movement of a hamster [159], or even from breathing and heartbeat of a rat [160], which demonstrate the potential applicability of NEMS on self-powering implanted nanodevices. High-output power nanogenerators have been also obtained by a rational assembling of ZnO nanowires in a 2-D array. The obtained nanogenerators are able to power real devices as a LED [161] or an LCD [162]. Power densities of 11 mW/cm^3 are experimentally demonstrated and by multilayer integration 1.1 W/cm^3 are predicted.

Still in the field of biomechanical energy harvesting, a very recent study solves the performance trade-off between piezoelectric coefficient and stretchability [163]. Typically, organic piezoelectric materials like PVDF (Polyvinylidene fluoride) are flexible, but show weak piezoelectricity and inorganic ceramic materials as PZT, ZnO or $BaTiO_3$ have piezoelectric coefficients one order of magnitude higher, but are brittle. PZT ribbons buckled by the attachment on a pre-stretched PDMS substrate display simultaneously high piezoelectricity and integrity under stretching and flexing operations [163]. Also the embedding of PZT nanofibers into a PDMS substrate is used to generate peaks of voltage and power around 1.6 V and 30 nW from external vibrations, respectively [164]. But not always organic means low piezoelectricity. The method to directly write PVDF nanofibers with energy conversion efficiencies one order of magnitude higher than those of thin films was developed [165]. The method, based on near-field electrospinning allows the mechanical stretching, polling and positioning of the nanofibers. Finally, a very smart example of inorganic piezoelectric into organic polymer embedding is of ZnO nanowires embedded into a PVC substrate [166]. The collective stretching of the nanowires produced by the temperature induced polymer shape-change allows achieving power densities around 20 nW/cm^3 at 65^{o}C by means of a non-conventional thermoelectric effect.

Solutions to unsolved challenges, such as a real co-design of the NEMS energy transducers and the power management circuitry or the introduction of unexplored materials to span the sensitivity to new energy sources, will define the future research tendencies in this field. As an example, suspended graphene nanoribbons have demonstrated to efficiently harvest the energy from thermal fluctuations due to the mechanical bistability induced by a controlled compressive stress [167].

10. Sumary and outlook

The progress in the field of NEMS has continued at good pace during the last years. The area of NEMS is entering into a more mature stage, addressing real applications in the areas of sensing, telecommunications, information processing and energy harvesting. A step forward is made for better understanding of nonlinear behaviour contributing to sensing and logic applications. The easy access to the nonlinear regime and the defect-free material properties make NEMS also excellent tools to study nonlinear dynamics in a more general context. Signal detection and sensitivity limits together with NEMS integration into complex systems at larger scale are continuously enhanced. Incorporation of new materials improves device performance in terms of sensitivity, working range and efficiency.

While device concepts and fundamental knowledge of the properties of NEMS structures are very much advanced, a fabrication technology that would fulfil the requirements for high dimensional precision, material compatibility and high throughput is still the limiting factor for commercial applications. In consequence, more effort in developing suitable fabrication methods adapted to industry is advisable to guarantee the future success of the field.

The field of nonlinear NEMS is emerging, and new phenomena are discovered which will be applicable in ultrasensitive detectors, mechanical signal processors and efficient energy harvesters. Weak signals can be amplified by making beneficial use of environmental noise, by employing processes like stochastic resonance. At weak driving devices may be optimized as to achieve nonlinear characteristics to reduce the electrical power consumed by the strongly vibrating NEMS. To this end, it is essential to understand the dissipation mechanisms in NEMS resonators. Modelling nonlinear NEMS requires numerical methods, which can be computationally intensive even for simple beam structures. More complex structures with multiple degrees of freedom can be hard to impossible to model quantitatively. Tight fabrication tolerances are required in order to predict and/or reproduce the dynamic behaviour in the nonlinear regime within a workable tolerance window. In order to employ noise-enhanced detection schemes, the barrier between the stable states of the bistable NEMS should be reduced. New ways to couple nonlinear NEMS in an efficient and adjustable way will further expand the NEMS toolbox. It allows the construction of extremely complicated dynamic systems, with many new concepts being discovered at present, and still a wide horizon to be explored.

Carbon-based mechanics is a relatively new research field, but the push for refining detection schemes and integrating carbon-based materials into silicon technology will undoubtedly lead to the construction of better sensors, which may eventually be quantum-limited. A bright future thus seems to being lying ahead for these miniature devices. From a fundamental physics point of view, challenges lie in improving detection schemes so that thermal motion at low temperatures and eventually zero-point motion can be detected. From a fundamental physics point of view, challenges lie in improving detection schemes so that thermal motion at low temperatures and eventually zero-point motion can be detected. The carbon-based resonators also provide a unique system to study the nonlinear properties of mechanical resonators especially in the quantum regime. Furthermore, it is presently still unknown what the limiting factor is in the intrinsic damping of carbon-based resonators. This is a more general issue in NEMS as damping in silicon resonators is also not understood in detail.

In the field of energy harvesting, the challenges to be faced are related not only to the efficient conversion, but also to the management and storage of the harvested energy at the nanoscale. Novel concepts and devices based on NEMS technology and oriented to the management/storage of the energy in a pure mechanical form would improve the energy efficiency of the overall harvesting process, since no conversions from the mechanical to the electrical domain would be needed. And finally, cchallenges making use of NEMS arrays in the biosensing realm can be thus foreseen both at the front-end for differential functionalisation of closely packed sensors and at the back-end, for the integration of actuation and sensing capabilities at nanodevice arrays levels.

Acknowledgements

The authors would like to thank organisations and fundations for the support of this work: Phantoms Foundation NanoICT, FOM, NWO (VICI grant), EU FP7 STREP projects QNEMS and RODIN (HvdZ, WJV), EU 7FP Multiplat (VA, JB), SNF Ambizione PZ00P2_139505 (VS, JB), SNSF 200020-121831 (MM, CH), OPACMEMS project (ENE2009-14340-C02-02) (GA).

11. References

[1] A. N. Cleland and M. L. Roukes, Nature 392 (1998) 6672, 160.

[2] W. Fon, K. C. Schwab, J. M. Worlock and M. L. Roukes, Phys. Rev. B 66 (2002) 4.

[3] K. Schwab, J. L. Arlett, J. M. Worlock and M. L. Roukes, Physica E-Low-Dimensional Systems & Nanostructures 9 (2001) 1, 60.

[4] K. Schwab, E. A. Henriksen, J. M. Worlock and M. L. Roukes, Nature 404 (2000) 6781, 974.

[5] K. Schwab, W. Fon, E. Henriksen, J. M. Worlock and M. L. Roukes, Physica B 280 (2000) 1-4, 458.

[6] A. N. Cleland, A. D. O'Connell, M. Hofheinz, M. Ansmann, R. C. Bialczak, M. Lenander, E. Lucero, M. Neeley, D. Sank, H. Wang, M. Weides, J. Wenner and J. M. Martinis, Nature 464 (2010) 7289, 697.

[7] J. D. Teufel, T. Donner, D. L. Li, J. W. Harlow, M. S. Allman, K. Cicak, A. J. Sirois, J. D. Whittaker, K. W. Lehnert and R. W. Simmonds, Nature 475 (2011) 7356, 359.

[8] M. L. Roukes, M. D. LaHaye, J. Suh, P. M. Echternach and K. C. Schwab, Nature 459 (2009) 7249, 960.

[9] A. Bachtold, B. Lassagne, Y. Tarakanov, J. Kinaret and D. Garcia-Sanchez, Science 325 (2009) 5944, 1107.

[10] G. A. Steele, A. K. Huttel, B. Witkamp, M. Poot, H. B. Meerwaldt, L. P. Kouwenhoven and H. S. J. van der Zant, Science 325 (2009) 5944, 1103.

[11] M. L. Roukes, A. K. Naik, M. S. Hanay, W. K. Hiebert and X. L. Feng, Nat Nanotechnol 4 (2009) 7, 445.

[12] M. L. Roukes, Y. Y. Yang, Y. T., C. Callegari and X. L. Feng, Nano Lett 11 (2011) 4, 1753.

[13] M. I. Dykman, M. Khasin, J. Portman and S. W. Shaw, Phys. Rev. Lett. 105 (2010) 23.

[14] R. Lifshitz and M. C. Cross, in *Reviews of nonlinear dynamics and complexity*, edited by H. G. Schuster (Wiley-VCH, Weinheim, 2008), Vol. 1.

[15] G. Weick, F. Pistolesi, E. Mariani and F. von Oppen, Phys. Rev. B 81 (2010) 12.

[16] J. Atalaya, A. Isacsson and M. I. Dykman, Phys. Rev. Lett. 106 (2011) 22.

[17] R. B. Karabalin, M. C. Cross and M. L. Roukes, Physical Review B 79 (2009) 16.

[18] R. B. Karabalin, R. Lifshitz, M. C. Cross, M. H. Matheny, S. C. Masmanidis and M. L. Roukes, Phys. Rev. Lett. 106 (2011) 9, 094102.

[19] H. J. R. Westra, M. Poot, H. S. J. van der Zant and W. J. Venstra, Phys. Rev. Lett. 105 (2010) 11, 117205.

[20] A. Bachtold, A. Eichler, J. Moser, J. Chaste, M. Zdrojek and I. Wilson-Rae, Nat Nanotechnol 6 (2011) 6, 339.

[21] K. L. Ekinci, A. Sampathkumar and T. W. Murray, Nano Lett 11 (2011) 3, 1014.

[22] O. Basarir, S. Bramhavar and K. L. Ekinci, Appl. Phys. Lett. 97 (2010) 25.

[23] M. R. Freeman, N. Liu, F. Giesen, M. Belov, J. Losby, J. Moroz, A. E. Fraser, G. McKinnon, T. J. Clement, V. Sauer and W. K. Hiebert, Nat Nanotechnol 3 (2008) 12, 715.

[24] H. X. Tang, M. Li and W. H. P. Pernice, Nat Nanotechnol 4 (2009) 6, 377.

[25] H. X. Tang, M. Li, W. H. P. Pernice, C. Xiong, T. Baehr-Jones and M. Hochberg, Nature 456 (2008) 7221, 480.

[26] H. Okamoto, D. Ito, K. Onomitsu, H. Sanada, H. Gotoh, T. Sogawa and H. Yamaguchi, Phys. Rev. Lett. 106 (2011) 3.

[27] M. Li, W. H. P. Pernice and H. X. Tang, Nat Photonics 3 (2009) 8, 464.

[28] A. N. Cleland and M. L. Roukes, Sensors and Actuators A 72 (1999) 3, 256.

[29] I. Bargatin, I. Kozinsky and M. L. Roukes, Appl. Phys. Lett. 90 (2007) 9.

[30] S. C. Masmanidis, R. B. Karabalin, I. De Vlaminck, G. Borghs, M. R. Freeman and M. L. Roukes, Science 317 (2007) 5839, 780.

[31] R. B. Karabalin, M. H. Matheny, X. L. Feng, E. Defay, G. Le Rhun, C. Marcoux, S. Hentz, P. Andreucci and M. L. Roukes, Appl. Phys. Lett. 95 (2009) 10.

[32] P. A. Truitt, J. B. Hertzberg, C. C. Huang, K. L. Ekinci and K. C. Schwab, Nano Lett 7 (2007) 1, 120.

[33] H. X. Tang, H. Bhaskaran, M. Li, D. Garcia-Sanchez, P. Zhao and I. Takeuchi, Appl. Phys. Lett. 98 (2011) 1.

[34] J. P. Kotthaus, Q. P. Unterreithmeier and E. M. Weig, Nature 458 (2009) 7241, 1001.

[35] I. Bargatin, E. B. Myers, J. Arlett, B. Gudlewski and M. L. Roukes, Appl. Phys. Lett. 86 (2005) 13.

[36] V. Sazonova, Y. Yaish, H. Ustunel, D. Roundy, T. A. Arias and P. L. McEuen, Nature 431 (2004) 7006, 284.

[37] C. Y. Chen, S. Rosenblatt, K. I. Bolotin, W. Kalb, P. Kim, I. Kymissis, H. L. Stormer, T. F. Heinz and J. Hone, Nat Nanotechnol 4 (2009) 12, 861.

[38] A. Ayari, V. Gouttenoire, T. Barois, S. Perisanu, J. L. Leclercq, S. T. Purcell and P. Vincent, Small 6 (2010) 9, 1060.

[39] N. Kacem, S. Hentz, D. Pinto, B. Reig and V. Nguyen, Nanotechnology 20 (2009) 27.

[40] R. B. Karabalin, S. C. Masmanidis and M. L. Roukes, Appl. Phys. Lett. 97 (2010) 18.

[41] K. L. Ekinci, Y. T. Yang, X. M. H. Huang and M. L. Roukes, Appl. Phys. Lett. 81 (2002) 12, 2253.

[42] X. L. Feng, C. J. White, A. Hajimiri and M. L. Roukes, Nat Nanotechnol 3 (2008) 6, 342.

[43] J. Arcamone, M. A. F. van den Boogaart, F. Serra-Graells, J. Fraxedas, J. Brugger and F. Perez-Murano, Nanotechnology 19 (2008) 30.

[44] M. Faucher, B. Grimbert, Y. Cordier, N. Baron, A. Wilk, H. Lahreche, P. Bove, M. Francois, P. Tilmant, T. Gehin, C. Legrand, M. Werquin, L. Buchaillot, C. Gaquiere and D. Theron, Appl. Phys. Lett. 94 (2009) 23, 233506.

[45] E. Colinet, C. Durand, P. Audebert, P. Renaux, D. Mercier, L. Duraffourg, E. Oilier, F. Casset, P. Ancey, L. Buchaillot and A. M. lonescu, presented at the IEEE International Solid-State Circuits Conference (ISSCC), 2008 (unpublished).

[46] D. Grogg and A. M. Ionescu, IEEE Transactions on Electron Devices 58 (2011) 7, 2113.

[47] D. Weinstein and S. A. Bhave, Nano Lett 10 (2010) 4, 1234.

[48] D. N. Guerra, A. R. Bulsara, W. L. Ditto, S. Sinha, K. Murali and P. Mohanty, Nano Lett 10 (2010), 1168.

[49] N. Liu, F. Giesen, M. Belov, J. Losby, J. Moroz, A. E. Fraser, G. McKinnon, T. J. Clement, V. Sauer, W. K. Hiebert and M. R. Freeman, Nat. Nanotechnology 3 (2008), 715.

[50] Q. P. Unterreithmeier, E. M. Weig and J. P. Kotthaus, Nature 458 (2009), 1001.

[51] J. Suh, M. D. LaHaye, P. M. Echternach, K. C. Schwab and M. L. Roukes, Nano Lett 10 (2010), 3990.

[52] R. B. Karabalin, X. L. Feng and M. L. Roukes, Nano Lett 9 (2009), 3116.

[53] A. K. Naik, M. S. Hanay, W. K. Hiebert, X. L. Feng and M. L. Roukes, Nat. Nanotechnology 4 (2009), 445.

