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Status and perspectives of nanoscale device modelling

M Macucci[1], G Iannaccone[1], J Greer[2], J Martorell[3], D W L Sprung[4], A Schenk[5], I I Yakimenko[6], K-F Berggren[6], K Stokbro[7] and N Gippius[8]

[1] Dipartimento di Ingegneria dell'Informazione, Università di Pisa, Via Diotisalvi, 2 I-56126 Pisa, Italy
[2] National Microelectronics Research Center, Lee Maltings, Cork, Ireland
[3] Departament d'Estructura i Constituents de la Materia, Facultat de Física, Universitat de Barcelona, E-08028 Barcelona, Spain
[4] Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada
[5] Swiss Federal Institute of Technology, Integrated Systems Laboratory, Gloriastrasse 35, CH-8092, Zürich, Switzerland
[6] Department of Physics and Measurement Technology, Linköping University, S-58183, Linköping, Sweden
[7] MIC-Technical University of Denmark, DK-2800, Kgs. Lyngby, Denmark
[8] General Physics Institute, RAS Vasilova 38, 117333 Moscow, Russia

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Abstract
During the meetings of the theory and modelling working group, within the MEL-ARI (Microelectronics Advanced Research Initiative) and NID-FET (Nanotechnology Information Devices–Future and Emerging Technologies) initiatives of the European Commission, we have been discussing the current status and the future perspectives of nanoscale device modelling. The outcome of such a discussion is summarized in the present paper, outlining the major challenges for the future, such as the integration of nonequilibrium phenomena and of molecular-scale properties. We believe that modelling has a growing importance in the development of nanoelectronic devices and must therefore make a move from physics to engineering, providing valid design tools, with quantitative predictive capabilities.

1. Introduction

In tandem with the increasing complexity of fabrication technologies and the consequent rising development costs, device modelling is becoming more and more important: it allows preliminary parameter optimization and, in an early design phase, it can provide information on the feasibility of a proposed new technology. This latter issue is particularly relevant, because several times a new device concept has been proposed and has been evaluated on the basis of very approximate and idealized models, thus neglecting aspects that, in the real world, would later present formidable obstacles to its actual implementation. Simulation based on realistic models, yielding quantitatively reliable predictions, could have saved many resources that in the past have been devoted to the pursuit of technologies which involved intrinsic practical difficulties.

For this purpose, models must have good predictive capabilities, which means that they must be based on first principles or be carefully tuned on the basis of experimental data. In essence, we need to develop for nanoelectronics what has been done, with great success, for microelectronics, for which a wide range of extremely reliable simulation tools are currently available, tools that are key to the current steady pace of growth.

However, since technologies for nanoscale devices are still at the early research stage, as opposed to the mature production stage of VLSI (very large scale integration) technologies, in the short- to medium-term modelling tools for nanoscale devices should be more oriented towards device prototyping and towards the early evaluation of the potential of a device structure.

It is apparent that simulation codes for nanoelectronics are more difficult to develop than those for mainstream devices, because at dimensional scales below 100 nm quantum effects play an important role (and therefore classical approaches are often inadequate) and also because the accumulated experience in the fabrication and operation of nanostructures is minuscule

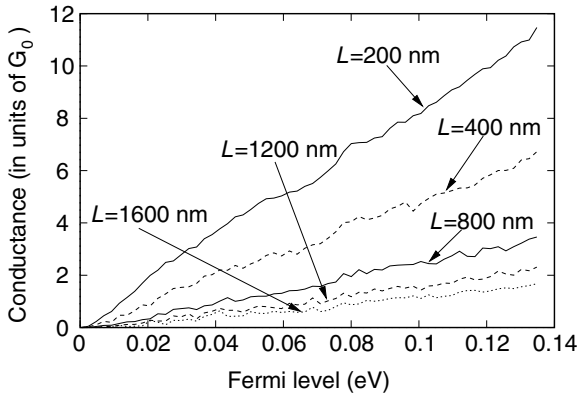

Figure 1. Conductance of a diffusive quantum wire (200 nm wide) as a function of the Fermi energy, for a constant concentration of scatterers and for several values of the wire length.

