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- **Status of Modelling for Nanoscale Information Processing and Storage Devices**
- **Atomic & Molecular Scale Devices and Systems and Bio-Chemistry Based Information Systems**

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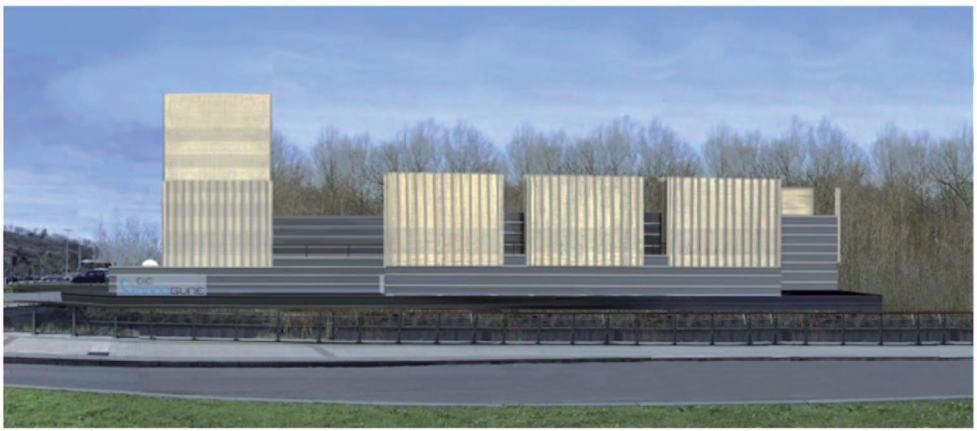

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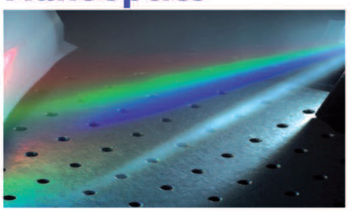

Self-assembly

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Nanodevices

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Dear Readers,

This E-nano Newsletter issue contains two reports providing insights in two relevant areas: modelling at the nanoscale and scientific EU policy.

The nanoICT position paper provides an analysis of the current status of modelling at the nanoscale information processing and storage devices in Europe and a comparison with that in the rest of the world. The previous version of the present paper (resulting from the 2008 nanoICT Working Group meeting) has been updated reflecting the new issues that have been recognised as relevant and of significant current interest.

The EU report summarises the discussions that took place end of October 2009 during a "Future and Emerging Technologies" (FET) expert consultation workshop and gives a list of proposed challenges for the 2011-2012 FET work programme.

We would like to thank all the authors who contributed to this issue as well as the European Commission for the financial support (project nanoICT No. 216165).

Dr. Antonio Correia
Editor - Phantoms Foundation

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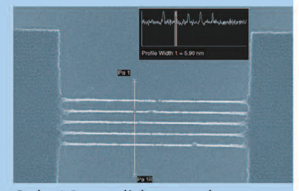

Sub 10 nm lithography

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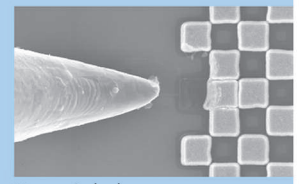

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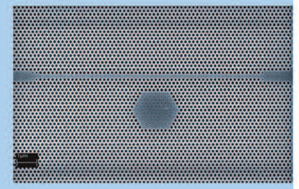

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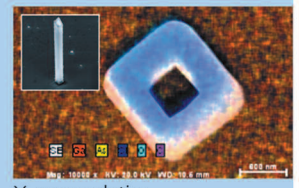

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Status of modelling for nanoscale information processing and storage devices[a]

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], G. Cuniberti[13] and H. Sevincli[13]

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During the 2009 meeting of the Theory and Modelling working group the current status of modelling for nanoscale information processing and storage devices has been discussed and the main issues on which collaboration within the modelling community is needed have been pointed out. An analysis of the current situation in Europe in comparison with that in the rest of the world has been performed, too. The previous version of the present report (resulting from the 2008 meeting) has been updated reflecting the new issues that have been recognized as relevant and of significant current interest.

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.

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 and easily accessible computational power (in particular considering the recent advances in terms of GPU-based general purpose computing) make the time ripe for a real leap forward in the scope and performance of computational approaches for nanotechnology and nanosciences.

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 mobi-

a 2nd Position Paper for nanoICT Theory and Modelling Working Group

lity. 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 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.

Commercial v.s. 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 32 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 32 nm MOS devices. However the need for full-band Monte-Carlo codes together with band structure 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 32 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 band structure 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.

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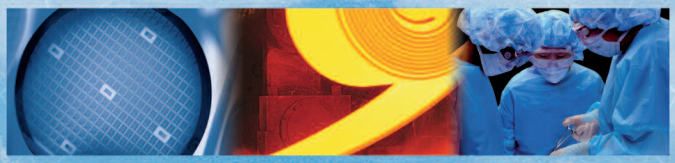

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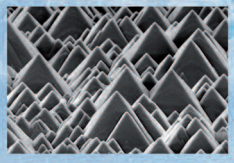

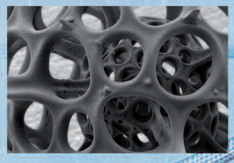

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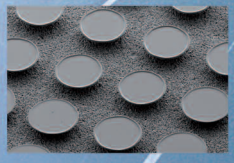

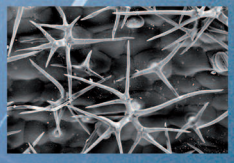

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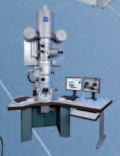

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Efficient modelling tools, as well as accurate physics highlights, would certainly bring a significant competitive advantage for the development and the optimization of the 32 nm CMOS technology and for future technologies, including molecular devices.

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 nanotransistor microscopically different from its neighbours [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 tunnelling, 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 infor-

mation 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.

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

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- Amplitude up to 300Vpp
- Auxiliar DC output up to 50V

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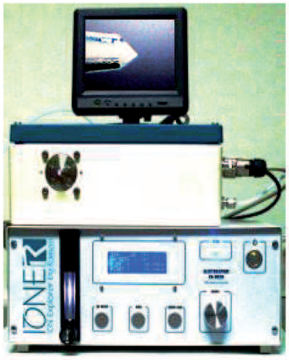

Fluid-electrodynamic device that generates an electrically charged nanoparticles or ions from a dispersion or solution.

- Can be operated downwards, upwards or horizontally
- Easy maintenance
- Separate control module (pressure, voltage and sheath gas flowrate) and spraying head for greater versatility.
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- No radioactive source, no cumbersome paperwork.
- Especially effective for ultrafine particles.
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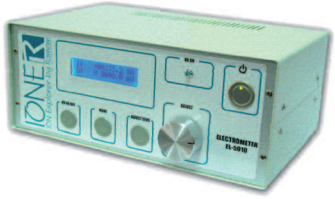
- Includes high DC voltage source
- Current measurement

Electrometers



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- Noise: < 1 fA (RMS)
- A/D effective resolution: 21 bits
- Selectable digital filter
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- Labview control software
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EL-5020, compact electrometer (16 x 6 x 3 cm), battery-powered (8 working hours) and communicated through wireless protocol Zig-Bee, especially conceived for the measurement of ultra-low current at high voltages. It is PC-controlled, with an option of a console for manual interface.