[54] T.-H. Lee, S. Bhunia and M. Mehregany, Science 329 (2010), 1316.

[55] M. Li, E. B. Myers, H. X. Tang, S. J. Aldridge, H. C. McCaig, J. J. Whiting, R. J. Simonson, N. S. Lewis and M. L. Roukes, Nano Lett 10 (2010), 3899.

[56] C. Guthy, R. M. Das, B. Drobot and S. Evoy, J. Appl. Phys. 108 (2010), 014306.

[57] T.-H. Lee, S. Bhunia and M. Mehregany, Science 329 (2010) 5997, 1316.

[58] E. Gil-Santos, D. Ramos, J. Martıínez, M. Fernández-Regúlez, R. García, A. S. Paulo, M. Calleja and J. Tamayo, Nat. Nanotechnology 5 (2010), 641.

[59] P. Ivaldi, J. Abergel, M. H. Matheny, L. G. Villanueva, R. B. Karabalin, M. L. Roukes, P. Andreucci, S. Hentz and E. Defaÿ, J. Micromech. Microeng. 21 (2011), 085023.

[60] Ü. Sökmen, A. Stranz, A. Waag, A. Ababneh, H. Seidel, U. Schmid and E. Peiner, J. Micromech. Microeng. 20 (2010), 064007.

[61] J. Sulkko, M. A. Sillanp, P. Hkkinen, L. Lechner, M. Helle, A. Fefferman, J. Parpia and P. J. Hakonen, Nano Lett 10 (2010), 4884.

[62] D. Vick, V. Sauer, A. E. Fraser, M. R. Freeman and W. K. Hiebert, J. Micromech. Microeng. 20 (2010), 105005.

[63] P. Sievilä, N.Chekurov and I. Tittonen, Nanotechnology 21 (2010), 145301.

[64] L. Bischoff, B. Schmidt, H. Langea and D. Donzevb., Nucl. Instr. Meth.B 267 (2009), 1372.

[65] G. Rius, J. Llobet, X. Borrisé, N. Mestres, A. Retolaza, S. Merino and F. Perez-Murano, J.Vac. Sci. Technol.B 27 (2009), 2691.

[66] www.nanovlsi.com.

[67] I. Martin-Fernandez, X. Borrisé, E. Lora-Tamayo, P. Godignon and F. Perez-Murano, J.Vac. Sci. Technol.B 28 (2010), C6P1.

[68] J. L. Lopez, J. Verd, J. Teva, G. Murillo, J. Giner, F. Torres, A. Uranga, G. Abadal and N. Barniol, J. Micromech. Microeng. 19 (2009), 015002.

[69] J. Arcamone, M. Sansa, J. Verd, A. Uranga, G. Abadal, N. Barniol, M. v. d. Boogaart, N. Barniol, J. Brugger and F. Perez-Murano, Small 5 (2009), 176.

[70] J. L. Lopez, J. Verd, A. Uranga, J. Giner, G. Murillo, F. Torres, G. Abadal and N. Barniol., IEEE Electron Device Letters 30 (2009), 718.

[71] J. Verd, M. Sansa, A. Uranga, F. Perez-Murano, J. Segura and N. Barniol, Lab on a Chip 11 (2011), 2670.

[72] W.-C. Chen, W. Fang and S.-S. Li, J. Micromech. Microeng. 21 (2011), 065012.

[73] O. Englander, D. Christensen and L. W. Lin, Appl. Phys. Lett. 82 (2003) 26, 4797.

[74] D. S. Engstrom, N. L. Rupesinghe, K. B. K. Teo, W. I. Milne and P. Bogild, J. Micromech. Microeng. 21 (2011) 1, 7.

[75] C. Kallesoe, C. Y. Wen, K. Molhave, P. Boggild and F. M. Ross, Small 6 (2010) 18, 2058.

[76] L. Luo, L. Lin and Ieee, in *Transducers '07 & Eurosensors Xxi, Digest of Technical Papers, Vols 1 and 2* (IEEE, New York, 2007), pp. U205-U206.

[77] L. Luo, B. D. Sosnowchik and L. W. Lin, Nanotechnology 21 (2010) 49.

[78] K. Molhave, B. A. Wacaser, D. H. Petersen, J. B. Wagner, L. Samuelson and P. Boggild, Small 4 (2008) 10, 1741.

[79] B. D. Sosnowchik, L. W. Lin and O. Englander, J. Appl. Phys. 107 (2010) 5, 14.

[80] K. L. Zhang, Y. Yang, E. Y. B. Pun and R. Q. Shen, Nanotechnology 21 (2010) 23, 7.

[81] O. Englander, in *Micro- and Nanotechnology Sensors, Systems, and Applications Ii*, edited by T. George, M. S. Islam and A. K. Dutta (Spie-Int Soc Optical Engineering, Bellingham, 2010), Vol. 7679.

[82] D. S. Engstrom, V. Savu, X. N. Zhu, I. Y. Y. Bu, W. I. Milne, J. Brugger and P. Boggild, Nano Lett 11 (2011) 4, 1568.

[83] C. Kallesoe, K. Molhave, K. F. Larsen, D. Engstrom, T. M. Hansen, P. Boggild, T. Martensson, M. Borgstrom and L. Samuelson, J.Vac. Sci. Technol.B 28 (2010) 1, 21.

[84] B. R. Burg, T. Helbling, C. Hierold and D. Poulikakos, J. Appl. Phys. 109 (2011) 6, 064310.

[85] M. Muoth, T. Helbling, L. Durrer, S. W. Lee, C. Roman and C. Hierold, Nature Nanotech. 5 (2010) 8, 589-592.

[86] J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, S. Blankenburg, M. Muoth, A. P. Seitsonen, M. Saleh, X. Feng, K. Mullen and R. Fasel, Nature 466 (2010) 7305, 470-473.

[87] M. A. Sillanpää, J. Sarkar, J. Sulkko, J. Muhonen and P. J. Hakonen, Appl. Phys. Lett. 95 (2009), 011909.

[88] N. Kacem, J. Arcamone, F. Pérez-Murano and S. Hentz, J. Micromech. Microeng. 20 (2010), 045023.

[89] G. Tosolini, G. Villanueva, F. Perez-Murano and J. Bausells, Microelectron. Eng. 87 (2010), 1245.

[90] J.-S. Wenzler, T. Dunn, S. Erramilli and P. Mohanty, J. Appl. Phys. 105 (2009), 094308.

[91] P. Unterreithmeier, T. Faust, S. Manus and J. P. Kotthaus, Nano Lett 10 (2010), 887.

[92] K. Y. Fong, W. H. P. Pernice, M. Li and H. X. Tang, Appl. Phys. Lett. 97 (2010), 073112.

[93] M. Li, W. H. P. Pernice and H. X. Tang, Appl. Phys. Lett. 95 (2010), 183110.

[94] J. Lee, W. Shen, K. Payer, T. P. Burg and S. R. Manalis, Nano Lett 10 (2010), 2537.

[95] A. S. Sadek, R. B. Karabalin, J. Du, M. L. Roukes, C. Koch and S. C. Masmanidis, Nano Lett 10 (2010), 1769.

[96] D. V. Scheible and R. H. Blick, New J. Phys. 12, 023019.

[97] X. L. Feng, M. H. Matheny, C. A. Zorman, M. Mehregany and M. L. Roukes, Nano Lett 10 (2010), 2891.

[98] A. Ayari, P. Vincent, S. Perisanu, M. Choueib, M. Gouttenoire, V. Bechelany, D. Cornu and S. Purcell, Nano Lett 7 (2007), 2252.

[99] S. Perisanu, T. Barois, P. Poncharal, T. Gaillard, A. Ayari, S. T. Purcell and P. Vincent, Appl. Phys. Lett. 98 (2011), 063110.

[100] E. Colinet, L. Duraffourg, S. Labarthe, P. Andreucci, S. Hentz and P. Robert, J. Appl. Phys. 105 (2009), 124908.

[101] Y.-C. Liu, M.-H. Tsai, W.-C. Chen, S.-S. Li and W. Fang, Transducers`2011, 934.

[102] W.-L. Huang, Z. Ren, Y.-W. Lin, H.-Y. Chen, J. Lahann and C. T.-C. Nguyen, Tech. Digest, 21st IEEE Int. Conf. on Micro Electro Mechanical Systems (MEMS’08), Tucson, Arizona, Jan. 13-17, 2008, 10.

[103] J. Verd, A. Uranga, G. Abadal, J. L. Teva, F. Torres, J. Lopez, F. Perez-Murano, J. Esteve and N. Barniol, IEEE Electron Device Letters 29 (2008), 146.

[104] M. K. Zalalutdinov, J. D. Cross, J. W. Baldwin, B. R. Ilic, W. Zhou, B. H. Houston and J. M. Parpia, J. Microelectromech. Syst. 19 (2010), 807.

[105] D. A. Czaplewski, G. A. Patrizi, G. M. Kraus, J. R. Wendt, C. D. Nordquist, S. L. Wolfley, M. S. Baker and M. P. d. Boer, J. Microelectron. Eng. 19, 085003.
[106] D. Roodenburg, J. W. Spronck, H. S. J. van der Zant and W. J. Venstra, Appl. Phys. Lett. 94 (2009) 18, 183501.
[107] T.-J. K. Liu, J. Jeon, R. Nathanael, H. Kam, V. Pott and E. Alon, Prospects for MEM logic switch technology, IEDM10 424 (2010).
[108] F. Chen, M. .Spencer, R. Nathanael, C. Wang, H. Fariborzi, A. Gupta, H. Kam, V. Pott, J. Jeon, T.-J. K. Liu, D. Markovic, V. Stojanovic and E. Alon, IEEE International Solid-State Circuits Conference (2010), 150.
[109] K. Akarvardar, D. Elata, R. Parsa, G. C. Wan, K. Yoo, J. Provine, P. Peumans, R. T. Howe and H.-S. P. Wong, Design Considerations for Complementary Nanoelectromechanical Logic Gates, IEDM 2009, 299.
[110] K. Akarvardar and H. S. P. Wong, IEEE Electron Device Letters 30 (2009), 1143.
[111] H. W. C. Postma, I. Kozinsky, A. Husain and M. L. Roukes, Appl. Phys. Lett. 86 (2005) 22, 223105.
[112] I. Kozinsky, H. W. C. Postma, I. Bargatin and M. L. Roukes, Appl. Phys. Lett. 88 (2006) 25, 253101.
[113] J. M. Nichol, E. R. Hemesath, L. J. Lauhon and R. Budakian, Appl. Phys. Lett. 95 (2009) 12, 123116.
[114] R. B. Karabalin, M. C. Cross and M. L. Roukes, Phys. Rev. B 79 (2009) 16, 165309.
[115] Q. Chen, L. Huang, Y.-C. Lai, C. Grebogi and D. Dietz, Nano Lett 10 (2010) 2, 406.
[116] B. Hälg, IEEE Transactions on Electron Devices 37 (1990) 10, 2230.
[117] B. Charlot, W. Sun, K. Yamashita, H. Fujita and H. Toshiyoshi, J. Micromech. Microeng. 18 (2008) 4, 045005.
[118] G. Weick, F. von Oppen and F. Pistolesi, Phys. Rev. B 83 (2011) 3, 035420.
[119] Q. P. Unterreithmeier, T. Faust and J. P. Kotthaus, Phys. Rev. B 81 (2010) 24, 241405.
[120] W. J. Venstra, H. J. R. Westra and H. S. J. van der Zant, Appl. Phys. Lett. 97 (2010) 19, 193107.
[121] S. Perisanu, T. Barois, A. Ayari, P. Poncharal, M. Choueib, S. T. Purcell and P. Vincent, Phys. Rev. B 81 (2010) 16, 165440.
[122] I. Mahboob and H. Yamaguchi, Nat Nanotechnol 3 (2008) 5, 275.
[123] I. Mahboob, C. Froitier and H. Yamaguchi, Appl. Phys. Lett. 96 (2010) 21, 213103.
[124] S.-B. Shim, M. Imboden and P. Mohanty, Science 316 (2007) 5821, 95.
[125] I. Mahboob, E. Flurin, K. Nishiguchi, A. Fujiwara and H. Yamaguchi, Nature Communications 2 (2011), 198.
[126] M. L. Roukes, IEEE International Electron Devices Meeting 2004: IEDM technical digest. IEEE , Piscataway, NJ (2004), 539.
[127] M. Freeman and W. Hiebert, Nat Nanotechnol 3 (2008) 5, 251.
[128] L. Gammaitoni, P. Hanggi, P. Jung and F. Marchesoni, Reviews of Modern Physics 70 (1998) 1, 223.
[129] R. L. Badzey and P. Mohanty, Nature 437 (2005) 7061, 995.
[130] R. Almog, S. Zaitsev, O. Shtempluck and E. Buks, Appl. Phys. Lett. 90 (2007) 1, 013508.
[131] D. N. Guerra, T. Dunn and P. Mohanty, Nano Lett 9 (2009) 9, 3096.
[132] F. Cottone, H. Vocca and L. Gammaitoni, Phys. Rev. Lett. 102 (2009) 8, 080601.
[133] R. L. Badzey, G. Zolfagharkhani, A. Gaidarzhy and P. Mohanty, Appl. Phys. Lett. 85 (2004) 16, 3587.
[134] A. M. van der Zande, R. A. Barton, J. S. Alden, C. S. Ruiz-Vargas, W. S. Whitney, P. H. Q. Pham, J. Park, J. M. Parpia, H. G. Craighead and P. L. McEuen, Nano Lett 10 (2010) 12, 4869.
[135] M. Poot and H. S. J. van der Zant, submitted to Physics Reports (2011).
[136] B. Babić, J. Furer, S. Sahoo, S. Farhangfar and C. Schönenberger, Nano Lett 3 (2003), 1577.
[137] P. Poncharal, Z.L. Wang, D. Ugarte and W. A. deHeer, Science 283 (2003) 199, 1513.
[138] S. T. Purcell, P. Vincent, C. Journet and V. T. Binh, Phys. Rev. Lett. 89 (2002), 276103.
[139] K. Jensen, J. Weldon, H. Garcia and A. Zettl, Nano Lett 7 (2007), 3508.
[140] B. Lassagne, D. Garcia-Sanchez, A. Aguasca and A. Bachtold, Nano Lett 8 (2008), 3735.
[141] B. Witkamp, M. Poot and H. S. J. v. d. Zant, Nano Lett 6 (2006), 2904.
[142] V. Gouttenoire, T. Barois, S. Perisanu, J.-L. Leclercq, S. T. Purcell, P. Vincent and A. Ayari, Small 6 (2010) 1060.
[143] B. Witkamp, M. Poot, H. Pathangi, A. K. Hüttel and H. S. J. v. d. Zant, Appl. Phys. Lett. 93 (2008), 111909.

[144] B. Lassagne, Y. Tarakanov, J. Kinaret, D. Garcia-Sanchez and A. Bachtold, Science 325 (2009), 1107.