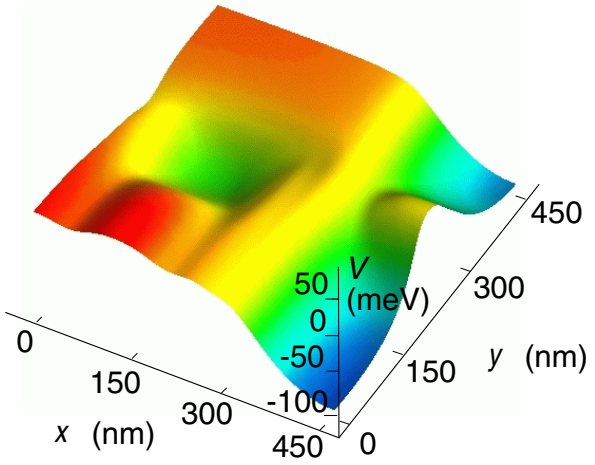

Figure 2. Confinement potential profile for a noninvasive charge detector: the depression on the left represents the quantum dot whose charge is to be detected, and the saddle potential on the right corresponds to the quantum point contact.

compared to that available for microelectronic devices.

2. State of the art and future perspectives

The study of mesoscopic devices has so far been performed mainly with the aim of understanding basic physical properties, and has therefore been focused on structures operating in the simplest possible conditions, in order to isolate one effect at a time. For example, most of the work so far has involved quasi-equilibrium conditions, where conductance properties are much simpler to understand and model. If we want to move from the investigation of fundamental aspects to the development of actual devices, from a physics based approach to an engineering based approach, we need to set up quantitative models for nonequilibrium conditions, which will most probably prevail in actual applications. This is a major issue, that can be approached by means of rather complex techniques such as those based on nonequilibrium Green's functions [1]. These, however, have so far been applied mainly to very simplified models. A major effort is needed to turn such techniques into practical tools for the simulation of realistic structures.

Most of the quantum models developed so far are elastic, omitting dissipation phenomena that play an important role in any real device. There are formulations that include coupling to a thermal bath, but, due to their analytical and numerical complexity, these approaches still represent a very rough approximation of reality. Dissipation is intrinsically difficult to model, because it essentially consists in the coupling of the device under investigation to the innumerable degrees of freedom of the macroscopic environment. On the one hand, it is possible to make a detailed investigation of the interaction of a single phonon with the device, but even a toy model for coupling to a single localized phonon may require a significant computational effort. On the other hand, phenomenological approaches are also conceivable, in which dissipation is introduced via a complex potential [2], but they are often too rough to provide a completely satisfactory description of device properties.

There are, however, other nonballistic regimes that we are already able to model accurately, such as the diffusive regime, which is attained when the length of the device along the direction of current flow is still much smaller than the inelastic mean free path, but already much larger than the elastic mean free path. This condition can be reproduced with the introduction, in a purely ballistic quantum mechanical model, of many localized scatterers that reproduce, for example, the random fluctuations of the electrostatic confinement potential, due to charged impurities. This approach has been tested [3] on the model of a mesoscopic conductor (a quantum wire) 200 nm wide and with a length variable between 200 and 1600 nm. Square scatterers ($12 \times 12\ \mathrm{nm}^2$) have been randomly distributed in the hard-wall defined wire, with a density of 562 $\mu\mathrm{m}^{-2}$. The transmission coefficient through the wire, related to the conductance via the Landauer–Büttiker formula, has then been computed by means of the recursive Green's function method [4, 5]. The resulting conductance is shown in figure 1 in terms of elementary conductance units ($2e^2/h$, where e is the electron charge and h Planck's constant) as a function of the Fermi level (and therefore of the number of propagating modes in the wire) for different values of the wire length. If we observe the conductance values at a given position of the Fermi level, we realize that the inverse proportionality of the conductance to the device length, typical of the diffusive regime, is correctly retrieved. The same approach has been shown [3] to properly reproduce shot noise suppression effects associated with diffusive transport [6].