EL-5030, electrometer for the measurement of ultra-low currents generated by ionized gases and electrically charged aerosols. It includes, besides the electronics for the measurement of the current, a Faraday cup with a HEPA filter inside for the collection of nanoparticles and a flowmeter for the calculation of the concentration of particles or ions.

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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.

cal, 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 nanoelectronics 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.

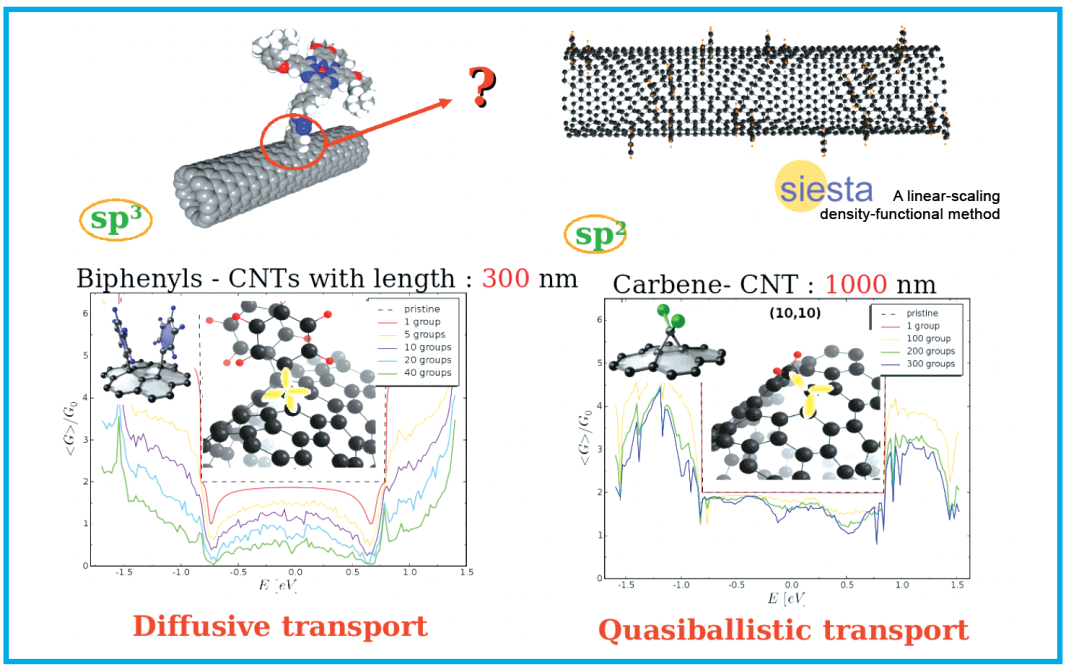

Fig. 1: Codes such as SIESTA can be used for the ab-initio simulation of relatively large structures.

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 nanoelectronics 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 flavours: 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 fotings. 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

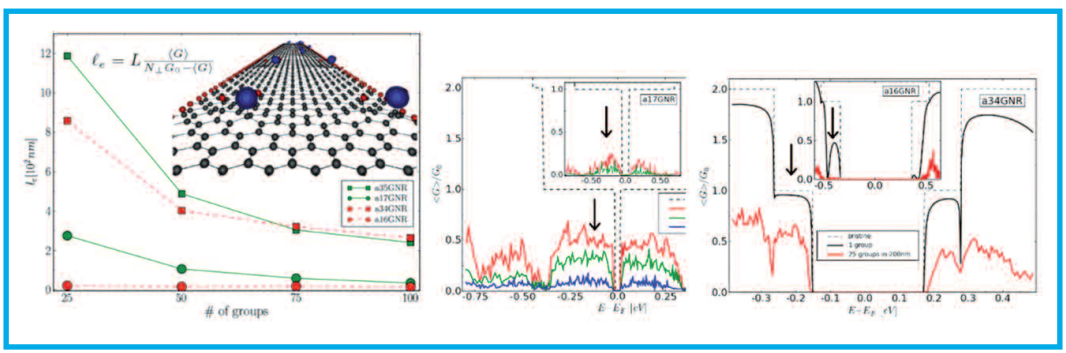

Fig. 2: With the help of ab-initio calculations, the effect of functionalization on graphene nanoribbon conductance can be evaluated.

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.

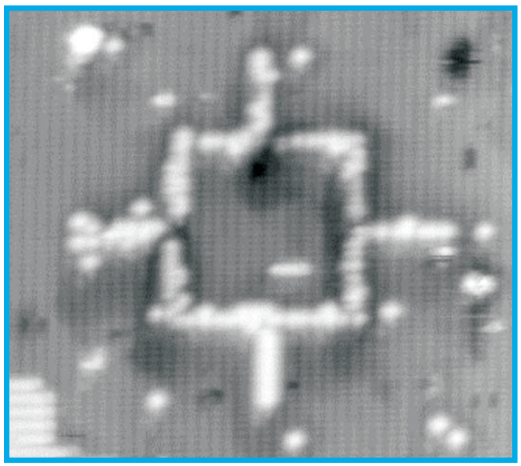

Fig. 3: Ultra-high-vacuum STM image of a substrate after the fabrication with single-atom manipulation, of a complete interconnection circuit for an OR gate, obtained by removing hydrogen atoms from a silicon hydride surface.

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 ge-

ometry, 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.

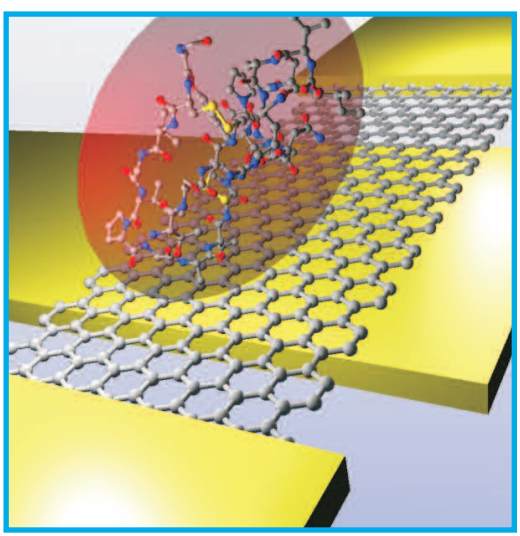

Fig. 4: Functionalized graphene nanoribbons can be used to detect organic molecules.

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 nanodevice 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.

Thus, one of the main challenges for modelling in the next few years is the creation of well organized collaborations with a critical mass sufficient for the develop-

ment of integrated simulation platforms and with direct contacts with the industrial world.

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.