[145] A. K. Hüttel, G. A. Steele, B. Witkamp, M. Poot, L. P. Kouwenhoven and H. S. J. van der Zant, Nano Lett 9 (2009), 2547.

[146] A. Eichler, J. Moser, J. Chaste, M. Zdrojek, I. Wilson-Rae and A. Bachtold, Nat. Nanotechnology 6 (2011), 339.

[147] K. Jensen, K. Kim and A. Zettl, Nat. Nanotechnology 4 (2009), 445.

[148] K. L. Ekinci, Y. T. Yang and M. L. Roukes, J. Appl. Phys. 95 (2004), 2682.

[149] T. M. Squires, R. J. Messinger and S. R. Manalis, Nat. Biotechnology 26 (2008), 417.

[150] B. Ilic, Y. Yang, K. Aubin, R. Reichenbach, S. Krylov and H. G. Craighead, Nano Lett 5 (2005), 925.

[151] B. Ilic, Y. Yang and H. G. Craighead, Appl. Phys. Lett. 85 (2004), 2604.

[152] P. E. Sheehan and L. J. Whitman, Nano Lett 5 (2005), 803.

[153] P. R. Nair and M. A. Alam, Appl. Phys. Lett. 88 (2006), 698.

[154] A. Sampatkhumar, K. L. Ekinci and T. W. Murray, Nano Lett 11 (2011), 1014.

[155] M. Li, R. B. Bhiladvala, T. J. Morrow, J. A. Sioss, K. K. Lew, J. M. Redwing, C. D. Keating and T. S. Mayer, Nat. Nanotechnology 3 (2008), 88.

[156] R. Agrawal and H. D. Espinosa, Nano Lett 11 (2011), 786.

[157] H. J. Xiang, J. Yang, J. G. Hou and Q. Zhu, Appl. Phys. Lett. 89 (2006), 223111.

[158] C. Sun, J. Shi and X. Wang, J. Appl. Phys. 108 (2010), 034309.

[159] R. Yang, Y. Qin, C. Li, G. Zhu and Z. L. Wang, Nano Lett 9 (2009), 1201.

[160] Z. Li, G. Zhu, R. Yang, A. C. Wang and Z. L. Wang, Adv. Mater. 22 (2010), 2534.

[161] G. Zhu, R. Yang, S. Wang and Z. L. Wang, Nano Lett 10 (2010) 3155.

[162] Y. Hu, Y. Zhang, C. Xu, G. Zhu and Z. L. Wang, Nano Lett 10 (2010), 5025.

[163] Y. Qi, J. Kim, T. D. Nguyen, B. Lisko, P. K. Purohit and M. C. McAlpine, Nano Lett 11 (2011), 1331.

[164] X. Chen, S. Xu, N. Yao and Y. Shi., Nano Lett 10 (2010), 2133.

[165] C. Chang, V. H. Tran, J. Wang, Y.-K. Fuh and L. Lin, Nano Lett 10 (2010), 726.

[166] X. Wang, K. Kim, Y. Wang, M. Stadermann, A. Noy, A. V. Hamza, J. Yang and D. J. Sirbuly, Nano Lett 10 (2010) 4901.

[167] M. López-Suárez, R. Rurali, L. Gammaitoni and G. Abadal, Phys. Rev. B 84 (2011), 161401.

4. Annex 2
nanoICT
groups & statistics

List of nanoICT registered groups

Biotecgen SRL www.biotecgen.it Italy Chiesa, Maurizio m.chiesa @biotecgen.it University of Vigo New Materials Group www.laser.uvigo.es Spain Chiussi, Stefano schiussi@uvigo.es Commissariat à l'Energie Atomique INAC/SPINTEC www.spintec.fr France Chshiev, Mairbek mair. chshiev@cea.fr University of Calabria Micro elec tronics and Microsystems Laboratory www.deis.unical.it Italy Cocorullo, Giuseppe crupi@unical.it University of Mons Laboratory for Chemistry of Novel Materials http://morris.umh.ac.be/ BelgiumCornil,JérômeJerome.Cornil@umons.ac.be Fundacion Phantoms Nanotechnology www.phantomsnet.net Spain Correia,Antonioantonio@phantomsnet.netDresden University of Technolog Chair of materials science and nanotechnology http://nano.tu-dresden.de Germany Cuniberti, Gianaurelio office@nano.tu-dresden.de Technical University of Denmark DyNEMSgroup www.nanotech.dtu.dk Denmark Davis, Zachary J. zachary.davis@nanotech.dtu.dk University of Sheffield Semiconductor materials and devices www.sheffield.ac.uk UnitedKingdomDeSouza, Maria Merlyne m.desouza@ sheffield.ac.uk Commissariatàl Energie Atomique LEM (LaboratoiredElectroniqueMoélculaire)http://iramis.cea.fr/sp ec /lem FranceDerycke, Vincent vincent. derycke @cea. fr Université de la MéditerranéeCNRS-CINaM www.cinam.univ-mrs.fr France Didier, Tonneau tonneau@cinam.univ-mrs.fr University of Paris-SudCNRS Nanoelectronics Group www.ief.u-psud.fr France Dollfus, Philippe philippe.dollfus@u-psud.fr Universitry of Castilla la Mancha, UCLM Femtoscience and single molecule microscopy www.uclm.es/centro /inamol/grupoi02.aspSpainDouhal,Abderrazzakabderrazzak.d ouhal@uclm.es B.S. Abdur Rahman University Polymer Nano Technology Centre www.bsauniv.ac.in India Manikandan, Elayaperumal maniphysics@gmail.com Universidad del Pais V

List of nanoICT registered groups

Institution	Group / Web	Country	Contact Person / Email
Technical Research Center of Finland	VTT Micro and Nanoelectronics www.vtt.fi	Finland	Ahopelto, Jouni jouni.ahopelto@vtt.fi
CNRS-University Bordeaux	BioInspired Nanotechnology and Carbon Nanotube www.cnanogso.org	France	Aimé, Jean-Pierre jp.aime@cnanogos.org
Aalto University	Micronova Nanofabrication Centre www.micronova.fi	Finland	Airaksinen, Veli-Matti veli-matti.airaksinen@tkk.fi
CEA-LETI / MINATEC	Micro/nanosystems Laboratory (LCMS) www.leti.fr	France	Arcamone, Julien julien.arcamone@cea.fr
Cambridge University	Institute for Manufacturing www.ifm.eng.cam.ac.uk	United Kingdom	Athanassopoulou, Nikol. naa14@cam.ac.uk
Unversity of Bologna	Microelectronics Group www.arces.unibo.it	Italy	Baccarani, Giorgio gbaccarani@arces.unibo.it
Centre Investigacions Nanociencia Nanotecnologia (CSIC-ICN) Barcelona	Quantum NanoElectronics www.nanocat.org/qne	Spain	Bachtold, Adrian adrian.bachtold@cin2.es
The Institute of Photonic Sciences ICFO	Nanophotonics Laboratory www.icfo.es	Spain	Badenes, Goncal goncal.badenes@icfo.es
CEA-Grenoble	www.cea.fr	France	Baptist, Robert robert.baptist@cea.fr
Universitat Autonoma de Barcelona	Electronic Circuits and Systems Group www.uab.es	Spain	Barniol, Nuria nuria.barniol@uab.es
AMO GmbH - Gesellschaft für amgewandte Mikro- und optoelektronik mit beschränkter Haftung	www.amo.de	Germany	Baus, Matthias baus@amo.de
Leiden University	Nanophysics www.lorentz.leidenuniv.nl/beenakker	Netherlands	Beenakker, Carlo beenakker@lorentz.leidenuniv.nl
Italian National Institute of Nuclear Physics-Laboratori Nazionali di Frascati	Nanotechnology www.lnf.infn.it	Italy	Bellucci, Stefano bellucci@lnf.infn.it
CIC nanoGUNE Consolider	Nanomagnetism www.nanogune.eu	Spain	Berger, Andreas a.berger@nanogune.eu
CIC nanoGUNE Consolider	Self-Assembly www.nanogune.eu	Spain	Bittner, Alexander a.bittner@nanogune.eu
University of Copenhagen	Nano-Science Center, NanoChemistry http://nano.ku.dk	Denmark	Bjørnholm, Thomas tb@nano.ku.dk
QuantumWise A/S	www.quantumwise.com	Denmark	Blom, Anders anders.blom@quantumwise.com
Commissariat à l'Energie Atomique	CEA Nanoscience Program www.cea.fr	France	Bourgoin, Jean-Philippe Jean-Philippe.Bourgoin@cea.fr
Technical University of Denmark	Theoretical Nanoelectronics www.nanotech.dtu.dk/TNE	Denmark	Brandbyge, Mads mads.brandbyge@nanotech.dtu.dk
University of Oxford	Quantum Nanomaterials www.materials.ox.ac.uk	United Kingdom	Briggs, Andrew andrew.briggs@materials.ox.ac.uk

Annex 2 nanoICT groups & statistics

List of nanoICT registered groups

Institution	Group / Web	Country	Contact Person / Email
Institut pluridisciplinaire de recherche sur l´environnement et les matériaux	Chimie physique http://iprem-ecp.univ-pau.fr	France	Brown, Ross ross.brown@univ-pau.fr
Ecole Polytechnique Fédérale de Lausanne	Microsystems laboratory – 1 http://lmis1.epfl.ch	Switzerland	Brugger, Juergen juergen.brugger@epfl.ch
CNRS	Institut d Electronique de Microelectronique et de Nanotechnologie www.iemn.fr	France	Buchaillot, Lionel lionel.buchaillot@iemn.univ-lille1.fr
TU Kaiserslautern	Magnetism Group www.physik.uni-kl.de/hillebrands/home/	Germany	Burkard, Hillebrands hilleb@physik.uni-kl.de
University of Geneva	Mesoscopic physics group http://mpej.unige.ch/~buttiker/	Switzerland	Buttiker, Markus Markus.Buttiker@unige.ch
Universidad Politecnica de Madrid	Instituto de Sistemas Optoelectrónicos y Microtecnología www.isom.upm.es	Spain	Calle, Fernando fernando.calle@upm.es
Consorzio Interuniversitario Nazionale per la Scienza e Technologia dei Materiali	Laboratory of Molecular Magnetism www.instm.it	Italy	Caneschi, Andrea andrea.caneschi@unifi.it
CNRS - Ecole Supérieure de Physique et de Chimie Industrielles - ParisTech	Institut Langevin and Laboratoire Photons et Matière www.espci.fr	France	Carminati, Rémi remi.carminati@espci.fr
Universitat Autonoma de Barcelona	Nanoelectronica Computacional www.uab.cat/grup-recerca/nanocomp	Spain	Cartoixa, Xavier Xavier.Cartoixa@uab.es
Università di Firenze	European Laboratory for Nonlinear Spectroscopy www.lens.unifi.it	Italy	Cataliotti, Francesco fsc@lens.unifi.it
University Paris Sud	Institut Electronique Fondamentale www.ief.u-psud.fr	France	Chappert, Claude chappert@ief.u-psud.fr
Université catholique de Louvain	Unité de Physico-Chimie et de Physique des Matériaux (PCPM) www.uclouvain.be	Belgium	Charlier, Jean-Christophe jean-christophe.charlier@uclouvain.be
Biotecgen SRL	www.biotecgen.it	Italy	Chiesa, Maurizio m.chiesa@biotecgen.it
University of Vigo	New Materials Group www.laser.uvigo.es	Spain	Chiussi, Stefano schiussi@uvigo.es
Commissariat à l'Energie Atomique	INAC/SPINTEC www.spintec.fr	France	Chshiev, Mairbek mair.chshiev@cea.fr
University of Calabria	Microelectronics and Microsystems Laboratory www.deis.unical.it	Italy	Cocorullo, Giuseppe crupi@unical.it
University of Mons	Laboratory for Chemistry of Novel Materials http://morris.umh.ac.be/	Belgium	Cornil, Jérôme Jerome.Cornil@umons.ac.be
Fundacion Phantoms	Nanotechnology www.phantomsnet.net	Spain	Correia, Antonio antonio@phantomsnet.net
Dresden University of Technolog	Chair of materials science and nanotechnology http://nano.tu-dresden.de	Germany	Cuniberti, Gianaurelio office@nano.tu-dresden.de
Technical University of Denmark	DyNEMS group www.nanotech.dtu.dk	Denmark	Davis, Zachary J. zachary.davis@nanotech.dtu.dk
University of Sheffield	Semiconductor materials and devices www.sheffield.ac.uk	United Kingdom	De Souza, Maria Merlyne m.desouza@sheffield.ac.uk

Institution	Group / Web	Country	Contact Person / Email
Commissariat à l Energie Atomique	LEM (Laboratoire d Electronique Moélculaire) http://iramis.cea.fr/spec/lem	France	Derycke, Vincent vincent.derycke@cea.fr
Université de la Méditerranée	CNRS-CINaM www.cinam.univ-mrs.fr	France	Didier, Tonneau tonneau@cinam.univ-mrs.fr
University of Paris-Sud - CNRS	Nanoelectronics Group www.ief.u-psud.fr	France	Dollfus, Philippe philippe.dollfus@u-psud.fr
Universitry of Castilla la Mancha, UCLM	Femtoscience and single molecule microscopy www.uclm.es/centro/inamol/grupoi02.asp	Spain	Douhal, Abderrazzak abderrazzak.douhal@uclm.es
B.S. Abdur Rahman University	Polymer Nano Technology Centre www.bsauniv.ac.in	India	Manikandan, Elayaperumal maniphysics@gmail.com
Universidad del Pais Vasco and Donostia International Physics Center	Condensed Matter Physics www.ehu.es	Spain	Echenique, Pedro wapetlap@ehu.es
Institut de Ciència de Materials de Barcelona- CSIC	Materials Magnètics i Òxids funcionals www.icmab.es/dmag/	Spain	Fontcuberta, Josep fontcuberta@icmab.es
Ecole Polytechnique Federale de Lausanne	Laboratory of Semiconductor Materials http://lmsc.epfl.ch	Switzerland	Fontcuberta i Morral, Anna anna.fontcuberta-morral@epfl.ch
Universidad de Granada	Nanoelectronics http://electronica.ugr.es	Spain	Gamiz, Francisco fgamiz@ugr.es
Fundación I+D en Nanotecnología (FideNa)	www.fidena.es	Spain	Garcia, Oscar info@fidena.es
Instituto de Cerámica y Vidrio-CSIC	Surface Plasmon in Nanostructures www.icv.csic.es	Spain	García García-Tuñon, Miguel A. magarcia@icv.csic.es
Instituto de Microelectronica de Madrid - CSIC	Magnetic nanostructures and Magnetoplasmonics www.imm-cnm.csic.es	Spain	Garcia-Martin, Antonio antonio@imm.cnm.csic.es
Catalan Institute of Nanotechnology	Phononics and Photonics Nanostructures Group www.icn.cat	Spain	García-Martínez, Yamila yamila.garcia@uv.es
International Centre of Biodynamics	www.biodyn.ro	Romania	Gheorghiu, Eugen office@biodyn.ro
Laboratoire de Photonique et de Nanostructures - CNRS	Ultimately Focused Ion Beams www.lpn.cnrs.fr	France	Gierak, Jacques jacques.gierak@lpn.cnrs.fr
Nanotec Electronica	www.nanotec.es	Spain	Gil, Adriana adriana.gil@nanotec.es
Tyndall National Institute	Electronic Theory Group www.tyndall.ie	Ireland	Greer, Jim jim.greer@tyndall.ie
INSA LYON	INL www.insa-lyon.fr	France	Guillot, Gérard gerard.guillot@insa-lyon.fr
Dresden University of Technology	www.nano.tu-dresden.de/	Germany	Gutiérrez, Rafael rafael.gutierrez@tu-dresden.de
CEA	PTA www.pta-grenoble.fr	France	Haccart, Thibault thibault.haccart@cea.fr
CEA Grenoble	SiNaPS - Nano Silicon Lab. www-inac.cea.fr	France	Hadji, Emmanuel emmanuel.hadji@cea.fr
CNRS	ELPHYSE www.lpn.cnrs.fr/en/ELPHYSE/ELPHYSE.php	France	Harmand, Jean-Christophe jean-christophe.harmand@lpn.cnrs.fr