Another approximation that should be lifted, at least for devices exhibiting material discontinuities on a scale of a few nanometres or less, is represented by the effective mass assumption, whose validity becomes more and more debatable as the number of atoms in each separate region of the devices decreases. New methods for performing full-band calculations are being developed [7], which involve a much smaller computational burden, compared to previous full-band approaches, and which could therefore be suitable for inclusion in realistic simulators. The challenge here is represented by the maximum detail that can be included in the model while keeping it numerically viable.

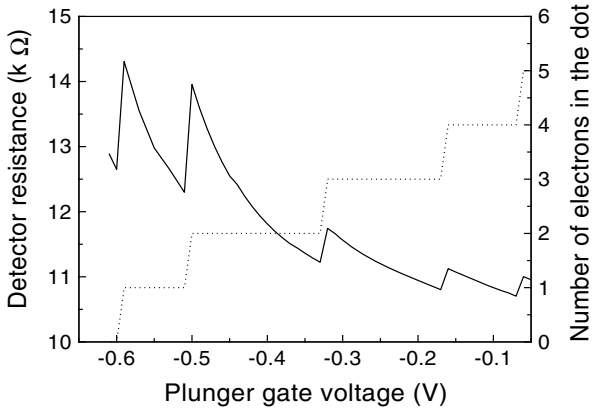

Figure 3. Detector resistance (solid line) and number of electrons in the quantum dot (dotted line) as a function of the plunger gate voltage.

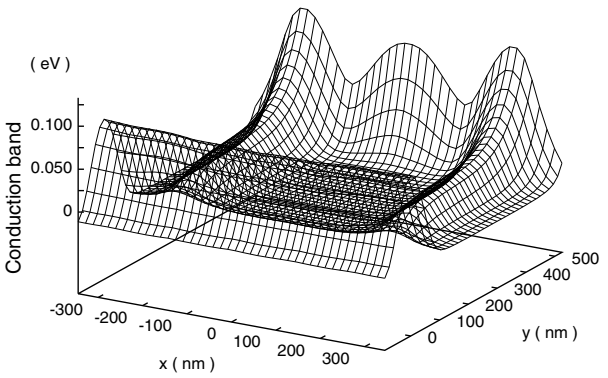

Figure 4. Confinement potential for a strongly isolated pumped dot, obtained with a Poisson–Thomas–Fermi simulation.

With present computational facilities, one cannot hope to model whole systems, containing a large number of elementary building blocks, while including every detail. The system must be subdivided into 'cells' and the model must be constructed in terms of the 'internal' and 'external' cell properties and their interconnections. This type of 'hierarchical' simulation can be exemplified with a practical case, such as the calculation of the resistance variation through a quantum point contact as a function of the number of electrons in a nearby quantum dot [8]. Such a device acts as a noninvasive charge detector and can be studied by determining the confinement potential with a semiclassical Poisson solver (as represented in figure 2), and then partitioning the structure into two regions: the quantum dot (corresponding to the depression on the left of figure 2) is treated with a self-consistent Poisson–Schrödinger solver, while the quantum point contact (defined by the saddle potential visible on the right of figure 2) is studied by subdividing it into many slices and then evaluating the transmission coefficient with the recursive Green's function approach. Results for the quantum point contact resistance, in good qualitative agreement with experimental data [9], are reported in figure 3 with a solid line, as a function of the voltage applied to the plunger gate that is used to deplete the quantum dot. The dotted line represents, again as a function of the plunger gate voltage, the number of electrons in the dot: each time a new electron enters the dot a clear jump can be seen in the resistance of the detector, due to the effect of the new charge on the confinement potential of the quantum point contact. In order to achieve good qualitative agreement, full self-consistency must be introduced, which in turn requires improvements of the numerical algorithms to keep simulation times within reasonable limits.