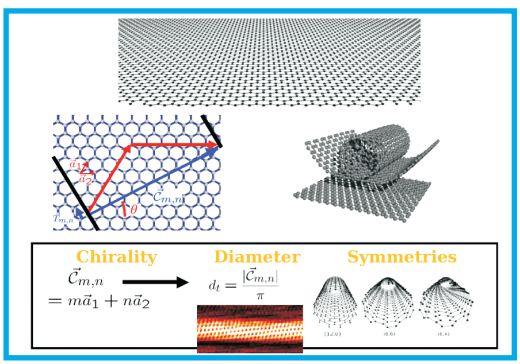

Fig. 5: A carbon nanotube consists of a rolled up sheet of graphene.

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 [39] has opened a promising avenue for future carbon-based spintronic applications. The further demonstration of spin injection in graphene [40] and the observation of long spin relaxation times and lengths [41] 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 [42]. A gate-tunable spin valve has been experimentally demonstrated [43]. Finally, a ferromagnetic insulator, such as EuO, may be used to induce ferromagnetic properties into graphene, through the proximity effect [44] and also to control the spin polarization of current by a gate voltage [45, 46]. 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" [47-49] 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 [50-52], and may be exploited for spintronics. Using first-principles calculations, very large values of magnetoresistance have been predicted in GNR-based spin valves [53,54].

Additionally, the potential for 3D based organic spintronics has been recently suggested by experimental studies [55]. 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 Al2O3. 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 [56].

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

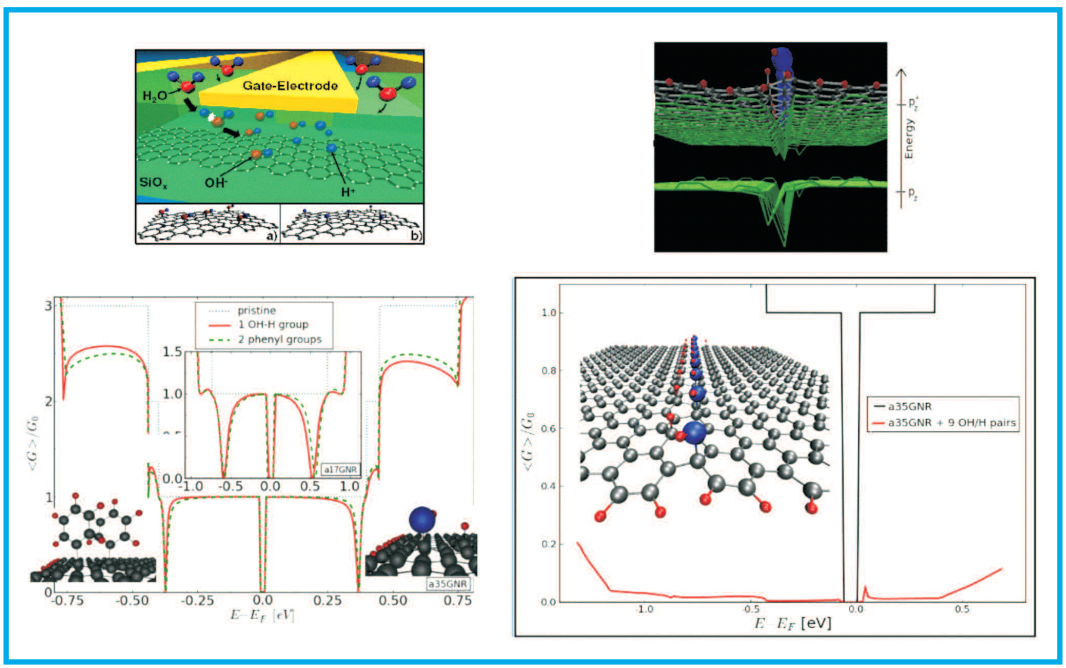

Fig. 6: Functionalization of graphene nanoribbons

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Six Positions for young technicians to work in our clean room and Characterization Laboratories. Selected candidates will have the possibility of career development in an international organization and specific training in selected Nanotechnology Centers in the Iberian Peninsula, while INL´s laboratory infrastructure is not completed.

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Low-field and solid-state NMR applied to food quality control (in collaboration with Dr N. C. Nielsen, iNano University of Aarhus and Aalborg, Denmark).

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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 [57,58].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 [59].

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 [60]. 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 [61]. 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.

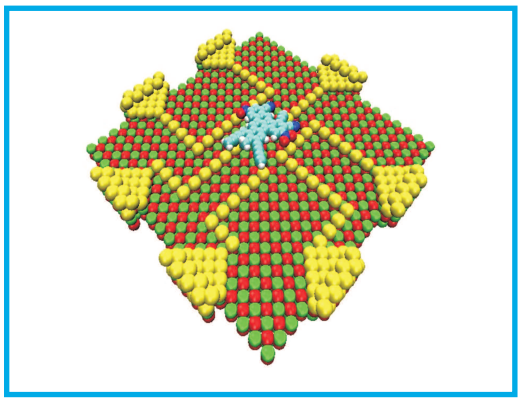

*Fig 7: Molecule connected to seven atomic wires on a ionic crystal. This setup is composed of 2025 atoms and more than 9700 atomic orbitals are needed to accurately calculate the function of the molecule (from "Picotechnologies : des techniques pour l'échelle atomique", C. Joachim, A. Gourdon and X. Bouju in Techniques pour l'ingénieur **NM130**, 1-16 (2009).*

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 [62,63]. 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 [64]. Still, the position of the molecular levels is also strongly influenced by the dynamical screening induced by the metallic leads [65,66]. 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 [68].

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 [69]. 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 [70]. In these cases more sophisticated methods are necessary, the coupling of which to ab initio DFT simulations is still an open question.

molecules in information processing, the use of multiscale tools [71] 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 in the time-dependent response of the molecules to external voltages and their interaction with light needs to be studied.

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 [72].

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

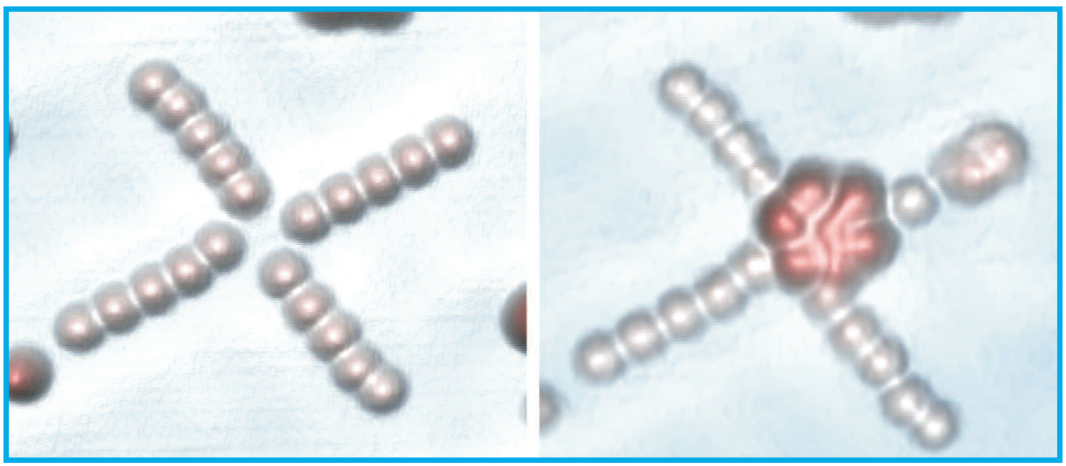

Fig. 8: Connection of a molecule to four atomic wires. Each wire has been fabricated (left panel) with five gold atoms deposited on the substrate; the molecule has then been placed at the center of the device (right panel), slightly modifying the structure of one of the wires.