Annex 2 nanoICT groups & statistics

List of nanoICT registered groups

Institution	Group / Web	Country	Contact Person / Email
CSEM SA	CSEM Nanotechnology & Life Sciences www.csem.ch	Switzerland	Heinzelmann, Harry harry.heinzelmann@csem.ch
ETH Zurich	Micro and Nanosystems www.micro.mavt.ethz.ch	Switzerland	Hierold, Christofer hierold@micro.mavt.ethz.ch
CIC nanoGUNE Consolider	Nanooptics www.nanogune.eu	Spain	Hillenbrand, Rainer r.hillenbrand@nanogune.eu
Tehran university	Nano technology http://ut.ac.ir	Iran	Hosseini far, Rahman rahman.hoseyni@gmail.com
CIC nanoGUNE Consolider	Nanodevices www.nanogune.eu	Spain	Hueso, Luis l.hueso@nanogune.eu
Swedish Defence Reserach Agency FOI	Antennas and Electromagnetic Compatibility www.foi.se/FOI/templates/Page____7265.aspx	Sweden	Höijer, Magnus magnus@foi.se
LPN-CNRS	Laboratoire de Photonique et de Nanostructures www.lpn.cnrs.fr	France	Jabeen, Fauzia fauzia.jabeen@lpn.cnrs.fr
University College London	Diamond Electronics Group www.london-nano.com	United Kingdom	Jackman, Richard r.jackman@ucl.ac.uk
University of Melbourne	Microanalytical Research Centre www.ph.unimelb.edu.au/~dnj	Australia	Jamieson, David d.jamieson@unimelb.edu.au
University of the Basque country	Solid state an materials chemistry www.dqi.ehu.es	Spain	Jimenez de Aberasturi, D. djimenezdeab001@ikasle.ehu.es
CNRS	LPN/PHYNANO www.lpn.cnrs.fr	France	Jin, Yong yong.jin@lpn.cnrs.fr
CNRS (Toulouse)	Nanoscience Group www.cemes.fr	France	Joachim, Christian joachim@cemes.fr
RWTH Aachen University	Institute for Electromagentic Theory www.unibw.de/eit4_1	Germany	Jungemann, Christoph christoph.jungemann@ithe.rwth-aachen.de
CNRS	Centre Interdisciplinaire de Nanoscience de Marseille / STNO www.cinam.univ-mrs.fr/cinam/	France	Juvenal, Valérie abbes@cinam.univ-mrs.fr
Eberhard Karls Universität Tübingen [University]	Nanostructures and Mesoscopic Physics www.uni-tuebingen.de/nano/index.html	Germany	Kern, Dieter dieter.kern@uni-tuebingen.de
Chalmers University of Technology	Division of Condensed Matter Theory www.chalmers.se	Sweden	Kinaret, Jari jari.kinaret@chalmers.se
Jacobs University Bremen	Theoretical Physics and Biophysics Group www.jacobs-university.de/ses/ukleinekathoefer	Germany	Kleinekathöfer, Ulrich u.kleinekathoefer@jacobs-university.de
Eindhoven University of Technology	Physics of Nanostructures www.fna.phys.tue.nl	Netherlands	Koopmans, Bert b.koopmans@tue.nl
University Paris Sud	IEF - Silicon-based photonics http://silicon-photonics.ief.u-psud.fr/	France	Laurent, Vivien laurent.vivien@u-psud.fr
THALES R&T and Ecole Polytechnique	Nanocarb www.polytechnique.edu	France	Legagneux, Pierre pierre.legagneux@thalesgroup.com
Fraunhofer Institute Material and Beam Technology IWS	www.iws.fraunhofer.de	Germany	Leson, Andreas birgit.schaub@iws.fraunhofer.de
Aalto University	Nanotechnology nano.tkk.fi/en	Finland	Lipsanen, Harri harri.lipsanen@aalto.fi
CNRS	NanoBioSystems www.laas.fr/NBS/	France	Liviu, Nicu nicu@laas.fr
Instituto de Ciencia de Materiales de Madrid	Photonic Crystals Group http://luxrerum.icmm.csic.es/	Spain	Lopez, Cefe cefe@icmm.csic.es

Institution	Group / Web	Country	Contact Person / Email
Universidad Complutense de Madrid	Aperiodic Structures in Condensed Matter http://material.fis.ucm.es/	Spain	Macia, Enrique emaciaba@fis.ucm.es
University of Pisa	Nanoelectronics Group www.unipi.it/	Italy	Macucci, Massimo macucci@mercurio.iet.unipi.it
NANOTIMES	www.nanotimes.fr	France	Magoga, Michael gaston.nicolessi@nanotimes.fr
CEA	Laboratory of Inorganic and Biological Chemistry http://inac.cea.fr/scib	France	Maldavi, Pascale pascale.maldivi@cea.fr
University of Minho	Physics of Nano-Crystalline Materials www.uminho.pt	Portugal	Martín Sánchez, Javier javier.martin.nano@gmail.com
Parc de Recerca UAB	http://parc.uab.cat	Spain	Martinez, Ana Belén parc.recerca@uab.cat
ISOM - Universidad Politecnica de Madrid	Nanofabrication and Nanodevices www.isom.upm.es	Spain	Martinez, Javier javier.martinez@isom.upm.es
Universidad de Salamanca	Semiconductor Devices Research Group www.usal.es/gelec/	Spain	Mateos, Javier javierm@usal.es
University of Ulster	Nnaotechnology and Integrated Bioengineering Centre www.nibec.ulster.ac.uk	United Kingdom	McLaughlin, Jim jad.mclaughlin@ulster.ac.uk
Fundacion CIDETEC	Nanotecnology Unit www.cidetec.es	Spain	Mecerreyes, David dmecerreyes@cidetec.es
University of Cambridge	EDM www-g.eng.cam.ac.uk/edm/	United Kingdom	Milne, Bill wim@eng.cam.ac.uk
Lund University	http://nano.lth.se	Sweden	Montelius, Lars fredrik.boxberg@ftf.lth.se
Jacobs University Bremen	Nanoelectronics/Nanomolecular science www.jacobs-university.de/ses/vwagner/research/group	Germany	Mousavi, Sayed Alireza a.mousavi@jacobs-university.de
CIC nanoGUNE Consolider	Nanobiotechnology www.nanogune.eu	Spain	Nabiev, Igor i.nabiev@naogune.eu
Universität Hamburg	Multifunctional Nanostructures www.physnet.uni-hamburg.de/institute/IAP/Group_K/multifunctional_nanostructures.htm	Germany	Nielsch, Kornelius knielsch@physnet.uni-hamburg.de
University of Copenhagen	Mogens Brøndsted Nielsen (SINGLE project) http://mbn.kiku.dk/mbn_home.htm	Denmark	Nielsen, Mogens B. mbn@kiku.dk
CSIC	Teoria y simulación de materiales www.icmm.csic.es/mnv/	Spain	Nieto Vesperinas, Manuel mnieto@icmm.csic.es
Centro de Investigación en Nanociencia y Nanotecnología	Theory and Simulation www.cin2.es/groups/theory	Spain	Ordejon, Pablo pablo.ordejon@cin2.es
University of Copenhagen	NanoTheory www.nbi.ku.dk/paaske	Denmark	Paaske, Jens paaske@fys.ku.dk
CEA Saclay	Chemistry of Surfaces and Interfaces http://iramis.cea.fr/spcsi/index.php	France	Palacin, Serge serge.palacin@cea.fr
CNR Istituto Nanoscienze	www.nano.cnr.it/	Italy	Pellegrini, Vittorio vp@sns.it
Consejo Superior de Investigaciones Científicas	Nanofabrication and Functional Properties of Nanostructres www.imb-cnm.csic.es	Spain	Perez-Murano, Francesc Francesc.Perez@imb-cnm.csic.es
CNRS	Unité Mixte de Physique CNRS/Thales www.trt.thalesgroup.com/ump-cnrs-thales/	France	Petroff, Frederic frederic.petroff@thalesgroup.com