Poisson–Schrödinger is the acknowledged way to go beyond simple 'macroscopic' modelling of quantum dots defined by electrostatic confinement. However for dots of complicated gate geometry, including connections to the external 2DEG (two-dimensional electron gas), and so on, further simplification is necessary. The Poisson–Thomas–Fermi (PTF) approach in 3D has been found useful in determining the confining potential in these complex configurations. Some testing of its predictions (pinch-off values) has been made for specially designed gate layouts [10]. However, difficulties remain on the experimental side: devices that have apparently the same gate layouts produce different pinch-off values when measured, probably as a consequence of surface imperfections or of randomly distributed dopants.

The usefulness of PTF in making quantitative predictions for the barrier shapes enclosing a dot has been tested, studying the lifetimes of electrons escaping from a strongly isolated pumped dot [11]. Figure 4 shows the results of one such PTF simulation. The barriers thus determined are then the input for a model of the tunnelling of electrons from the dot, that reproduces the main trends found in the experiment. What is particularly remarkable is the stability of the experimental results on a time scale of many hours. Sequences of up to nine consecutive decays have been measured in several runs. Statistical analysis of the escape times accumulated for each of these decays is in excellent agreement with the exponential decay law. This allows extraction of quite reliable values for the corresponding lifetime constant, ranging from tens of seconds for the shortest decays to thousands for the slowest. These results show that PTF allows one to model the emission of electrons from dots out of equilibrium with the surrounding electron gas.

Another technique that can be applied to the investigation of partitioned structures is the scattering matrix approach [12], which allows the calculation of the transmission properties of the whole system, provided that the scattering matrices of the constituent parts are known. The main advantage of the scattering matrix and of the recursive Green's functions method is their capability to treat complicated structures in a recursive manner. For example, transport through a sequence of a large number of elements can be calculated at a reasonable computational cost: first the calculation of the scattering matrix (or the Green's function) for a single element is performed and then a combination procedure is applied to compute the scattering matrix (Green's function) for the whole chain.

In a perfectly periodical structure the electron energy spectrum exhibits formation of a sequence of mini-bands. The transport properties of electrons propagating along the one-dimensional chain with energies within mini-bands depend on the specific structure and size of channel imperfections.

The scattering matrix and the recursive Green's function approaches, although derived through two quite different procedures, are substantially equivalent from a conceptual

point of view, as can be guessed from the formal similarity of the equations. The incorporation into these computational techniques of nonequilibrium transport methods relying on the Keldysh formalism and of first principle approaches is a challenging direction in nanoelectronic device modelling. Unfortunately, there are limitations on the extent to which nanoelectronic circuits can be partitioned in simulations. A simple example suffices to provide an understanding of the problem: circuits made up of single-electron transistors cannot in general be reduced down to a SPICE-like model, in which each component can be studied independently and represented by means of its current–voltage characteristic, thereby requiring only the solution of an electrical network. Such a simplification, always allowed in the case of classical devices, is possible only if the capacitances (stray and intentional) of the nodes connecting the devices are much larger than those internal to the devices themselves. Therefore circuit simulators for nanoelectronics are intrinsically more complex than those for classical circuits, and require the development of original approaches to keep computational complexity under control.

In order to obtain modelling tools with predictive capability, validation of the models is particularly important. This can be achieved through close interaction with experimental groups, based on the fabrication and characterization of properly designed test structures. This issue has received little attention until now, but is of primary importance if simulation tools are to be profitably used by industrial technology developers, in order to accelerate the pace of technological evolution of nanoelectronic devices.