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 high-level NEGF or other sophisticated methods [73,74]. The concept of a molecular logic gate has emerged recently and specific approaches including quantum Hamiltonian computing [75] will be used for a numerical integration.

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).

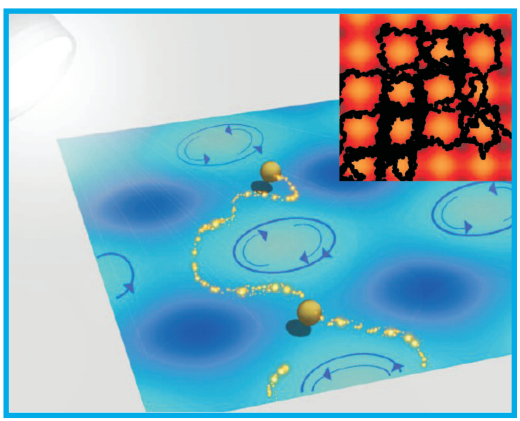

Fig. 9: Diffusion processes are of fundamental importance in many disciplines of physics, chemistry and biology. A low diffusion rate may hinder progress in many issues related to technology and health improvement. For example high viscosity may prevent tailored chemical reactions or work as an undesired barrier for targeted nano-engineered drug delivery in bio-chips. The classical diffusion of a small particle in a fluid can be greatly enhanced by the light field of two interfering laser beams. Langevin Molecular Dynamics simulations show that radiation pressure vortice, due to light interference, spin the particle out of the whirls sites leading to a giant acceleration of free diffusion. The effective viscosity can then be notably reduced by simply increasing the laser intensity. [Albaladejo et al., Nano Letters 9, 3527 (2009)]

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.

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 [76].
Quasi one-dimensional quantum wires [77], engineered molecular junctions [78,79], superlattices of quantum dots [80] 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 [81].

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 [82].
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 [83]. 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 [84]. 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.

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 effects 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 [85,86]. 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 [87], ferroelectric tunnel junctions [88] or novel oxide superlattices [89], 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.

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 32 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. 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.

New computational approaches

The development of highly parallel and computationally efficient graphic processors has recently provided a new and extremely powerful tool for numerical simulations. Modern Graphic Processing Units (GPU) approach a peak performance of a Teraflop (1012 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. In particular, GPU hardware is specialized for matrix calculations (fundamental for 3D graphic rendering), which do represent also the main computational burden in many types of device simulations.

As a result, speed ups of the order of 30 - 40 have been observed, for tasks such as the simulation of nanoscale transistors, with respect to state-of-the-art CPUs. Up to now the main disadvantage was represented by the availability, in hardware, only of single-precision operations, but last generation GPUs, such as the FireStream 9170 by AMD, are advertised as capable of handling 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. Overall, this is a field that deserves investing some time and effort on the part of the de-

vice modelling community, because it could result in a real breakthrough in the next few years.

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 NCN survey [23], 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 EU funded "Phantoms network of excellence" and has been active for several years; it is currently being revived with some funding within the nanoICT coordination action. (www.europa.iet.unipi.it)

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 defragmentation 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.

Other initiatives such as the "Report on multiscale approaches to modelling for nanotechnology" [90] intends to provide an overview, albeit limited and certainly not exhaustive, of relevant aspects of modelling at the nanoscale, pointing out some important issues that are still open and affording the reader that is not yet active in the field with an introduction to several widely used techniques and with a large body of references.

This review has been written by experts in the fields of computational modelling; most of them have strongly contributed to the development of European excellence in recent years, and have been leading EU-initiative over FP5, FP6 and FP7. Although more efforts will be needed to bridge different communities from ab initio development to device simulation, such initiatives need to be supported considering that contributors of this report are overviewing promising methodologies to fill the gap between scientific communities, establishing some framework for further promoting European-based networking activities and coordination.

Past, present and future European advances in computational approaches.

This novel initiative should be able to bridge advanced ab-initio/atomistic computational approaches to ulti-

mate 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.

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 down scaling.

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, are emerging, with an impressive potential for device fabrication and with completely new requirements for simulation.

A unique opportunity is now surfacing, with powerful new modelling 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.

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PhD Position (Centre Investigacions Nanociencia Nanotecnologia (CSIC-ICN)(CIN2), Spain): *"Quantum Transport in Carbon Nanotubes"*

The research will be focused on the electrical and mechanical properties of structures with dimensions of a few nanometers, such as carbon nanotubes or graphene. These structures are so tiny that quantum effects start to play a dominant role. For e.g. the energy levels are quantized, just like in atoms and molecules. Interestingly, these structures are large and robust enough to be implemented in a variety of different microfabricated devices, which allow the tuning of their quantum properties.
This work will be carried within the Quantum Nano-Electronics group, which is part of the Centre Investigacions Nanociencia Nanotecnologia (CSIC-ICN). The group is located at the Campus Universitat Autonoma de Barcelona. The funding for the salaries comes from an EURYI award.

The deadline for submitting applications is April 08, 2010
For further information about the position, please contact: **Adrian Bachtold (adrian.bachtold@cin2.es)**

PhD Position (CIC nanoGUNE, Spain): "Nanomagnetism"

The Nanomagnetism Group at the CIC nanoGUNE Research Center in San Sebastian (Spain) is currently looking for a motivated PhD Student (Physicists/Materials Scientists/Engineers) who is interested in working in an inspiring international and interdisciplinary environment in the following research areas:

- Time resolved magneto-optic Kerr microscopy with subnanosecond time resolution for studying the magnetization dynamics (e.g., fast magnetic switching).
- Laterally patterned magnetic nanostructures that are fabricated by means of electron beam lithography and thin film and multilayer deposition techniques.

The deadline for submitting applications is March 31, 2010
For further information about the position, please contact: **Paolo Vavassori (p.vavassori@nanogune.eu)**

Job Vacancy (CIC nanoGUNE, Spain): *"Electron Microscopy Technician"*

CIC nanoGUNE Consolider, located in San Sebastian, Basque Country (Spain), is a R&D center created recently with the mission of conducting basic and applied world-class research in nanoscience and nanotechnology, fostering training and education excellence, and supporting the growth of a nanotechnology-based industry.
An electron microscopy facility is currently being established to accompany nanoGUNE´s already ongoing research activities by means of a high-level structural characterization laboratory, including Cs corrected TEM, FIB and ESEM. In order to provide qualified assistance to the Staff Microscopist that is managing these facilities, we have an immediate opening for an Electron Microscopy Technician. We are searching for a highly motivated and creative person with a solid technical/engineering background, mechanical and electronic design and construction skills, and experience in operating and maintaining TEM sample preparation facilities.