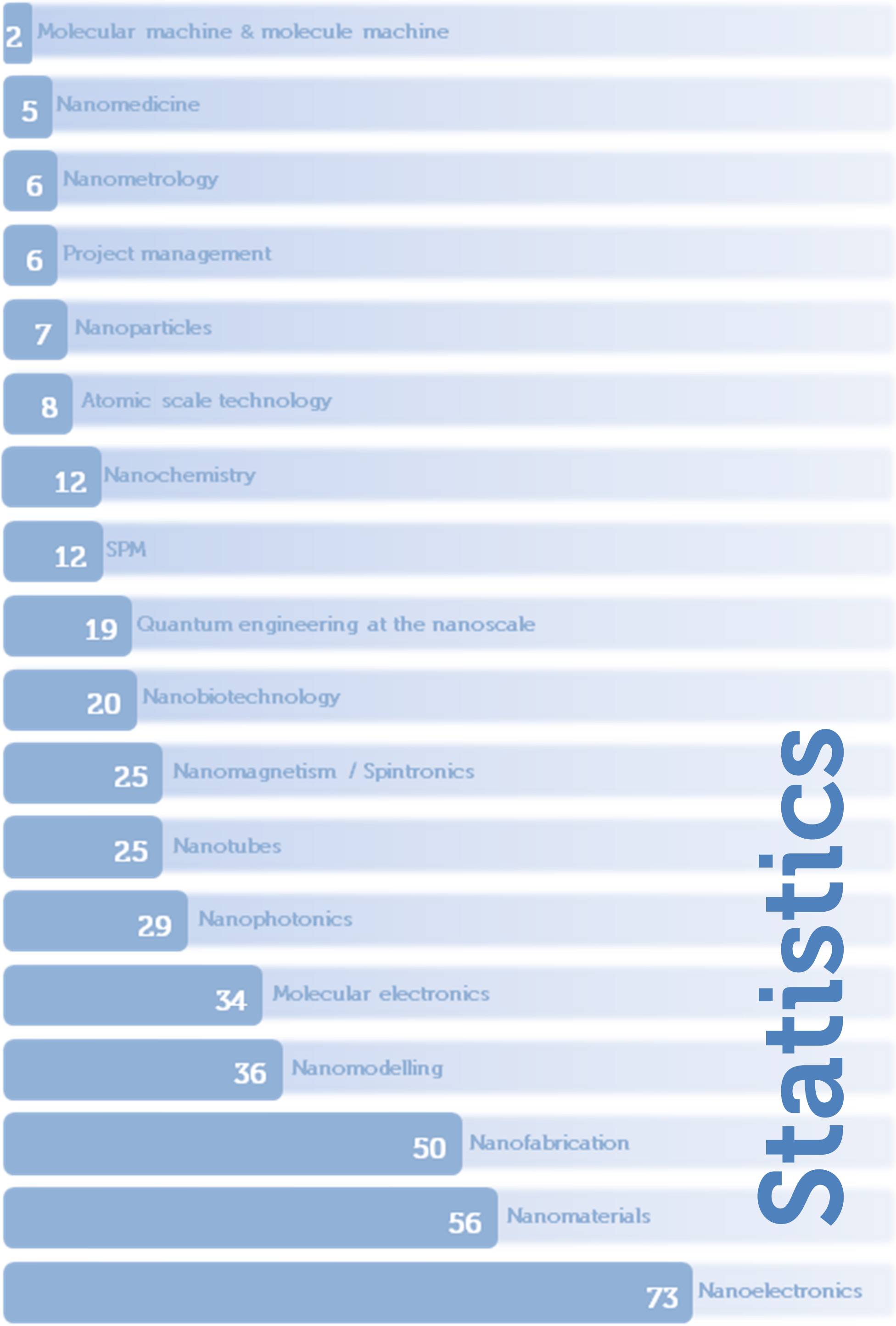
Annex 2 nanoICT groups & statistics

List of nanoICT registered groups

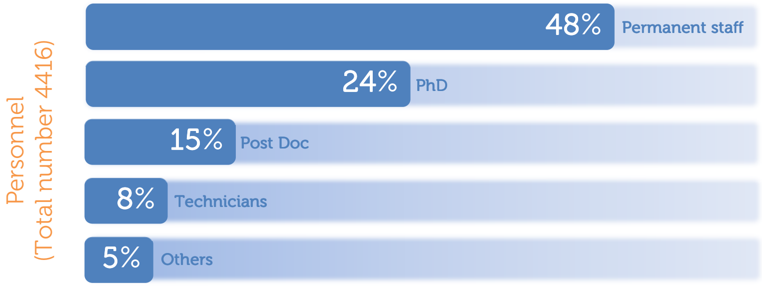
Institution	Group / Web	Country	Contact Person / Email
Instituto de Microelectronica de Madrid	Molecular Beam Epitaxy www.imm-cnm.csic.es/mbe	Spain	Postigo, Pablo Aitor aitor@imm.cnm.csic.es
Archimedes Foundation	www.archimedes.ee	Estonia	Raamat, Rivo rivo.raamat@archimedes.ee
Johannes Gutenberg-Universität	Nanofibre Photonics and Quantum Optics www.quantum.physik.uni-mainz.de/en/fibres/index.html	Germany	Rauschenbeutel, Arno arno.rauschenbeutel@uni-mainz.de
Università del Salento	CMTG http://cmtg1.unile.it/	Italy	Reggiani, Lino lino.reggiani@unisalento.it
CNR - IMM Institute for Microelectronic and Microsystems	Sensors and biosensors group www.imm.cnr.it	Italy	Rella, Roberto roberto.rella@le.imm.cnr.it
University of Regensburg	Mesoscopic Physics www.physik.uni-regensburg.de/forschung/richter/richter/	Germany	Richter, Klaus klaus.richter@physik.uni-r.de
IBM Research GmbH	Nanoscale Electronics www.zurich.ibm.com/	Switzerland	Riel, Heike hei@zurich.ibm.com
Georg-August University Goettingen	Group III-N based Functional Hetero- and Nanostructures www.uni-goettingen.de/en/105305.html	Germany	Rizzi, Angela rizzi@ph4.physik.uni-goettingen.de
University of Cambridge	EDM www-g.eng.cam.ac.uk/edm	United Kingdom	Robertson, John jr@eng.cam.ac.uk
Catalan Institute of Nanotechnology	Theoretical and Computational Nanoscience www.icn.cat/index.php/research	Spain	Roche, Stephan stephan.roche@icn.cat
Instituto de Ciencia de Materiales de Sevilla	Thin Film Engineering and Plasma Technology www.sincaf-icmse.es	Spain	Rodríguez, Agustín arge@icmse.csic.es
UPV/EHU	Solid state and materials chemistry www.ehu.es/qi/	Spain	Rojo Aparicio, Teófilo teo.rojo@ehu.es
INRS	Nano(meter)-Femto(second) Laboratory www.nanofemtolab.qc.ca	Canada	Rosei, Federico rosei@emt.inrs.ca
Universidad del País Vasco	Nano-bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF) http://nano-bio.ehu.es/	Spain	Rubio, Ángel angel.rubio@ehu.es
Universidad Autonoma de Madrid	MOLE-UAM www.uam.es/gruposinv/MoLE/	Spain	Sáenz Gutiérrez, Juan José juanjo.saenz@uam.es
Institute for Bioengineering of Catalonia	Nanobioengineering group www.ibecbarcelona.eu/nanobioengineering	Spain	Samitier, Josep jsamitier@ub.edu
Lund University	The Nanometer Structure Consortium http://nano.lu.se	Sweden	Samuelson, Lars Lars.Samuelson@ftf.lth.se
CEA	SPSMS/Laboratory for Quantum Electronic Transport and Superconductivity http://inac.cea.fr/en/Phocea/Vie_des_labos/Ast/ast_visu.php?id_ast=208	France	Sanquer, Marc marc.sanquer@cea.fr
Sapienza University of Rome	EMC Lab w3.uniroma1.it/cnis/	Italy	Sarto, Maria Sabrina mariasabrina.sarto@uniroma1.it
UJF-CNRS-CEA	SPINTEC www.spintec.fr	France	Schuhl, Alain alain.schuhl@cea.fr

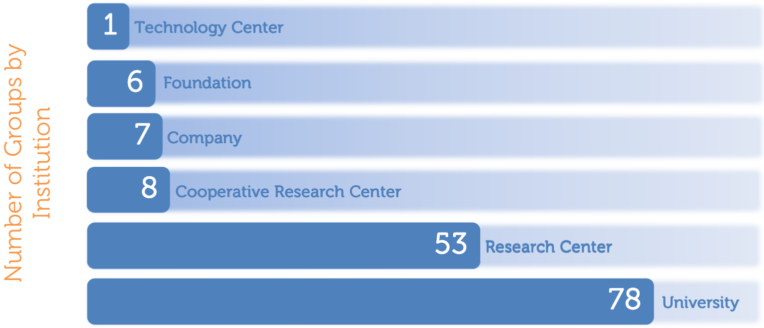
Institution	Group / Web	Country	Contact Person / Email
CEA	Laboratory for Innovative NAnophotonic systems (LINA) www.leti.fr	France	Segolene, Olivier segolene.olivier@cea.fr
Technische Universität Wien	Institute for Microelectronics www.iue.tuwien.ac.at	Austria	Selberherr, Siegfried Selberherr@TUWien.ac.at
Università degli Studi di Udine	Nano Electronics www.diegm.uniud.it/selmi	Italy	Selmi, Luca luca.selmi@uniud.it
Instituto de Ciencia de Materiales de Madrid (CSIC)	Condensed Matter Theory www.icmm.csic.es/Teoria/	Spain	Serena Domingo, Pedro A. pedro.serena@icmm.csic.es
Universita di Roma	Università di Roma www.uniroma1.it	Italy	Sibilia, Concita concita.sibilia@uniroma1.it
Institut Català de Nanotecnologia	The Phononic and Photonic Nanostructures Group (P2N) www.nanocat.org	Spain	Sotomayor Torres, Clivia clivia.sotomayor@icn.cat
Institut Jean Lamour	Nanomagnetism & Spintronic group www.lpm.u-nancy.fr/nanomag/	France	Stephane, Mangin stephane.mangin@ijl.nancy-universite.fr
Jagiellonian University	NANOSAM www.if.uj.edu.pl/NANOSAM/	Poland	Szymonski, Marek ufszymon@cyf-kr.edu.pl
AIXTRON	www.aixtron.com	United Kingdom	Teo, Ken k.teo@aixtron.com
University of Salerno	Lab of Electromagnetic Characterization of Materials www.dieii.unisa.it	Italy	Tucci, Vincenzo vtucci@unisa.it
TUDelft	MED http://kavli.tudelft.nl/	Netherlands	van der Zant, Herre h.s.j.vanderzant@tudelft.nl
IMEC	Functional Nanosystems www.imec.be	Belgium	Van Roy, Wim vanroy@imec.be
Comissariat à Energie Atomique	Laboratoire dElectronique et des Technologies de lInformation www-leti.cea.fr	France	Viala, Bernard bernard.viala@cea.fr
Freie Universitaet Berlin	Theory of quantum transport www.physik.fu-berlin.de/en/einrichtungen/ag/ag-von-oppen/	Germany	von Oppen, Felix vonoppen@physik.fu-berlin.de
Institute for Electronics Microelectronics and Nanotechnology	Molecular Nanostructures & Devices group ncm.iemn.univ-lille1.fr	France	Vuillaume, Dominique dominique.vuillaume@iemn.univ-lille1.fr
Forschungszentrum Juelich GmbH	Electronic Materials www.fz-juelich.de/iff	Germany	Waser, Rainer r.waser@fz-juelich.de
National Physical Laboratory	Multi-Functional Materials www.npl.co.uk	United Kingdom	Weaver, Paul paul.weaver@npl.co.uk
University of Stuttgart, Institute of Biology	Nanobiotechnology Group www.uni-stuttgart.de/bio/bioinst/molbio/	Germany	Wege, Christina christina.wege@bio.uni-stuttgart.de
Ludwig-Maximilians-University	Nanomechanics Group nano.physik.uni-muenchen.de/nanomech	Germany	Weig, Eva weig@lmu.de
European Laboratory for Non Linear Spectroscopy	Optics of Complex Systems www.complexphotonics.org	Italy	Wiersma, Diederik wiersma@lens.unifi.it
Hitachi Europe Ltd	Hitachi Cambridge Laboratory www.hitachi-eu.com/r&d/rdcentres/Cambridge.pdf	United Kingdom	Williams, David jj302@cam.ac.uk
Julius-Maximilians-Universität Würzburg	Nanoelectronics http://www.physik.uni-wuerzburg.de/index.php?id=5272	Germany	Worschech, Lukas worschech@physik.uni-wuerzburg.de
Linköping University	Theoretical Physics www.ifm.liu.se	Sweden	Yakimenko, Irina irina@ifm.liu.se, kfber@ifm.liu.se

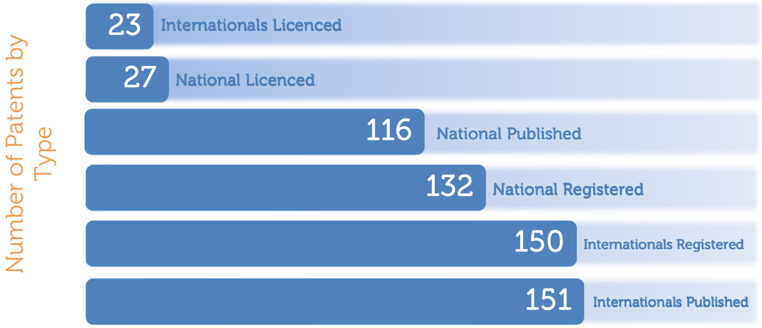
Statistics

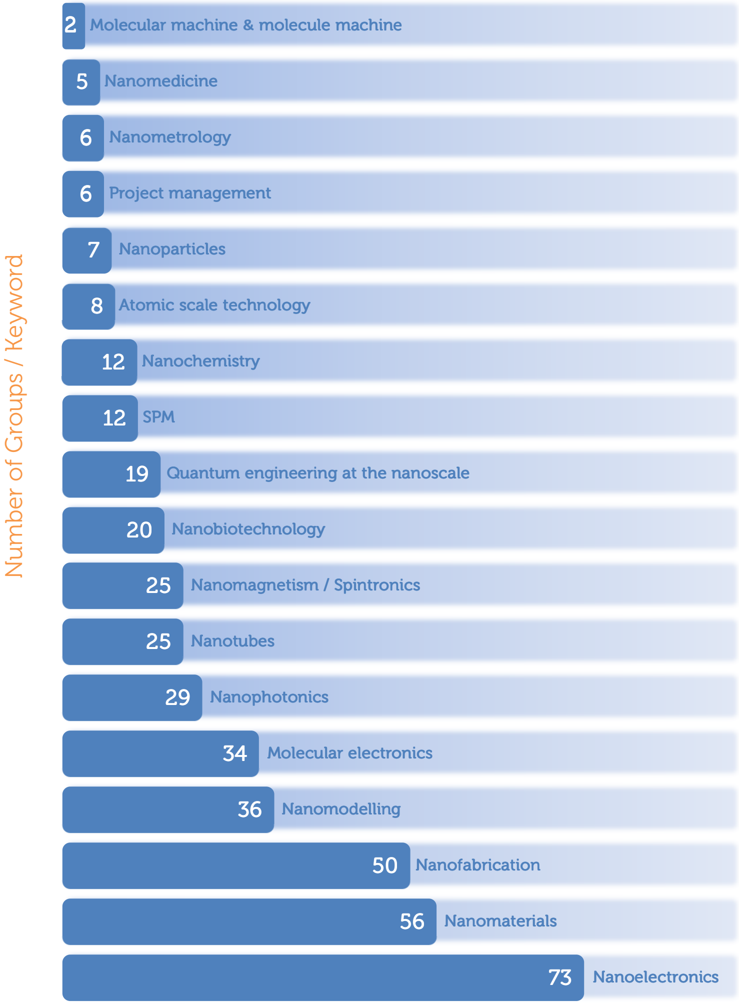

2 Molecular machine & molecule machine
5 Nanomedicine
6 Nanometrology
6 Project management
7 Nanoparticles
8 Atomic scale technology
12 Nanochemistry
12 SPM
19 Quantum engineering at the nanoscale
20 Nanobiotechnology
25 Nanomagnetism / Spintronics
25 Nanotubes
29 Nanophotonics
34 Molecular electronics
36 Nanomodelling
50 Nanofabrication
56 Nanomaterials
73 Nanoelectronics

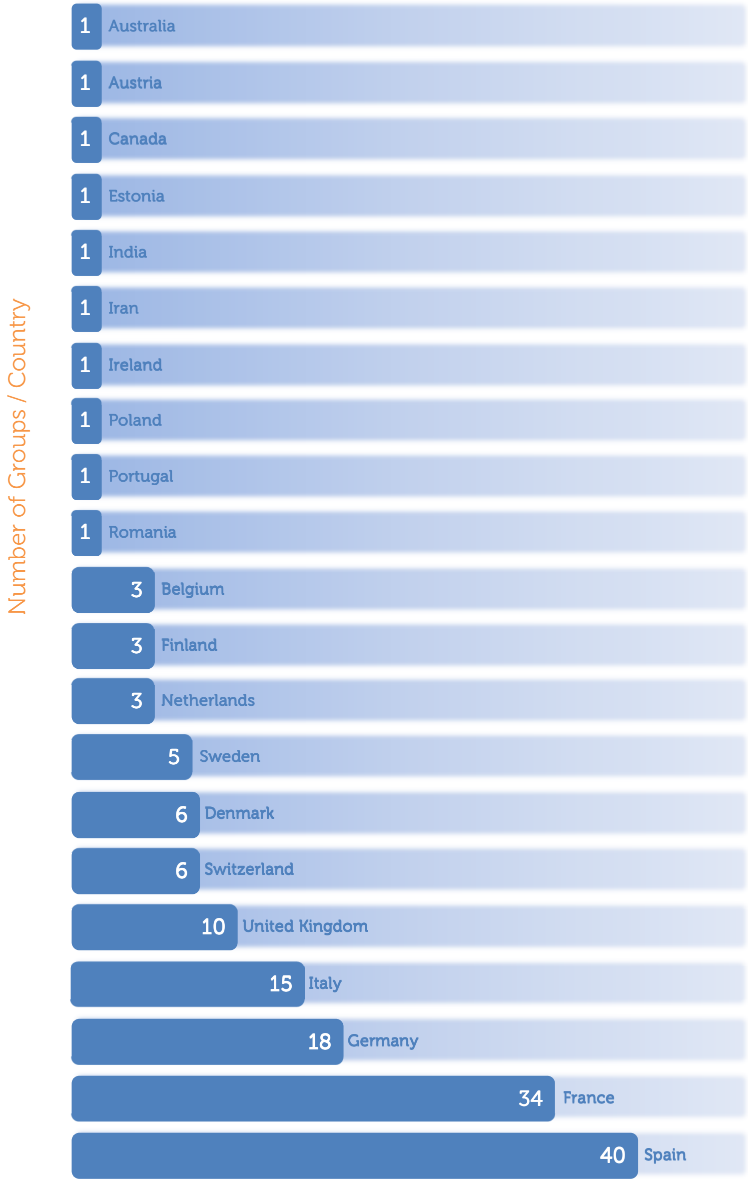
Statistics


Personnel
(Total number 4416)
48% Permanent staff
24% PhD
15% Post Doc
8% Technicians
5% Others


Number of Groups by
Institution
1 Technology Center
6 Foundation
7 Company
8 Cooperative Research Center
53 Research Center
78 University


Number of Patents by
Type
23 Internationals Licenced
27 National Licenced
116 National Published
132 National Registered
150 Internationals Registered
151 Internationals Published


Number of Groups / Keyword
2 Molecular machine & molecule machine
5 Nanomedicine
6 Nanometrology
6 Project management
7 Nanoparticles
8 Atomic scale technology
12 Nanochemistry
12 SPM
19 Quantum engineering at the nanoscale
20 Nanobiotechnology
25 Nanomagnetism / Spintronics
25 Nanotubes
29 Nanophotonics
34 Molecular electronics
36 Nanomodelling
50 Nanofabrication
56 Nanomaterials
73 Nanoelectronics


Number of Groups / Country
1 Australia
1 Austria
1 Canada
1 Estonia
1 India
1 Iran
1 Ireland
1 Poland
1 Portugal
1 Romania
3 Belgium
3 Finland
3 Netherlands
5 Sweden
6 Denmark
6 Switzerland
10 United Kingdom
15 Italy
18 Germany
34 France
40 Spain

5. Annex 3

National & regional funding schemes study

National & regional funding schemes study

1. Science Funding Agencies in Europe

Nanoscience, transformed in Nanotechnology, is taking now its first steps outside the laboratories and many small and large companies are launching a first wave of nanoproducts into the markets. However, the actual power of Nanotechnology resides in an immense potential for the manufacture of consumer goods that, in many cases, will not be commercialized before a couple of decades, thus bringing tangible and promising results for the economy. Because this huge expected economic impact, nanotechnology has roused great interest among the relevant public and private R&D stakeholders of the world's most developed countries: funding agencies, scientific policymakers, organisations, institutions and companies.