It is also important to mention that one of the inherent problems of nanoscale electronics consists in the unavoidable randomness that results from any fabrication technology. Induced disorder, background charges and the increasing effect of unwanted surface states which, e.g., degrade retention times due to resonant tunnelling, pose serious limitations to the functionality of nanoelectronic devices and in particular to their ultra-large scale integration. Simulation has already shown that even a promising device for room-temperature application like the quantum-dot floating gate EEPROM (electrically erasable programmable read only memory), requires the placement of doping atoms with a precision in the 1 nm range, if single-electron effects on the threshold voltage are to be utilized. TCAD (technology computer-aided design) should be also regarded as a useful tool for the identification of principal limits, the quantification of disturbing effects and, therefore, the assessment of potential applications. Irregularities due to discrete dopant atoms create much more disorder in the potential defining quantum dots than that due to lithographic imperfections, which is already preventing the successful implementation of some nanoelectronic device ideas [13].

Also for classical MOS (metal-oxide semiconductor) devices the random distribution of dopants represents an important issue, particularly when they are scaled down to decananometre dimensions and conduction band fluctuations start having a strong influence on the behaviour of the device (see figure 5). In order to get statistically valid results, simulations must be repeated many times, starting from different, randomly generated, distributions of dopants. Recent contributions [14, 15] have shown that atomistic effects

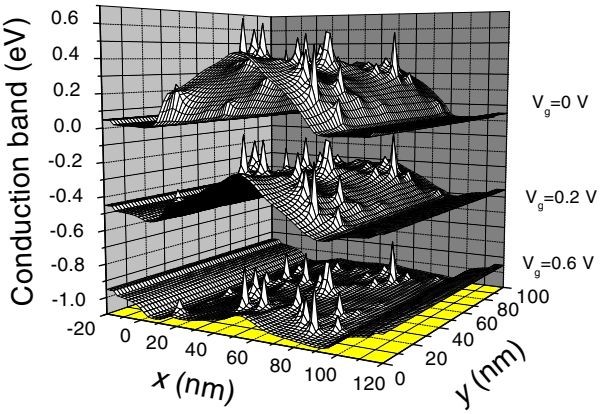

Figure 5. Conduction band profile in an MOS transistor for different values of the gate voltage, in the presence of randomly distributed dopants.

can cause significant fluctuations of the threshold voltage and have helped in determining technological steps that may alleviate these problems.

For device dimensions below 10 nm, simulation problems approach those of molecular modelling, since the exact potential produced by each atom has to be taken into consideration. There is therefore a seamless transition from semiconductor simulation to that of molecular devices, which represent the future frontier of integration and miniaturization. Existing models used within the field of molecular electronics to determine the 'electric' properties of molecules, are often too crude, in contrast to the refinement achieved by calculations of electronic structure in quantum chemistry.

Nanotechnology in general is concerned with the manipulation of matter on the nanometre scale, and it is natural that nanotechnology design will rely heavily on the computational methods and tools developed to study the chemistry and physics of materials on the atomic scale. Electronic structure theory, which has been extremely successful in the calculation and prediction of molecular and solid properties, is foremost amongst the tools available for nanotechnology design. Electronic structure theory is the area of computational chemistry and physics concerned with direct solution of the Schrödinger equation for quantum and many electron systems, atoms, molecules and solids. The techniques of electronic structure theory are already finding their way into the technology computer-aided design hierarchy applied by the microelectronics industry. The microelectronics industry is routinely concerned with the manipulation of matter on the atomic scale, with atomic layer deposition (ALD) being the latest example. The methods of quantum chemistry have been applied to the study of chemical vapour deposition (CVD), dopant–defect interactions after ion implantation, chemical and plasma etching, and thin film sputtering. First principles calculations on the atomic scale remain computationally demanding, so they are often used to formulate and identify basic reaction mechanisms or electronic properties. This information is then incorporated into conventional process and device simulators. For example, the steps involved in chemical vapour deposition may be elucidated through quantum chemistry methods, but the time and length scales for a fully first principles treatment of film growth remain beyond