The deadline for submitting applications is March 01, 2010
For further information about the position, please contact: **nano@nanogune.eu**

PhD Position (University of Castilla – La Mancha, Spain): *"Ultrafast spectroscopy of cyclodextrin-based drug nanocarriers"*

The Laboratory of Ultrafast Spectroscopy at the University of Castilla – La Mancha, Toledo, Spain under the supervision of Prof. Abderrazzak Douhal is seeking an outstanding PhD candidate to carry out studies on **interaction of drugs with cyclodextrin-based nanocarriers** using steady state and fs- to ms-time resolved spectroscopic techniques of absorption and emission, as well as time- and space resolved single molecule spectroscopy.

The deadline for submitting applications is February 28, 2010
For further information about the position, please contact: **Abderrazzak Douhal (Abderrazzak.Douhal@uclm.es)**

PostDoctoral Position: *"Ultrafast spectroscopy of cyclodextrin-based drug nanocarriers"*

A postdoctoral position for a period of 18 months is available at the University of Castilla – La Mancha, Toledo, Spain.
The Laboratory of Ultrafast Spectroscopy at the University of Castilla-La Mancha (Toledo, Spain) is looking for an outstanding postdoctoral candidate for a European-funded research project (Cyclon, FP7, Marie Curie ITN Network) based on the use of ultrafast techniques

to study the **interaction of drugs with cyclodextrin-based nanocarriers**. The Laboratory of Ultrafast Spectroscopy is equipped with femtosecond fluorescence up-conversion, transient-absorption and time- and spectrally-resolved single-molecule fluorescence microscopy techniques.

The deadline for submitting applications is February 28, 2010
For further information about the position, please contact: **Abderrazzak Douhal (Abderrazzak.Douhal@uclm.es)**

Scholarships (National Science Council of Taiwan (NSC): *"10 scholarships will be allocated to Spanish graduate students to undergo 2-month summer trainings in Taiwanese research institutes"*

In order to promote a further collaboration with Spanish Education and Research authorities, the National Science Council of Taiwan (NSC) intends to provide 10 Spanish graduate students - PhD or Master students in science and social sciences and humanities - of first-hand research experience in Taiwan, an introduction to its science and technology policy infrastructure, and orientation to the culture and language.
The goals of the program are to introduce students to Taiwanese scientific and technological development in the context of a research laboratory, and to initiate personal relationships that will better enable them to collaborate with foreign counterparts in the future.

The deadline for submitting applications is February 15, 2010
For further information about the position, please contact: **Charles Peng (fran01@nsc.gov.tw)**

Scientist Positions (Madrid Institute for Advanced Studies of Materials, Spain):

"Virtual Processing of Structural Composites"
Virtual Processing of Structural Composites, including numerical simulation of curing and infiltration and design of optimum preforms (braiding, stitching, 3D weaving, knitting).

"Computational Design of Metallic Materials"
Computational Design of Metallic Materials to predict the influence of alloy composition and processing route on the microstructure (phases, precipitation, segregation, grain size and shape, texture, etc.) through advanced numerical modeling (computational thermodynamics, phase-field modeling, etc.).

"Advanced Processing of Structural Composites"
Advanced Processing of Structural Composites with particular emphasis on out-ofautoclave consolidation of prepegs, pultrusion, VARTM, RFI, and processing of thermoplastic composites (glass-mat strands and long fiber reinforced thermoplastics direct-process).

"Processing of Metallic Materials"
Processing of Metallic Materials to develop innovative strategies and to improve current methods of manufacturing near net-shape components for high temperature structural applications (Ni-based superalloys, intermetallics) and light weight alloys (Mg, Al) for the aerospace and automotive sectors. Techniques of particular interest include casting, secondary processing (forging, extrusion), and novel methodologies (rapid prototyping, electron-beam melting, direct-metal laser-sintering, etc.).

The deadline for submitting applications is February 04, 2010
For further information about the position, please contact: **IMDEA-Materials (https://www.imdea.org/internationalcall)**

PostDoctoral Position (Groupe Nanosciences - CEMES, France): *"Investigation of molecular adsorption on SiC surfaces by UHV-NC-AFM and STM"*

The successful candidate will participate in a project whose main objective is to use silicon carbide reconstructed surfaces as templates for adsorbed molecules, in a overage ranging from isolated molecules to one monolayer. He will be in charge of experimental studies based on Scanning tunneling microscopy (STM) and atomic force microscopy (AFM) in the non-contact mode. Two STM/AFM microscopes will be used. A room temperature STM/cantilever-based AFM and a low temperature (6 K) STM/tuning fork-based AFM, depending on the experimental requirements. The Nanosciences group in CEMES comprises experimental physicists, chemists specialized in the synthesis of molecules for nanoscience and theoreticians with a strong background in STM and AFM image calculations. The candidate will closely collaborate with the chemists and the theoreticians to optimize the molecules and for image interpretation and calculation.

The deadline for submitting applications is January 31, 2010
For further information about the position, please contact: **Sébastien Gauthier (Gauthier@cemes.fr)**

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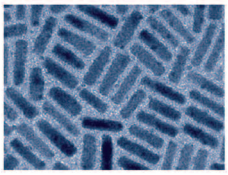
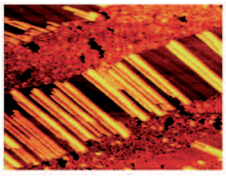
imdea nanociencia

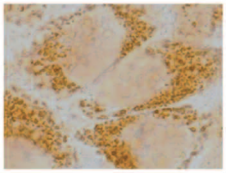
MOLECULAR NANOSCIENCE



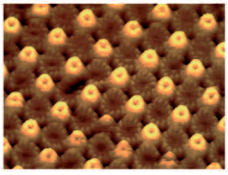
SCANNING PROBE MICROSCOPIES AND SURFACES



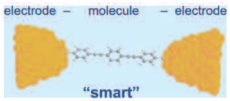
NANOMAGNETISM



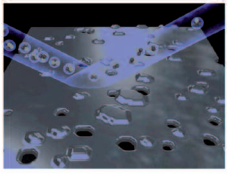
NANOBIOSYSTEMS: BIOMACHINES AND MANIPULATION OF MACROMOLECULES



NANOELECTRONICS AND SUPERCONDUCTIVITY



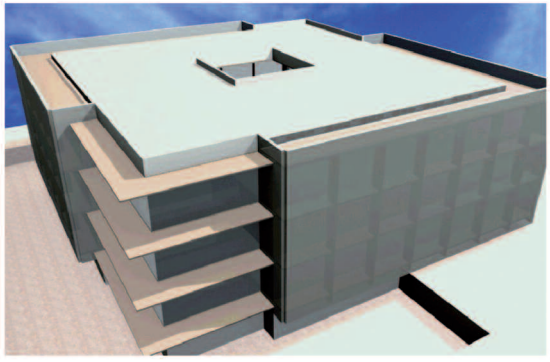
SEMICONDUCTING NANOSTRUCTURES AND NANOPHOTONICS



HORIZONTAL PROGRAM ON NANOFABRICATION AND ADVANCED INSTRUMENTATION

IMDEA-Nanociencia is a private Foundation created by joint initiative of the regional Government of Madrid and the Ministry of Education of the Government of Spain in February 2007 to manage a new research Institute in Nanoscience and Nanotechnology (IMDEA-Nanociencia), which is located in the campus of the Universidad Autónoma de Madrid, 12 km away from Madrid downtown with an excellent communication by public transportation with the Madrid-Barajas airport (25-30 min) and Madrid downtown (15-20 min).