N&N represent one of the fastest growing areas of R&D. In the period of 1997-2005 worldwide investment in Nanotechnology research and development has increased approximately nine times, from US$ 432 million to US$ 4200 million. This represents an average annual growth rate of 32%. A great example is the National Nanotechnology Initiative (NNI) that was established in 2000 and links 25 federal agencies closely related to activities in N&N. NNI budget allocated to the federal departments and agencies increased from US$ 464 million in 2001 to approximately US$ 1700 million in 2009. For 2011 the funding request for nanotechnology research and development (R&D) in 15 federal departments and agencies is US$ 1760 million, reflecting a continuous growth in strategic collaboration to accelerate the discovery and deployment of nanotechnology. In addition to the federal initiative, an important effort has been carried out by the different US state governments, as well as companies (Motorola, Intel, Hewlett-Packard, IBM, Amgen, Abbot Lab., Agilent, etc).

Industrialized Asian countries have promoted the development of Nanotechnology from the industrial and governmental sectors, with investments similar to those of USA. Countries as Taiwan and Korea have made a great effort to keep their current privileged positions in the control of Nanotechnology know-how. According to Mihail Roco, Japan increase their budget from US$ 245 million in 2000 to US$ 950 million in 2009, proving a significant rising of the investment from the Japanese Government. Taiwanese, Japanese and South Korean companies are leading the Nanotechnology investments in their respective countries. In the meantime, China has become a key player in the Nanotechnology field, leading sectors as the fabrication of nanoparticles and nanomaterials. Countries as Israel, Iran, India, Singapore, Thailand, Malaysia and Indonesia have launched specific programmes to promote the use of Nanotechnologies in many industrial sectors with local or regional impact (manufacture, textile, wood, agriculture, water remediation, etc).

Europe has intensively promoted Nanotechnology within the VI (FP6) and the VII (FP7) Framework Programme through thematic Areas denominated NMP[1] and ICT[2]. During the period of 2003-2006 the budget for NMP was 1429 million Euros and a remarkable increase of 3475 million Euros for funding N&N over the duration of FP7 (2007-2013). There's a proven commitment of the EU to strengthen research in Europe. Initiatives involving not only increased investment, but also stronger coordination and collaboration between all stakeholders like the FET flagship (ICT) are being implemented. In order to improve the competitiveness of European industry, to generate and ensure transformation from a resource-intensive to a knowledge-intensive industry were created the FET Flagships Initiatives. FET-Proactive acts as a pathfinder for the ICT program by fostering novel non-conventional approaches, foundational research and supporting initial developments on long-term research and technological innovation in selected themes. Under the FP7 program were created AMOL-IT, nanoICT and Towards Zero-Power ICT projects in order to focus resources on visionary and challenging long-term goals that are timely and have strong potential for future impact. There has been a boom of European initiatives dedicated to develop and popularize Nanotechnology and this area maintains its outstanding role in the FP7 Program.

Among the EU members, Germany stands right at the forefront of international Nanoscience and is considered as a key location for nano research. The Federal Government by exceptional funding programs is helping to turn Germany into the leading nano spot. In 2008 about 430 million Euros were invested by public funding in Nanotechnology. Nowadays, around 740 companies work on the development, application and distribution of nanotechnology products. Following similar long term strategies, on December 2009, French Government unveiled a 35000 million Euros national bond to prepare France for the challenges of the future. The spending spree over the coming years contemplates higher education and research as the main priorities, among others. Part of this amount will be applied to create new Campus of Excellence, develop research teams, boost competitiveness and increase efforts in biotechnology and nanotechnology. NanoNextNL[3] (2011-2016) consortium in Netherlands which supports research in the field of nano and microtechnology is another great example of the efforts made by the European Countries. This initiative embrace 114 partners and the total sum involved is 250 million Euros, half of which is contributed by the collaboration of more than one hundred businesses, universities, knowledge institutes and university medical centres and the other half by the Ministry of Economic affairs, Agriculture and Innovation. NanoNextNL is the successor of NanoNed and MicroNed programmes which were also greatly supported. In the same line, we must mention the Austrian NANO Initiative[4], a multi-annual funding programme for N&N that coordinates NANO measures on the national and regional levels and is supported by several Ministries, Federal provinces and Funding institutions, under the overall control of the BMVIT Federal Ministry for Transport,

---

[1] FP6 Thematic Area denominated "Nanotechnologies and nano-sciences, knowledge-based multifunctional materials and new production processes and devices" and FP7 denominated "Nanosciences, Nanotechnologies, Materials and new Production Technologies".

[2] ICT: Information and Communication Technologies.

[3] www.nanonextnl.nl

[4] www.nanoinitiative.at

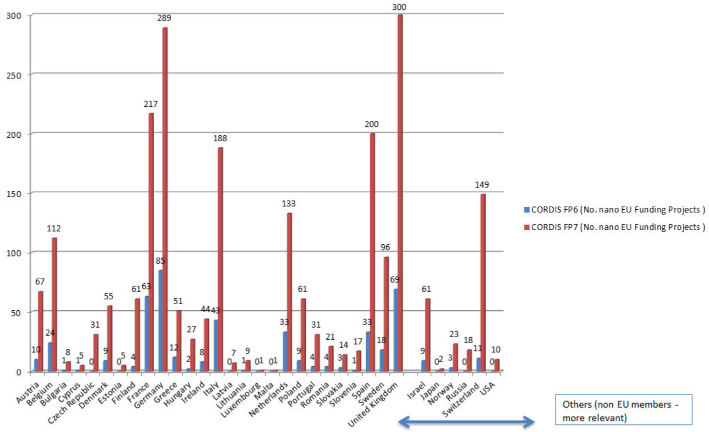


Figure 1. *Nº of nano EU funded projects (FP6 & FP7) per country*

Innovation and Technology. The orientation and the structure of the Austrian NANO Initiative have been developed jointly with scientists, entrepreneurs and intermediaries. The Austrian NANO Initiative has funded nine RTD project clusters involving more than 200 Austrian companies and research institutions.

EU authorities have also taken into account serious concerns on Nanotechnology, appearing in diverse social and economic forums during the last decade, in relation with its possible environmental and health effects. These non-desired drawbacks would provide a negative social perception on the development on Nanotechnology and could lead to an unexpected cut of private and public investments, with the subsequent delay in the arrival of the bunch of promised goods, devices and materials. In order to allow a coherent (rational, sustainable, non-aggressive, etc) development of Nanotechnology, the EU has promoted basic and applied research on nanoecotoxicology and different studies on social perception on N&N. Simultaneously, several EU Departments have launched initiatives to improve the communication and dissemination among population on the future advances and risks that Nanotechnology will bring. A good example is the European Project NanoCode[5], funded under the Program Capacities, in the area Science in Society, within the 7th Framework Program (FP7) which started in January 2010 in order to implement the European Code of Conduct for Responsible Nanosciences & Nanotechnologies.

In addition, EU has also promoted the generation of knowledge based on Nanotechnology emphasizing the role of this techno-scientific area as foundation for future convergence with other disciplines such as Biotechnology, Medicine, Cognitive Science, Communications and Information Technologies, Social Sciences, etc.

---

[5] www.nanocode.eu

Annex 3 National & regional funding schemes study

European Commission

http://ec.europa.eu/research/index.cfm
(See Figure 1).

ERC - European Research Council

http://erc.europa.eu/

European Research Council (ERC) grants support individual researchers of any nationality and age who wish to pursue their frontier research. In particularly, the ERC encourages proposals that cross disciplinary boundaries, pioneering ideas that address new and emerging fields and applications that introduce unconventional, innovative approaches.

ESF - The European Science Foundation

www.esf.org

EMBO - BIO

www.embo.org

EMBO is an organization of leading life scientist members that fosters new generations of researchers to produce world-class scientific results.

They support talented researchers, selected through impartial evaluation processes, so that they can go on to do great science with the creativity and passion to answer the unanswered. We provide platforms for scientific exchange and training in cutting-edge technologies so that the high standards of excellence in research practice are maintained. We help to shape science and research policy for a world-class European research environment.

The objective of the instruments under Science Strategy is to provide evidence-based foresight and advice on science, research infrastructure and science policy issues of European significance to underpin decisions on strategic directions and priorities, or on programmes of science-driven research. In the application of these instruments special attention is paid to promoting Europe's ability to open up new research areas in order to be a leader rather than a follower. The instruments in Science Strategy can have a real impact if the experts involved are of the highest authority. High quality output requires a critical awareness of the need for an impartial balance of interests.

These links to foreign science funding agencies (NSF counterparts) are provided as a resource for the US science community. Note that listing an agency is not an endorsement by NSF. Viewers will leave the NSF website when selecting a specific counterpart link.

Many countries have several science agencies. For more information related to a specific country or a country with no counterpart agency listed, contact the NSF Europe Regional Office (nsfeurope@nsf.gov) or the NSF OISE program officer listed for that country (www.nsf.gov/od/oise/country-list.jsp).

Armenia

National Academy of Sciences of Armenia (NAS RE)
www.sci.am

Austria

The Austrian Nano Initiative began life in March 2004, following a 2002 recommendation from the Austrian council for research and technology development for targeted support of nanotechnology. The Initiative has a budget of €35 million and targets research funding, networking, education and training. It is intended to spam research and industry, focusing on basic and applied research and pre-competitive development.

Austria has also issued seven calls for specific project clusters, such as NANOCOAT (Development of Nanostructured Coatings for the Design of Multifunctional Surfaces) in 2004. The goal of this project is to develop knowledge for “load orientated design of coatings and surfaces”. The project is coordinated by Materials Centre Leoben and has funded eight projects with €3.2 million over two years.

Additional funding for nanotechnology comes from the following agencies:

- The Austrian Research Promotion Agency (FFG), €8 million
- The Austrian Science Fund (FWF), €6 million
- Federal States, €0.3 million

These figures represent a yearly average.

The Austrian Nano Initiative also includes the project NanoTrust, which is intended to survey the state of knowledge regarding potential risks of nanotechnology, to act as a clearing house for information, and to promote discussion.

Austrian Academy of Sciences (OAW)
www.oeaw.ac.at/english/home.html
Austrian Science Fund (FWF)
www.oeaw.ac.at/english/home.html

Azerbaijian

Azerbajian National Science Foundation (ANSF)
www.ansf.az

Belgium

Belgian National Science Foundation (FWO) - Flanders
www.fwo.be
Fonds de la Recherche Scientifique (FNRS)
www1.frs-fnrs.be

Bulgaria

Bulgarian Academy of Sciences (BAS)
www.bas.bg
Bulgarian National Science Fund (NSFB)
www.nsfb.net

Croatia

Ministry of Science, Education and Sport
http://public.mzos.hr/Default.aspx

Cyprus

The Research Promotion Foundation
www.trainmor-knowmore.eu/0E7CAFFD.en.aspx

Czech Republic

Czech Science Foundation (GACR)
www.gacr.cz
Academy of Sciences of the Czech Republic (CAS)
www.cas.cz

Denmark

The Danish Agency for Science, Technology and Innovation
http://en.fi.dk/

Estonia

Estonian Science Foundation (ETF)
www.etf.ee/index.php?page=3&

Finland

The Finnish nanotechnology programme, FinNano, ran from 2005 to 2010 and had a total budget of €70 million, of which Tekes, the National Funding Agency for Research and Innovation, commited €45 million. FinNano funded cooperative, innovative and risk-intensive projects, preferably with a strong industrial component. Target sectors included ICT, Health and Wellbeing, Energy and

Environment, the Metals industry, and the Forest Cluster.

A biannual survey of Nanotechnology in Finnish Industry is carried out by Spinverse for Tekes. This study found that there were currently 202 active Finnish nanotechnology companies at the end of 2008, compared to 61 that existed in 2004. Of these companies 65 had commercial products or processes in 2008 (compared to 27 in 2004). A 'nanotechnology company' in this sense is defines as a company which has commercial products, research and development activities, or a strategy for how nanotechnology will impact their business. Revenue from nanotechnology-related products and activities were estimated at € 300 million in 2008, with employment of 3-4,000. Industrial funding (at € 56.6 million) exceeded public funding (€38 million) and venture capital (€ 9.5 million).

Academy of Finland (AKA)
www.aka.fi/en-gb/A/
National Technology Agency (TEKES)
www.tekes.fi/en/community/Home/351/Home/473/%20

France

Funding for nanotechnology research and development in France comes from several sources. The National Research Agency (ANR) supports a number of nanotechnology programmes, including Pnano, Materials and Processes, and Health, Environment and Health Work, which considers nanoparticles toxicity. France has three networks for advanced research (RTRA) which include nanotechnology in their research. These include the Triangle of Physics in the Paris area, the Strasbourg-based International Center for Frontier Research in Chemistry, and the Nanosciences Foundation in Grenoble (www.fondation-nanosciences.fr). The latter includes 32 laboratories in the Grenoble area, accounting for around 1000 researchers. France's Nano2012 programme is intended to develop technology to design and produce the next generation of integrated circuits. The industry/research alliance is driven by STMicroelectronics and has received € 450 million from the French government. The total cost of the programme is €2 billion.

Key Organisations:

National Research Agency (L'Agence nationale de la recherché - ANR)
www.agence-nationale-recherche.fr
Foundation Nanosciences
www.fondation-nanosciences.fr
Triangle of Physics
www.triangledelaphysique.fr
International Center for Frontier Research in Chemistry – Strasbourg
www.cirfc.fr
Centre National de la Recherche Scientifique(CNRS)
www.cnrs.fr

Germany

Germany has the highest public sector investment in nanotechnology of any European country, second only to the European Commission. The German Ministry of Education and Research (BMBF) claims that over half of all European nanotechnology companies are based in Germany, with the BMWi identifying 600 (mainly small) companies. Public investment in Germany reached €330 million in 2006, following regular annual increases of 5-10%. Nanotechnology development is guided by the Nano Initiative Action Plan 2010, which like the US NNI sets a framework for the activities of seven German Federal ministries. The main aim of this action plan is to improve the interface between research and implementation, and to open up new markets. This is being approached with a variety of measures, including branch-level industrial dialogues which highlight the research needs of particular sectors, describe application scenarios and constructs complete value chains. Other priorities of the Action Plan include keeping the public informed, ensuring responsible development, and identifying future demands for research.