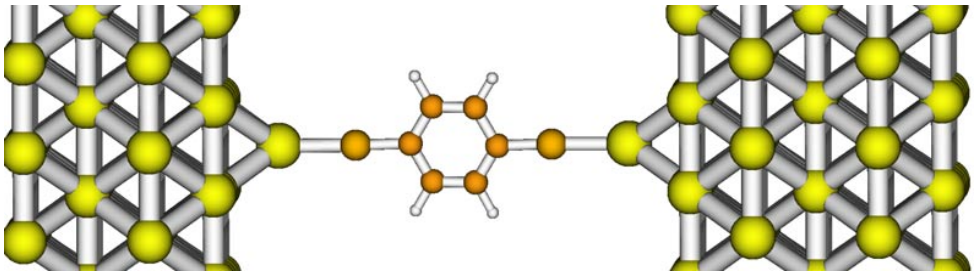

Figure 6. Example of a hybrid metal–molecule–metal structure: a dithiol-benzene molecule is connected between two gold (100) surfaces.

computational reach. To avoid these limitations, the *ab initio* data are fed into Monte Carlo or continuum treatments of film growth as reaction steps and rate constants.

Many problems posed by nanotechnology are directly describable by electronic structure methods. For molecular scale problems, quantum chemistry methods can yield important information on chemical bonding, vibrational spectra, electronic transitions and polarizabilities. However, with the advent of molecular electronics investigations, the methods of quantum chemistry need to be modified to allow for current injection into molecules, a situation that cannot presently be handled by commonly used *ab initio* programs. The formulation of efficient computational algorithms allowing for the treatment of current carrying states is under development in many research groups, and initial results are promising. However, it should be emphasized that this area of research is relatively new and has been to date primarily concerned with the flow of current through a single molecule bonded to metallic contacts. This is an important test case for the prototyping and understanding of molecular electronics, but must be viewed as a first step forward in the computational prototyping. Numerous fundamental difficulties remain for molecular electronic transport problems. The state of the art in transport simulations can handle self-consistency for the unperturbed atomic and molecular components, but they do not generally allow for self-consistency upon charge injection. A difficult issue to address is the accurate treatment of electron–electron interactions, the so called correlation problem, for charge transport. Explicitly correlated methods remain computationally too costly, but explicitly correlated methods are needed for multiple charging of quantum dots and for molecular problems in general.

Density functional methods are attractive in that they provide an accurate treatment of ground state correlations within a reasonable computational demand. However, it is still unexplored how well density-functional methods describe systems far from equilibrium. This is mainly because the description of systems out of equilibrium with density-functional methods is technically difficult, due to the need of a self-consistent solution of a one-electron Schrödinger equation with open boundary conditions. Some initial ground breaking work in which the leads connecting the nanostructure are described in terms of a jellium model has been performed [16, 17], giving quite promising results. However, to obtain predictive power, a more accurate description of the leads is necessary. Recently, two groups have independently implemented the density-functional method using non-equilibrium Green's functions that allow the description of systems out of equilibrium by taking into account the atomic structure of both the leads and the contact region [18, 19]. With such methods it will be possible to evaluate the accuracy of density functional theory in describing systems out of equilibrium. An example of a hybrid structure which can be treated with such approaches is shown in figure 6: a dithiol-benzene molecule is connected to two gold (100) surfaces.

Also the effect of the substrate, to which molecules must be attached in any conceivable structure for information processing, may alter their properties in ways that need to be predicted, which represents another very challenging modelling task. With technologies that could become available in the foreseeable future, it is not likely to be able to obtain virtually defect-free substrates, therefore the action of imperfections and stray charges must be considered and included in the assessment of any device idea.

A recent review of quantum chemistry methods applied to microelectronics problems is available [20]. Semi-empirical quantum chemistry methods applied to the study of molecular transport are compared in [21].