The Institute offers attractive opportunities to develop a career in science at various levels from Ph.D. students to senior staff positions.



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Atomic & Molecular Scale Devices and Systems and Bio-Chemistry Based Information Systems

Expert Consultation Workshop: 22 & 23 October 2009, Brussels (Belgium).

Executive Summary

Future and Emerging Technologies – Proactive Initiatives (FET – Proactive) is preparing the next work programme for 2011–2012 and later. As part of the process to identify new grand research challenges, FET organised a workshop on 22 and 23 October 2009, in Brussels, on the following two themes: Atomic & Molecular Scale Devices and Systems, and Bio-Chemistry Based Information Systems. Around 20 researchers covering the different relevant areas of research attended the meeting. The objective was to find new topics for future challenging and promising FET proactive initiatives for Information and Communication Technologies (ICT). The meeting covered also the possible affinities between its two themes, such as the emergent field of quantum effects in biological systems. This report summarises the discussions that took place during the workshop and gives a list of proposed challenges for the work programme.

1. Introduction

FET (Future Emerging Technologies) structures research in a number of proactive initiatives, which typically consist of a group of projects funded around a common theme. The themes are shaped through interaction with the research community, and focus on novel approaches, foundational research and initial developments on long-term research and technological innovation. This workshop discussed how both atomic & molecular scale systems, and bio-chemistry based information systems can be investigated to push for a new generation, and even paradigm, of information and communication technologies at a new and smaller scale, exploring both the quantum and the biological effects offered by nature. The expected outcomes from the meeting were:

- To obtain visionary scenarios for atomic scale and bio-chemical ICT systems and what is needed to develop, test and implement them.
- To identify the core challenges, their impact and ti mescale.
- To identify the adequate target research communities.
- To produce an outline of funding schemes and cooperation strategies to be deployed.

2. Synthesis of the discussions

The workshop included discussions amongst the members of both the Atomic & Molecular Scale Devices and Systems group and the Bio-chemistry Based Information Systems group, as well as joint discussions, namely to identify potential joint challenges. The following aspects were covered:

- The challenges faced and identified in these areas, namely as potential FET research topics
- The impact of successful projects on both society and research communities
- The identification of the core communities that should be involved
- The timescales for the uptake
- The instruments of funding most relevant
- International cooperation

Each of these points is discussed below giving a summary of the views expressed during the discussions.

In particular, the first four points are presented for both workshop themes: Atomic & Molecular Scale Devices and Systems, in section 3, and Bio-Chemistry Based Information Systems, in section 4. In section 5, the possible affinities and overlaps between these two themes are discussed. Finally the funding instruments and international cooperation are discussed in section 6.
As additional resources, the list of participants in the workshop is presented in annexe I, the terms of reference of the meeting are presented in annexe II, the written contributions of the experts consulted are available at:
ftp://ftp.cordis.europa.eu/pub/fp7/ict/docs/fet-proactive/wsconsult09-amolbio-02_en.pdf

3. Atomic & Molecular Scale Devices and Systems

The technological revolution brought about by the development of miniaturized information processing devi-

ces over the last 50 years has had an extraordinary impact on almost every aspect of our daily lives. At present essential properties of these technologies may still be understood semi-classically whereby quantum mechanical properties enter at the level of global material properties, but not as a basic functional resource. However, miniaturization is now reaching the quantum frontier where quantum properties are playing an essential role for the behaviour of systems that are either built, bottom-up, from individual atomic or molecular components or, top-down, from bio-molecular systems created through evolution. Nanofabricated devices can now be built to operate at this quantum frontier and bio-molecular systems can now be shown to exhibit quantum mechanical features in their dynamics.

Hence, quantum mechanics, the theory of the very small, is widely appreciated to be at the core of the next technological revolution and the development of methods for the creation, manipulation and control of atomic, molecular and bio-molecular devices at the quantum-classical frontier holds the promise of turning the quantum behaviour of such structures to our advantage, thus providing the foundations of atomic scale information technologies for the 21st century.

3.1. Research topics addressed (based on the participants' written contributions and presentations)

A large number of topics were addressed and discussed during the workshop, namely in the Atomic & Molecular Scale Devices and Systems break-out sessions. Taking also into account the written contributions, there emerged some common themes and topics, which the majority of contributors addressed and discussed. These may be summarised as being:

- Fabrication at the atomic scale
- Controlling and probing single atoms and molecular scale systems
- Embedding and connecting atomic and molecular quantum systems
- Understanding and utilizing the local nanoscale environment
- Experimental exploration of the quantum-classical interface
- Theoretical and numerical methods for modelling at the quantum-classical border
- Exploiting new functionalities in sensing, memory, logic and energy harvesting
- New information exchange mechanisms (spin, magnetism, light, etc.)
- Scalability and production methods
- Controlled doping at the nanoscale
- Efficient information extraction
- Thermodynamics at the molecular scale
- Quantum effects in biology
- Bio-inspired new paradigms of information coding and processing

It was also suggested that a future call on this theme would be better named *Atomic Scale Technologies*.

3.2. Challenges

Several important challenges were identified. Some addressed fundamental issues, while other focused on future applications of atomic-scale systems. Four interconnected challenges were mentioned:

1. ICT functionality from atomic and molecular design using top-down, bottom-up or a combination of both approaches

- Designing functionality from the guided assembly of atoms and molecules or by exploiting bio-molecules realized by nature
- Improving existing ICT technologies by pushing the limits of miniaturization to the atomic scale
- Characterizing atomic and molecular scale components
- Providing the routes towards cost effective fabrication at the atomic or molecular scale

2. Embedding and interfacing of atomic and molecular devices within a technological environment

- Embedding atoms and molecules in a controlled environment: fabrication and connection
- Engineering stability, uniformity and robustness
- Interconnecting atomic and molecular devices

- Interfacing atomic and molecular systems with the outside world, e.g. light-matter connectivity, electronic transport, spin resonance, mechanical response, etc.
- Investigating the effect of operation on device behavior

3. Exploit coherence, decoherence and the quantum-classical boundary for ICT

- Enhancing coherence to take advantage of the system's quantum behaviour
- Enhancing decoherence to turn the system classical in the shortest possible time
- Exploiting the interplay between decoherence and coherence for optimized performance in atomic, molecular and bio-molecular systems
- Exploiting dynamical control of molecular and atomic systems
- Exploiting coherence for sensing and metrology
- Developing techniques to probe and extract information efficiently from such systems

4. Develop experimental models and theoretical methods for atom, molecular and bio-molecular systems at the quantum-classical boundary

- Developing proof-of-concept experimental model systems for component functionalities
- Developing theoretical methods to describe multi-component connected quantum systems interacting with their environment

3.3. Impact

Developing atomic and molecular scale ICT devices takes us to the ultimate limit of miniaturization, where quantum physics can give us improved speed, precision and efficiency, as well as new functionalities, thereby contributing to the ongoing information revolution which benefits virtually all areas of society.