The Federal Ministry of Labour and Social Affair (BMAS) has an interest in nanotechnology both as a technology which will influence future economic development in Germany, and as a topic in occupational health and safety. The Federal Ministry for the Environment, Nature Conservation and Nuclear Safety similarly has a dual interest; the potential for nanotechnology to improve resource efficiency and improvements in environmental protection, as well developing greater understanding of the effects of nanoparticles on people and the environment.

Key Organisations:

Federal Ministry of Education and Research (BMBF)
www.bmbf.de/en/index.php
Federal Ministry of Labour and Social Affair (BMAS)
www.bmas.de/EN/Home/home.html
Federal Ministry for the Environment, Nature Conservation and Nuclear Safety (BMU)
www.bmu.de/english/aktuell/4152.php
Federal Ministry of Food, Agriculture and Consumer Protection (BMELV)
www.bmelv.de/EN/Homepage/homepage_node.html
Federal Ministry of Defence (BMVg)
www.bmvg.de/portal/a/bmvg
Federal Ministry of Health (BMG)
www.bmg.gv.at/cms/home/thema.html?channel=CH1013
Federal Ministry of Economics and Technology (BMWi)
www.bmwi.de/English/Navigation/root.html
German Research Association (DFG)
www.dfg.de/en/index.jsp

Key Documents:
Nano-Initiative Action Plan 2010
www.bmbf.de/pub/nano_initiative_action_plan_2010.pdf

Greece

Foundation for Research and Technology-Hellas (FORTH)
www.forth.gr

Hungary

Hungarian Academy of Sciences (MTA)
http://mta.hu/
Hungarian Scientific Research Fund (OTKA)
www.otka.hu

Ireland

Royal Irish Academy (RIA)
www.ria.ie
Science Foundation Ireland (SFI)
www.sfi.ie

Latvia

Latvian Council of Science (LCS)
www.lzp.lv

Lithuania

Lithuanian Academy of Science (LMA)
http://lma.lt/index.php?lang=en

Luxembourg

Fonds National de la Recherche (FNR)
www.fnr.lu

Malta

Malta Council for Science and Technology (MCST)
www.mcst.gov.mt

The Netherlands

The Netherlands has had one of Europe's most high profile nanotechnology programmes, NanoNed. The project partners include eight research centres and Phillips Electronics. Three further research centres are cooperation partners of the project. The programme has a total budget of € 235 million, of which 50% is provided by a grant from the Dutch government. € 80 million of the NanoNed budget is directed to an infrastructure element called NanoLab NL, and €5 million to a technology assessment programme which is intended to 'improve the interaction between science, technology and society'. The largest element of the project budget, €150 million goes to 11 'Flagship' programmes, which as of 2007 contained a total of 185 projects:

- NanoFabrication, 13 projects, lead by University of Twente
- NanoSpintronics, 22 projects, TU Eindhoven
- NanoFluidics, 24 projects, University of Twente
- Nanophotonics, 22 projects, AMOLF
- NanoInstrumentation, 18 projects, TNO
- Advanced NanoProbing, 15 projects, Radboud University
- NanoElectronic Materials, 25 projects, U Twente
- Bottom-Up Electronics, 12 projects, RU Groningen
- BioNano Systems, 13 projects, BioMade
- Chemistry and Physics of Individual Molecules, 12 projects, RU Groningen
- Quantum Computation, 9 projects, TU Delft

In 2009 it was announced that 125 million Euros in funding for nanotechnology R&D would be allocated from the Fonds Economische Structuurversterking (FES), under the auspices of the programme 'Towards a Sustainable Open Innovation Ecosystem'. This funding resulted in large part from the development of the Strategic Research Agenda of the Dutch Nano Initiative, which had been drawn up by Nanoned, FOM and STW. The total budget for this initiative is 300 million Euros, with the remaining 175 million coming from participating universities, institutes and companies.

Netherlands Organization for Scientific Research (NWO)
www.nwo.nl

Norway

In contrast to Sweden, Norway has a large scale programme on nanotechnology and new materials, called NANOMAT. This is one of seven such programmes (others address climate change, management of petroleum resources, aquaculture, for example) which each have a long term funding commitments and are targeted to research and technology development, as such involving research centres and companies. The NANOMAT programme runs from 2002 -2016 and aims to develop world leading research in specific areas, to provide a basis for innovation and growth, and to promote commercialisation. The budget for the programme in 2008 is €8.4 million, with €10.9 available for funding. Total funding from NANOMAT to projects has been €74.7 million.

The programme has four thematic areas:

- Energy and environment
- ICT and Microsystems
- Health and biotechnology
- Sea and food

Cross functional competences are being developed, including nanostructured materials and surfaces, and ELSA including health safety and environment. Just less than 50% of total funding has been allocated to the first two thematic priorities, Energy and ICT, with 42 projects funded in this area. Another large funding category is the expertise area 'New Functional and Nanostructured Materials', which has received €17.8 million for 42 projects. The intriguing 'Ocean and Food' thematic area has received just € 0.8 million for two projects. 104 projects are running in total.

Research Council of Norway
www.forskningsradet.no/no/Forsiden/1173185591033

Poland

Polish National Foundation (FNP)
www.fnp.org.pl
Poland Ministry of Science & Higher Education (NAUKA)
www.nauka.gov.pl

Portugal

Foundation for Science and technology (FCT)
http://alfa.fct.mctes.pt/

Romania

National University Research Council (CNCSIS)
www.cncsis.ro
Romanian Academy of Sciences
www.acad.ro/def2002eng.htm

Slovakia

Slovak Academy of Sciences (SAV)
www.sav.sk/?lang=en

Slovenia

Ministry of Education, Science and Sports (MVTZ)
www.mvzt.gov.si
Slovenian Science Foundation (SZF)
www.szf.si

Spain

At the end of 90´s, Spain had not any institutional framework nor initiative pointed towards the support and promotion of R&D in Nanotechnology. This fact pushed the scientific community to promote several initiatives to strengthen research in Nanotechnology and, at the same time, to raise the awareness of Public Administration and industry about the need to support this emergent field.

Among the initiatives that emerged in Spain in this last decade we can highlight the creation of thematic networks with a strong multidisciplinary character. These networks have enabled communication between scientific communities and different areas, improving the interaction between Spanish groups and improving the visibility of this community. NanoSpain network[6] is the clearest example of self-organization of scientists that helped to promote to the authorities and the general public the existence of this new knowledge, in order to generate and achieve competitive science, which can result into high value added products in the near future. NanoSpain network comprises nearly 330 R&D groups (see Figure 2) from universities, research centers and companies, distributed throughout the country. These groups respresent a research task force formed by more than 2000 scientists working in N&N. Despite being the meeting point of the continuously increasing Spanish nanotechnology community, NanoSpain network has received little support from Spanish Administration in contrast to those networks established in other countries.

Another Spanish initiative, which emerged from the scientific community and has

---

[6] www.nanospain.org

***Figure 2.** Regional Distribution of research groups – Nanospain Network.*

become an international benchmark, is the celebration of ten consecutive editions of the conference "Trends in Nanotechnology"[7]. These meetings, a true showcase of Spanish nanoscience and nanotechnology, have attracted the most prestigious international researchers, improving the visibility of Spanish scientists. The international event, ImagineNano[8], is also a step further, a meeting that gather nearly 1500 participants from all over the world, combining within the same initiative a set of high impact conferences and an industry exhibition with more than 160 institutions/companies.

In early 2003 the initiatives launched by the scientific community (networks, workshops, conferences) related to nanotechnology led to the incorporation of the Strategic Action in Nanoscience and Nanotechnology in the National Plan R+D+I for the 2004-2007 period. This Strategic Action has had its continuity in the current National Plan (2008-2011), also including topics related to new materials and production technologies. Both strategic actions maintained an increasing rate of investment in nanotechnology in the period of 2004-2009. For example, the effort made by the General State Administration (GSA) in the implementation of N&N has been over 82 million Euros in 2008. During the 2004-2007 period the Strategic Action focused on small scale projects whereas during the 2008-2011 period the funding was mainly allocated to large scale initiatives as the building of new R&D centers or public-private consortia and platforms.

	Grants (M€)	**Loans (M€)**
Ministry of Science and Innovation (MICINN)	56,4	16,3
Ministry of Industry, Tourism and Trade (MITYC)	4,2	6,3
TOTAL	**60,6**	**22,6**

***Table 1.** Fiscal effort made by Spanish government in the field of Nanoscience and Nanotechnology in the year 2008 (Source: Ministry of Science and Innovation of Spain).*

---

[7] www.tntconf.org

[8] www.imaginenano.com

The International Campus of Excellence program was discussed in 2008, first staged competitively in 2009 and in 2010 became firmly established and aims to put major Spanish universities among the best in Europe, promoting international recognition and supporting the strengths of the Spanish university system. The program is managed by the Ministry of Education in collaboration with other ministries and supported by the Autonomous Communities. In many cases, as the Excellence Campus of Universidad Autónoma de Madrid or the Universidad Autónoma de Barcelona include remarkable activities related to the promotion of N&N.

Under the policies of the General State Administration (GSA), the Ingenio 2010 program through programs such as CENIT, CONSOLIDER and AVANZA, allowed many economic resources in strategic areas such as nanotechnology. Currently, 8 CONSOLIDER and 9 CENIT projects are related to nanotechnology, with a total GSA funding of 37.9 and 127.8 million Euros, respectively. In the case of CENIT projects, participating companies provided an additional amount of 127.8 M €. Over the next few years we expect to see the results of these initiatives through several indicators. Another important initiative is the Biomedical Research Networking center in Bioengineering, Biomaterials and Nanomedicine[9] (CIBER-BBN), a consortia, created under the leadership of the Carlos III Health Institute (ISCIII) to promote research excellence in bioengineering and biomedical imaging, biomaterials and tissue engineering and nanomedicine, diagnosis and monitoring and related technologies for specific treatments such as regenerative medicine and nanotherapies.

In addition to GSA strategies, the regional governments expressed with more or less emphasis their interest in nanotechnology, including this topic in its regional plans of R&D and encouraging the creation of new regional networks. However, most palpable manifestation of the widespread interest in nanotechnology is the establishment of new research centers as joint projects of the Ministry of Science and Innovation, Autonomous Communities and Universities. (See Figure 3).

The International Iberian Nanotechnology Laboratory[10] (INL) is the result of a joint decision of the Governments of Portugal and Spain, taken in November 2005 whereby both countries made clear their commitment to a strong cooperation in ambitious science and technology joint ventures for the future. The new laboratory is established by Portugal and Spain, but in the future will be open to the membership of other countries of Europe and other regions of the world.

Some of the centers indicated in Fig. 3 are under construction and are expected to be fully operational during the decade 2010-2020. This set of centers, along with those already existing in the public research organizations, the network of Singular Scientific and Technological Infrastructures form a system of huge potential research in nanoscience and nanotechnology. The task of knowledge generation must be completed by the technology transfer offices of universities and public research organizations, the Technology Centers, and the many science and technology parks that have been successfully implemented in Spain[11]. Also emerge thematic "nano-networks" and “nano-platforms” oriented to productive sectors as RENAC[12] (Network for the application of nanotechnologies in construction and habitat materials and

---

[9] www.ciber-bbn.es

[10] www.inl.int

[11] www.apte.org

[12] www.nano-renac.com

Figure 3. *Main N&N Centres in Spain*

products), SUSCHEM[13] (Spanish Technology Platform on Sustainable Chemistry), Génesis[14] (Spanish Technology Platform on Nanotechnology and Smart Systems Integration), NANOMED[15] (Spanish Nanomedicine Platform), MATERPLAT[16] (Spanish Technological Platform on Advanced Materials and Nanomaterials) or Fotonica21[17] (The Spanish Technology Platform of Photonics), among many others.

These strategies for generation and transfer of knowledge are reinforced by other complementary activities aimed at both the internationalization of our scientific-technological results and the dissemination of science. As an example of the internationalization, the Spanish Institute of Foreign Trade (ICEX), through its "Technology Plan" in Nanotechnology (coordinated by Phantoms Foundation) encourages external promotion activities of research centers and companies, enabling the participation of Spain with pavilions and informative points in several international exhibitions as Nanotech Japan (2008-2011), one of the most important events in nanotechnology, NSTI fair (2009) in U.S. and Taiwan Nano (2010)[18].

More recently, a catalogue of N&N companies in Spain was compiled by Phantoms Foundation and funded by ICEX and gives a

---

[13] www.suschem-es.org
[14] www.genesisred.net
[15] www.nanomedspain.net
[16] www.materplat.es
[17] www.fotonica21.org
[18] www.phantomsnet.net/nanotech2008/; www.phantomsnet.net/nanotech2009/; www.phantomsnet.net/NSTI2009/; www.phantomsnet.net/Taiwan2010/

general overview of the enterprises working in this field. Since the year of 2000 until 2010, were created 36 companies mainly in nanomaterials, nanocomposites, nanobio and nanoparticles. So far 60 companies performing R&D in nanoscience and nanotechnology are listed and is predicted a significant increase in the upcoming years.

In terms of outreach efforts we can mention several initiatives. On one hand the edition of the first book in N&N issued by the Spanish Foundation for Science and Technology (FECYT), designed to spread among teachers in secondary and high school education along with books devoted to N&N dissemination that have been recently issued. On the other hand, events as "Atom by Atom" or "Passion for Knowledge" disclose the progresses, challenges and implications of various "nano-areas" to a broad and general audience. Furthermore, initiatives as the SPMAGE international contest[19] of SPM (Scanning Probe Microscopy) images or the exhibition "A walk around the nanowold" are succesful initiatives to disseminate N&N. Recently, an Iberoamerican Network for Dissemination and Training in N&N (NANODYF[20]) has been funded by the Iberoamerican Programme for Science and Technology (CYTED) in order to promote formal and non-formal education of N&N in Iberoamerican countries where more than 460 million people communicate in Spanish.

One could say that in this last decade we have seen an explosion of initiatives in the field of nanotechnology. All initiatives represent a clear commitment that Spain is situated in the medium term between the group of countries that can lead the change towards a knowledge-based society. However, it is necessary to maintain a constant tension to strengthen the settlement of all initiatives. The short-term challenge is to continue the investement, despite being in an economic crisis, and improve coordination of all players involved in the R+D+I. The next decade will confirm whether efforts have been sufficient to be amongst the most advanced economies, fulfilling the expectations for nanotechnology as an engine of Spanish industry in 2020. Everything achieved so far has required a great effort, but still we have a R&D system relatively weak compared with those countries which we want to look like. Any change in the sustained investment policies in our R&D system can take us back several years, as budget cuts are announced to overcome this period of crisis they can also be very harmful in an emerging issue as nanotechnology. We hope these cuts are punctual and that soon will regain the road of support R+D+I.