Many problems posed by nanotechnologists do not require electronic structure information, rather the questions posed resemble the problems faced by molecular biologists and it is natural that the simulation tools developed by molecular biologists are now being applied to nanotechnology, particularly within the field of self-assembly. Molecular biologists are often concerned with the interaction between large, organic molecules and these systems remain too large for a comprehensive electronic structure treatment. At a level of approximation above electronic structure theory methods, are the atomistic or molecular modelling approaches. For molecular modelling, one does not attempt to directly solve the Schrödinger equation. Molecular modelling rests on the premise that atoms and functional units occurring in molecules often behave similarly and can be described by simple, analytic interactions. Functional units in different molecules are assumed to behave similarly and their interactions are said to be transferable, an assumption in general applied to organic systems and less true for inorganic materials. Hence, problems such as DNA-base pair interactions or the docking of proteins are good candidates for molecular modelling studies,

and indeed such studies are widespread in the literature. For nanotechnology, these methods can be directly applied when one seeks to study the interactions of well-characterized organic systems. One can quickly construct test molecules to evaluate their suitability for a specific application. Molecular modelling tools allow design to link molecular functionality and chemical synthesis at the nanoscale.

Within microsystems, the integration of microelectronics systems with biological systems is emerging. Conventional microelectronic design tools for chip fabrication need to be coupled to computational fluid dynamics, mechanical and electrical simulation, and for microsystems geared to drug discovery and medical applications, a molecular modelling component emerges. In general, these various simulators have emerged from independent fields of enquiry and the coupling of the algorithms for microsystems applications remains an outstanding challenge. Typically, a simulation tool is developed with underlying physical assumptions restricting its applicability to limited length and time scales. Microsystems and nanotechnologies by their nature require these simulation tools to operate at the extreme limits of their applicability. For example, a microsystem could be designed requiring a molecular modelling tool to describe a large molecule and a small mechanical system. The mechanical system, such as a pump to circulate a fluid on a microsystem, may be many orders of magnitude larger than the molecules dissolved in the fluid it is pumping, but nonetheless the characteristic length for the pump is small whereas the characteristic length for molecules is large. For nanotechnology computer-aided design to extend beyond specific applications such as electronics or drug design, the coupling of electrical, mechanical, optical, thermal and chemical simulation tools will be required over length and time scales currently not achievable.

Modelling will play a fundamental role also in the effort for the physical realization of a quantum computer, which still poses formidable scientific and technological challenges. At a preliminary stage, it is necessary to evaluate the feasibility of different possible schemes for qubits and quantum gates as building blocks of quantum computers. In particular, one of the most promising schemes for quantum computing, which is based on the use of spin states of semiconductor quantum dots, is strongly related to nanoelectronics and to one of its currently most active branches, spintronics. Application of Kohn–Sham local spin-density functional formalisms has recently allowed significant understanding of the role played by spin effects in mesoscopic transport [22], and can shed light on the appearance of a conductance plateau at $0.72\,e^2/h$ that has been experimentally observed [23, 24]. Such simulation tools will be useful also for the development of spin injection into semiconductors [25, 26].

3. Conclusions

We can conclude that, as nanoelectronics moves closer to actual circuit implementation and device sizes are further shrunk, modelling is acquiring a growing importance, and must adapt more closely to the needs of experimental activities, in a move from physics to engineering.

To this purpose, and to assist the evaluation of new device proposals, models must have good quantitative predictive capabilities, which can be developed only through a constant collaboration with experimental groups capable of providing data from test structures.

On the one hand, the computational complexity is so large that we need to find ways to increasingly partition models following hierarchical approaches. On the other hand simplifying assumptions, such as those allowing the usage for classical devices of circuit simulators based on *I–V* characteristics, may break down at the nanometric scale, thereby effectively preventing partitioning. A careful balance is therefore needed between the development of simplified approaches, whenever they are possible and help in reducing the computational burden, and the usage of very detailed or even *ab initio* methods, required in those situations in which the actual behaviour of the system could not be otherwise described.

As device sizes are scaled down, modelling approaches for 'standard' nanoelectronic devices and for molecular devices are bound to converge, since they deal in both cases with structures at the molecular scale. Modelling can therefore derive inputs from the well-developed field of quantum chemistry and extend its approaches to non-equilibrium situations such as those found in devices that perform information processing and storage functions.

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