In particular, a profound impact is expected in the following two areas:

Science and industry: namely with the new ability to build and control multiscale systems, new measurement systems, new standards, new tools and ICT devices. A programme in this area would help define and give a leading role to the EU in molecular scale engineering and electronics.

Society: namely in increased and new areas of employment, improved man-machine interactions – in particular sensors (health, safety, environment and quality of life), improved energy efficiency and energy harvesting/scavenging from new sources.

3.4. Core Communities

These were identified as being the communities that can have an input in the project calls, in order to achieve the maximum benefit to the wider community and to ensure that all relevant technical areas are able to contribute to the projects in the most effective manner.
The core communities addressed by this call belong to the following fields:

- Physics
- Electronics and nano-science
- Chemistry
- Molecular biology
- Surface science

3.5. Timescale for uptake

The following short, medium and longer-term timescales were identified to meet the main challenge of progressing from concept to marketable molecular scale information systems:

- A shorter term of around five years is expected to be the timescale for sensors (but not single molecule sensors), basic proofs-of-concept and possibly some simpler molecular based devices.
- In the medium term (5-10 years) one could expect the development of new measurement systems and measurement references/standards to support the development of molecular electronics and their characterisation to emerge.
- In the longer term (10+ years) ICT using molecular technology which complements and integrates with CMOS would emerge.

4. Bio-chemistry Based Information Systems

Living cells and organisms input, manipulate and process information, and they do this in a way very different from our conventional digital computers. The information is embodied in complex biochemicals, and information processing includes the modification, construction, and replication of these chemicals. Our abilities to exploit these processes are still at an early stage. But once we have an understanding and control of biochemical information processing, we will be able to affect and change processes in living cells, with obvious medical applications. Furthermore, we will be able to develop analogous processes in non-living systems and engineer new materials with an enormous range of novel physical and information processing capabilities. Developing fundamental understanding, theories, techniques, and tools of embodied biochemical information processing, requiring novel inputs from computer science and from biochemistry, is crucial to developing these capabilities.

4.1. Research topics addressed (based on the participants' written contributions and presentations)

The Bio-chemistry Based Information Systems break-out group discussed a large and diverse range of topics, which are summarised below, taking also into account the written contributions:

- Processes and applications targeting living cells and organisms
- Self construction, self assembly, self organisation, self regulation, self destruction, feedback (internal, and via the environment) and emergence in bio-chemical systems, from the molecular scale upwards
- Making matter (biological or non-biological) "smarter"
- The importance of geometric issues (space, surface, scale, structure)
- The source of the information processing power: construction, replication, self-assembly, auto-catalytic networks
- The "self-consistent" (non-arbitrary) relationship between information and function
- Theoretical underpinnings will be more physical than logico-mathematical
- Abstraction of the functionality of molecules, and reimplementation in a different framework
- Developing appropriate computational and information processing models for these novel paradigms and abstractions, that are inherently stochastic and "soft"
- Interfacing with other microscopic and with macroscopic systems
- Safety as an architectural systems issue, not (just) a component issue

4.2. Challenges

The following 20-year vision was proposed for Bio-chemistry Based Information Systems: a mainstream technology based on programmable self-organising systems in which the generic components are physical constructors.

The overall challenge is to make substantial and significant steps in the directions of the vision: to design and program self-organising construction systems down to the molecular scale, that are able to perform information processing. This is broken down into the following requirements:

1. Theories, methods, tools, languages, architectures and simulations allowing self-organised systems to be programmed
2. Implementations of programmable physical systems
   Namely at levels including physical self-organising systems, synthetic chemistry, supra-molecular systems, reaction networks, sub-cellular/cellular systems, organism (single robots), and swarm robots
3. Nature-inspired design and fabrication processes for robust self-modifying systems
4. Environment and interface:

- Flexible reaction containers, flexible geometry, fine grained control of reactor topology, interplay between reactions and topology, for information processing, content sensitive systems
- Biology inspired strategies of information coding and exchanging

4.3. Impact

Bio-chemistry Based Information Systems is a rather

novel area and its impact is not easy to predict, but it offers the potential for ICT disruptive technology. It will provide novel sensors, interfaces, recognition systems, and actuators, with clear applications for health, the environment, and security. It offers new paradigms and architectures for computer science, of embodied decentralised pervasive information processing, as well as for robotics and its applications, which play such an important role in our society. It promises a range of completely novel "smart" materials that combine and exploit both physical properties and information processing capabilities. It provides a radical new outlook on sustainability of products that can be locally constructed and then sustainably dismantled when no longer needed.

4.4. Core Communities

These were identified as being those communities that will need to have an input in to the project calls so as to achieve the maximum benefit to the wider community and to ensure that all relevant technical areas are able to contribute to the projects in the most effective manner. The core communities need to be:

- Chemistry
- Biochemistry
- Molecular biology
- Physics
- Computer science
- Robotics
- Electronics
- Surface science

4.5. Timescale for uptake

An overarching 20-year vision was proposed for Bio-chemistry Based Information Systems, with four challenges that are four parallel strands that all have to be achieved to realise the vision.

Each strand has steps along the way to maturity, and the following global timescale was envisioned:

- After 5+ years, there should be laboratory prototypes (that solve most of the scientific problems)
- After 10+ years, there should be commercial prototypes (that solve most of the scaling-up and engineering problems)
- After 20 years, there should be ICT consumer products.

5. Atomic & Molecular vs. Bio-chemical based ICT

During the meeting were also discussed potential topics addressing both atomic & molecular and bio-Chemistry based information systems. The discussion has shown that we are still at a very early stage of a path that could reveal itself promising and technologically disruptive. This workshop has triggered a process by identifying potential directions exploring the affinities between these two areas, at an intermediate scale still little explored. In particular, the following topics were suggested:

- Guided self-assembly in a practical environment
- Connectivity and interfacing
- Advanced classical and quantum simulation of complex non-modular systems
- Nature-based optimization of information coding and processing
- Bio-molecular behaviour at the quantum-classical boundary

It was noted that the meeting could have benefited from the presence of more biology experts, including for laying out further perspectives for the emergent area of quantum effects in biological systems and its consequences for biology. Altogether it was suggested it would be important to further explore this path, possibly through an FP7 Coordination and Support Action, to help build the respective research community and establish its challenges.