In the meantime, before recovering the previous momentum, we need to implement new strategies intended to keep the path we started ten years ago under a more restrictive economic scenario. These strategies must be based in few ingredients, including among others: (i) the stimulus of the dialogue between Spain Ministries and Regional Goverments, on one side, and scientific community using existing networks that must be suitably funded on the other; (ii) the increasing coordination of research centres and large scale infrastrutures in order to optimize the access to scientific services of public and private groups; (iii) to enhace public-private cooperation through Technology Platforms, Industry Networks and Science and Technology Parks; (iv) an actual support to small N&N spin-offs emerging from research centres, (v) the formation of a new generation of PhD students and technicians highly skilled for multidisciplinary research through specific training programs (Master and PhD courses); and (vi) the involvement of society through well designed dissemination

---

[19] www.icmm.csic.es/spmage/
[20] www.nanodyf.org

activities using emerging communication technologies.

Sweden

Despite not having a formal nanotechnology programme, Sweden has directed public funding to the sector. Interest in nanotechnology began in the 1980s with the Micronics programme, followed by materials research consortia in the 1990s. During this decade, Sweden has directing funding from a number of sources, including five national agencies and three foundations:

- The Swedish Research Council;
- VINNOVA (The Swedish Governmental Agency for Innovation System)
- The Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning (Formas)
- The Swedish Energy Agency
- The Swedish Defence Research Agency (FOI)

Foundations:

- SSF, Foundation for Strategic Research
- KK-stiftelsen, The Knowledge Foundation
- MISTRA, the Foundation for strategic environmental Research

Together with the European Commission and the Nordic Innovation Centre, these organizations have committed approximately € 50 million in 2007. This has resulted in a structure in which there are 100 industrial actors and 15 universities engaged in nanotechnology-related activities. There is a debate in the country about the about to which the lack of an identified national programme has hampered development; whilst it has resulted in 'under-labelling' of nanotechnology activities, research and industrial activities is still relative.

Swedish Foundation for Strategic Research (SSF)
www.stratresearch.se

Switzerland

Swiss National Science Foundation (SNF)
www.snf.ch/e/Pages/default.aspx

United Kingdom

The United Kingdom lays claim to one of the earliest nanotechnology programmes, the LINK Nanotechnology Programme (LNP) National Initiative on Nanotechnology (NION). This was an initiative of the then Department of Trade and Industry (DTI) which began in 1988, and which directed around GBP 11.5 million over its lifetime. A contemporary assessment judged that the project had been relatively successful. After a lengthy interlude, in 2003 the former Science Minister Lord Sainsbury announced that GBP 90 million would be directed to funding nanotechnology commercialisation over the following six years. GBP 40 million was allocated to capital projects, which formed the basis for the current MNT Facilities Network. The intention of this project was to create a distributed network of facilities, which were intended to form a coherent national portfolio of capabilities – rather than being primarily intended for national development. The remaining GBP 50 million was allocated to collaborative research and development projects by the DTI.

In 2007 the Nanotechnology Knowledge Transfer Network (KTN) was established to continue these activities by facilitating interactions between organisations in the UK, as well as to provide input to future policy decisions. The Nanotechnology KTN is now under the auspices of the Technology Strategy Board, which is responsible for all 24 KTNs. The Technology Strategy Board was established in 2007 as an executive non-departmental public body, sponsored by the Department for Innovation, Universities and Skills. The Technology Strategy Board published its Nanoscale Technologies Strategy 2009-12 in October 2009. The strategy directs funding to nanotechnologies which address one of three specific challenges; Living with Environmental Change, Living with an Ageing and Growing Population, and Living in an Intelligence, Connected Modern World.

Key Organisations:
Technology Strategy Board
www.innovateuk.org
Engineering and Physical Science Research Council (EPSRC)
www.epsrc.ac.uk/Pages/default.aspx
Natural Environment Research Council (NERC)
www.nerc.ac.uk
Biotechnology and Biological Science Research Council (BBSRC)
www.bbsrc.ac.uk

Key Documents:
Nanoscale Technologies Strategy 2009-12
www.innovateuk.org/_assets/pdf/Corporate-Publications/NanoscaleTechnologiesStrategy.pdf
www.mvzt.gov.si
Slovenian Science Foundation (SZF)
www.szf.si

2. Profiles of Other World Regions

Russia

The Russian Corporation of Nanotechnologies (RUSNANO) was established in 2007 with a commitment of 130 billion roubles from the Russian government. The organisation has an explicit focus on the commercialisation of nanotechnology, though it takes a fairly broad view of this mission, funding projects in three areas:

- 'Nanoproduct' fabrication
- Scientific forecasting and roadmaps, standardisation, certification and safety
- Education and popularization

The bulk of the financial commitment; 3.28 billion USD is directed to Nanoproduct fabrication, with 0.54bn for education and 0.82bn for infrastructure, foresight, certification and standardisation. Investments are being ramped up to reach a level of 1.05 billion USD by 2012. Applications for projects are submitted to RUSNANO and assessed on their investment and scientific potential. Applications are reviewed by an external Technical and Scientific Board, and an Industrial Policy Committee, with final decisions being made by RUSNANO's Supervisory Board. Funding decisions which involve sums in excess of 1.3 billion roubles (1% of the organisation's funding) are made by the Advisory Board. The organisation essentially operates like a large venture fund, taking equity stakes (of less than 50%) in the projects to which it invests. Funding support is long term – over 10 years. The organisation states that when exiting it plans to sell to offset investment costs, rather than seeking to maximise profit.

By end 2009, RUSNANO had approved 61 projects, committing to investment of €2.4 billion (92.4 billion roubles). The organisation predicts that by 2015 the volume of nanotechnology production will reach 900 billion rubles per year (19,8BEUR), from a current volume of 4-5 billion rubles annually (88MEUR).

Russian Foundation for Basic Research (RFBR)
www.rfbr.ru/rffi/ru/pages/404

United States

The National Nanotechnology Initiative was established in 2000 and links 25 Federal Agencies whose work relates to nanoscience and nanotechnology. Overall authority for management of the NNI lies with the White House's Office of Science and Technology Policy. The NSET subcommittee coordinates the development of the NNI strategic plan, and the National Nanotechnology Coordination Office (NNCO) provides technical and administrative support, produces reports, and is a point of contact for the public. NNI investment in the period 2001-2009 totals almost $10 billion, with an annual budget that has increased from US$ 464 million in 2001 to US$ 1,527 billion in 2009 (requested). Funding is allocated to the Federal Agencies responsible for this project, with the largest recipients in 2009 being:

- Department of Defence, US$ 431 billion
- Department of Education, US$ 311 billion
- National Science Foundation, US$ 397 billion
- National Institutes of Health, US$ 226 billion
- National Institute of Standards and Technology, US$ 110 billion
- Other Organisations, US$ 52 billion

Funding can also be broken down by Program Component Area (PCA) which gives some indication of the target of each funding element:

1. Fundamental Nanoscale Phenomena and Processes US$550.8 billion
2. Nanomaterials, US$227,2 billion
3. Nanoscale Devices and Systems, US$327,0 billion
4. Instrumentation Research, Metrology, and Standards, US $81,5 billion
5. Nanomanufacturing, US $62,1 billion
6. Major Research Facilities and Instrument Acquisition, US$161,3 billion
7. EHS, US$76,4 billion
8. Education and Societal Issues, US$40,7 billion

One of the effects of the NNI has been the creation of the National Nanotechnology Infrastructure Network (NNIN), which involves 13 universities and houses 700 tools which are accessible for the wider research community. The NNI has also directed an increasing share of budget to Environment Health and Safety research. US$ 34.8 million was directed to EHS in 2005, rising to US$ 76.4 million in 2009.

The recent stimulus package also contains elements which may assist the development of nanotechnology, placing an emphasis on clean energy sources and infrastructure upgrades. The newly confirmed director of the Office of the Science and Technology Policy, John P. Holdren, commented that:4 …he was gratified that the stimulus bill passed by Congress recognized the importance of ongoing investments in innovation by including crucially needed funding for an array of science and engineering efforts with large potential payoffs for society – biotechnology, nanotechnology, information technology, renewable energy, and more efficient cars and buildings, among others. Also important, he noted, is that a portion of the recovery package is designated explicitly for high risk/high-reward research - “the kind that, when successful, proves truly transformative.”

For 2011, the National Nanotechnology Initiative has requested $1,8 billion, mainly to DOE, NSF, HHS/NIH and DOD. $511 million for nanotechnology was included in the Recovery Act stimulus Package

Japan

The main bodies in Japan’s innovation system are the Minister of State for Science and Technology Policy, and the Council for Science and Technology Policy in the Cabinet Office, inaddition to seven Ministries with S&T responsibilities. These include the Ministry of Economy, Trade and Industry (METI) under which falls the large New Energy and Industrial Technology Development Organization (NEDO). The Ministry of

Education Culture, Sports, S&T (MEXT) oversees the Japan Science and Technology Agency (JST) and the Japan Society for the Promotion of Science (JSPS). Japan is currently nearing the end of its 3rd Basic S&T Plan, which runs from 2006-2010. This plan has a total budget target of 25 trillion Yen (€162 billion), equivalent to 1% of Japan's GDP. One of the four priority areas of this plan is Nanotechnology and Materials; a priority originally introduced during the 2nd Basic Plan. Spending on nanotechnology research has been:

- 76.2 billion Yen (~ €494M) in Financial Year 2006
- 78.6 billion Yen (~ €510M) in Financial Year 2007
- 86.5 billion Yen (~ €562M) in Financial Year 2008

This level of funding is projected to be maintained until 2010. The nanotechnology and materials priority areas have been further broken down into ten strategic priorities:

- Materials for reducing costs of clean Energy
- Materials for replacing rare or deficit materials
- Nanotech and Materials supporting security and safety
- Materials for innovation
- Electronics for Break-through Devices
- Nano-biotechnology and Nano-medical Technology for very early diagnosis
- R & D for the Social Acceptance of Nanotechnology
- Advanced R & D at Innovation COE's for commercialization of Nanotechnology
- Nano-measurement and Nano-Processing technology
- X-ray Free Electron Lasers

Japan has seen high industrial investment in comparison to Europe – US$ 4.7 billion in 2005. However, concerns remain that the efficiency of the technology transfer process could be enhanced, with the International Advisory Committee for the evaluation of JST Basic Research Program reporting that Japan has seen "excellent scientific outcome, but some frustration in tech-transfer to innovation".

One of the efforts to investigate EHS issues has been the NEDO project "Risk Assessment & Management of Manufactured Nanomaterials", which runs from 2006-2010.

3. References

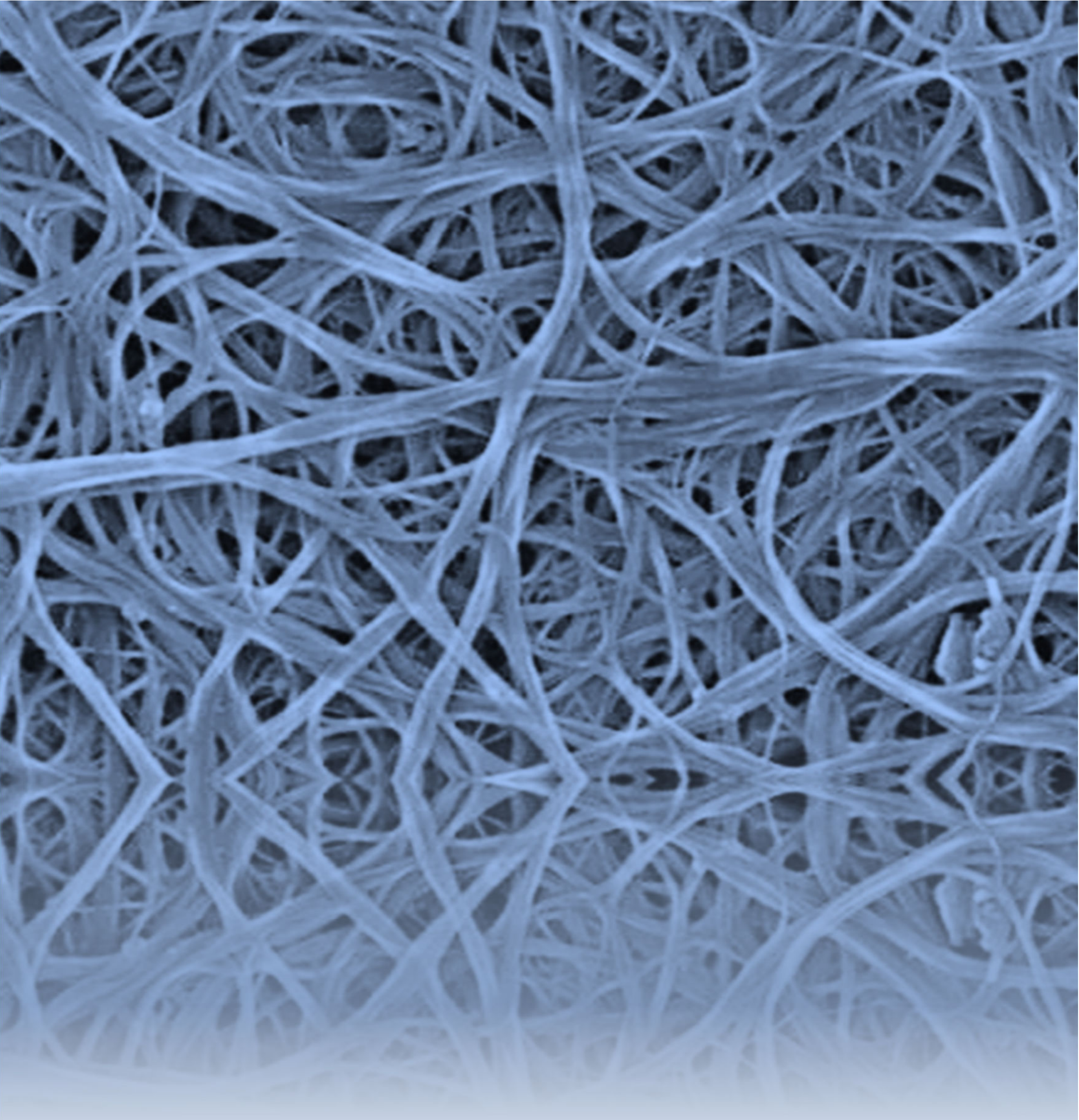
[1] Introduction to Nanotechnology, http://ec.europa.eu/nanotechnology/index_en.html

[2] http://www.berr.gov.uk/dius/innovation/innovation-statistics/evaluation-reports/page10795.html

[3] http://bfm.ru/news/2009/02/25/chubajs-rosnano-budet-prinosit-900-mlrd-rublej-k-2015-godu.html

[4] http://ostp.gov/galleries/press_release_files/holdren_confirmation_release_3-20-09.pdf

[5] Nanoscience and Nanotechnology in Spain, 2010/2011, Introduction. http://www.phantomsnet.net/Resources/nanodoc.php?project=1



Funded by

nanoICT coordination action

Edited by

Phantoms Foundation
Alfonso Gomez 17
28037 Madrid - Spain

info@phantomsnet.net
www.phantomsnet.net
www.nanoict.org