6. Instruments and International Cooperation

6.1. Instruments

The various types of instruments open for consideration were briefly discussed, as well as possible modifications to those mechanisms. Both for Atomic & Molecular Scale Devices and Systems (which, it was suggested, should be renamed *Atomic Scale Technologies*) and for Bio-chemistry Based Information Systems, it was generally thought that smaller projects were the most appropriate for these novel areas, but it was noted that

their three-year lifetime may be too short for the type of challenges envisioned. The possibility of having calls that would accept projects of any size, competing for the same budget, was also suggested.
Regarding the emergent area overlapping between the two main themes of the workshop, namely quantum effects in biological systems, it was pointed out that instruments such as training network would be a very important step to train young European researchers and interweave the community in these emerging research fields. Such a structure could be the basis for subsequent STREP-like projects.

Finally, it was noted that Coordination and Support Actions could be explored for two purposes: to help develop the more embryonic topics, and to build connections towards related FET initiatives.

6.2. International Cooperation

The members of the workshop briefly discussed the role of international cooperation. It was considered that it is in general beneficial for EU research groups to cooperate with top research groups/centres from other countries, namely from the USA, Japan and Australia, amongst others, specially in the novel and emergent areas, where there are still not that many groups in the world. No national programs that could complement FET schemes were identified.

Annex I: List of Participants

Robert Baptist
CEA Leti
Erik Dujardin
CEMES
Jerzy Gorecki
Polish Academy of Sciences
Thomas Jung
Paul Sherrer Institute
Zoran Konkoli
Chalmers University of Technology
John McCaskill
Ruhr University, Bochum
Barry McMullin
Dublin City University
Yasser Omar
Technical University of Lisbon (*rapporteur*)
Vittorio Pellegrini
Scuola Normale Superiore, Pisa
Martin Plenio
Technical University of Ulm
Alfonso Rodriguez-Paton
Universidad Politécnica de Madrid
Jörg Schmiedmayer
Tech. University of Vienna (*AMS moderator)*
Pierre Seneor
THALES
Michele Simmons
Centre for Quantum Computer Technology
Susan Stepney
University of York *(Bio-Chem moderator)*
Herre Van der Zant
TU Delft
Ian Walmsley
University of Oxford
Lukas Worschech
University of Würzburg
Klaus-Peter Zauner
University of Southampton

Annex II: Terms of Reference

Atomic & Molecular Scale Devices and Systems and Bio-Chemistry Based Information Systems (22-23 October 2009, Brussels)

1. Context

The ICT Future and Emerging Technologies (FET) Proactive scheme fosters frontier research that opens up new avenues across the full breadth of **future information** technologies. FET acts as a pathfinder promoting the exploration of radically new ideas and trends for future research and innovation and provides sustained support to emerging areas that require fundamental research to be carried out over a long period. It aims to go beyond the conventional boundaries of ICT and ventures into uncharted areas, often inspired by and in close collaboration with other scientific disciplines. Radical breakthroughs in ICT increasingly rely on fresh synergies, cross-pollination and convergence between different scientific disciplines.

One research area pursued within FET is frontier research at the **atomic and molecular** scale which requires both operating in a world dominated by quantum

effects and linking it to the environment, be it electronic, mechanical, optical, organic or of another type. This convergence of scale and function calls for interdisciplinary collaborations and combination of knowledge from a wide range of sciences.

FET also embraced the emerging research field of **biochemical and bio-inspired information processing**. This denominator covers research challenges, such as e.g.; how to exploit nature's information processing capabilities, how to address evolution, (bio-) immersive computing, interfacing traditional silicon-based IT and (immersed) wetware, how to deal with formalisms, etc.

Fundamental research in the area of nanoelectronics, quantum information and bio-chemistry has been pursued in FET since FP6, indicating the sustained and growing importance of these areas (for more details see website http://cordis.europa.eu/fp7/ict/fet-proactive/areas_en.html):

- **FP6, call 3: Emerging Nanoelectronics (E-Nano)** aimed at advancing research in hybrid and molecular electronics, and prepared the bases for an extension of integrated circuit technology beyond the limits of CMOS scaling. The selected projects started in September 2005.
- **FP7, call 1: Nano-scale ICT Devices and Systems (Nano-ICT)** aimed at demonstrating unconventional solutions to increase computing performance, functionality or communication speed, or to reduce cost, size and power consumption of ICT components beyond the expected limits of CMOS technology. The selected projects started in January 2008.
- **FP7, call 4: Bio-Chemistry-based information technologies (Chem-IT)** aimed at developing the foundations for a radically new kind of information processing technology, inspired by chemical processes in living systems. The selected projects are under negotiation and are supposed to start in February 2010.
- **FP7, call 4: Quantum Information Foundations and Technologies (QI-FT)** aimed at research in quantum information theory, entanglement-enabled quantum technologies, scalability of quantum processing systems and long distance quantum communication. The selected projects are under negotiation and are supposed to start in February 2010.

2. Objectives of the Consultation Workshop

This consultation is targeted to scientists interested in atomic & molecular scale devices and systems, in quantum information foundations and technologies, in biochemistry based information systems, in the move towards zero-power ICT and in the interconnection of tera-scale devices to shape monolithic information systems. The purpose is to identify new topics for future challenging and promising FET proactive initiatives. This meeting will concentrate on topics related to **Atomic & Molecular Scale Devices and Systems** and **Bio-Chemistry Based Information systems** with a view on those grand challenges that should be included in the FET work programme 2011 – 2012 or later to tackle them. The contributions and discussion are expected to serve at the level of research programmes rather than at the level of single project ideas. Suggestions regarding the means to implement the research are also welcome – whether the projects should be big or small, or whether networking or coordination between researchers should be fostered.

FUNDING OPPORTUNITIES from the FUTURE & EMERGING TECHNOLOGIES scheme

http://cordis.europa.eu/fp7/ict/fetproactive/calls_en.html

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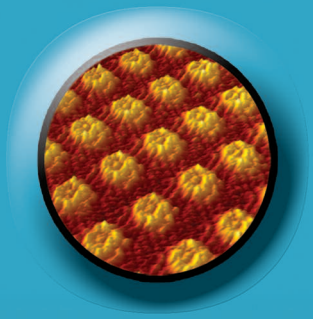
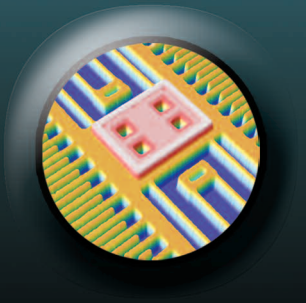


AFM / STM

Materials, polymers, biology, electrochemistry...

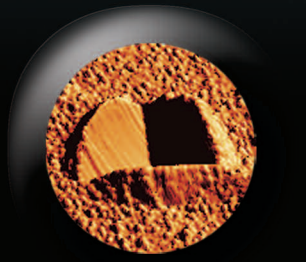
SNOM Microscopy

Reflection, transmission, Apertureless...
SECM, Deep Trench, nanopipette probes...



3D Optical Profilometry

New confocal technology...
Interferometry (PSI/VSI)...



And also...

Mechanical profilometry, nano-indentation...

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