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1. Executive Summary

The development of novel devices at the nanometer scale with potential for large-scale integration and room temperature operation is a formidable task. Over the years, many ideas have been proposed on the basis of very qualitative reasoning or simplified physical models: typically, the demonstration of working prototypes is achieved, while the fabrication of complex logic circuits proves to be unfeasible. While in some cases insufficient maturity of the available technology is responsible for the undesired outcome, most often fundamental problems are present. The extreme sensitivity of device operation to the presence of defects, stray charges, and other parasitics, the requirement of prohibitively tight fabrication tolerances, very slow switching times, or even the weakness of the physical effect on which the device is based, may easily prevent proper operation at large scale, or, possibly, room temperature.

The NANOTCAD Project was mainly motivated by the belief that many of the difficulties and of the limits of candidate technologies for nanoelectronics and molecular electronics could be predicted, anticipated and, hopefully, solved if detailed modeling tools of realistic devices and structures were available. The same modeling tools could be used to design more robust devices, and to select molecules and device structures with potential for use in large-scale integrated circuits. For these reason, the main objectives of the project, refocused after the first year, were the following:

- Development and validation of a hierarchical set of software tools for the simulation and the design of a wide spectrum of devices, based on semiconductors and on transport through single molecules.
- Demonstration of a procedure for the realization of prototype nano-scale devices based on detailed modeling.
- Design, fabrication, characterization and optimization of single and double quantum-dot HFETs for use as single /few electron memories, and resonant tunneling diodes, and nanoscale HFETs.
- The design, fabrication, characterization and optimization of devices in which transport occurs via one/few molecules connected to metal electrodes.

The project consortium consists of six partners: four of them are directly involved in the theoretical activity of model and code development, and two partners are involved in the fabrication and characterization of state-of-the-art nanoscale devices and structures, to experiment a method for prototype realization and transport investigation strongly intertwined with nanostructure modeling. In detail, University of Pisa (DII-IET) and ETH Zürich focused on semiconductor modeling in quasi equilibrium, for devices including subregions with different degree of quantum confinement (quantum dots, quantum wires, and quantum wells). ETHZ, in addition, focused on the coupling of quantum simulation based on density functional theory with commercial semiclassical TCAD tools of semiconductor devices, based on drift-diffusion and energy-balance transport models. TU Vienna was involved in the development of models and tools for Quantum Monte Carlo modeling, to account for far from equilibrium transport in quantum devices. NRMC Cork focused on molecular devices, developing a model and an associated numerical code for transport through single molecule that would not depend on a single particle picture or on a density function approach.

Experimental partners were the University of Würzburg, covering fabrication and characterization of semiconductors nanostructures and nanodevices, and Max-Planck Institut Stuttgart (MPG), covering the realization and characterization of devices in which transport occurs through single/few molecules. University of Pisa was in charge of Project coordination.

Project objectives have been largely met. A set of software tools have been developed and freely distributed to the european nanotechnology community through the Phantoms Simulation Hub (www.phantomshub.com) and comprehensive manuals have been prepared for non expert users. Such tools include codes for the self-consistent solution of Poisson-Schrödinger equation in semiconductor nanostructures with regions subjected to strong quantum confinement based on density functional theory (NANOTCAD1D, NANOTCAD2D, NANOTCAD3D), a quantum Monte Carlo code for the physically detailed simulation of one-dimensional devices operating in far from equilibrium conditions and in presence of strong dissipative phenomena (VMC), a code for the simulation of transport through single molecules contacted with metal electrodes immersed in a generic scalar potential (VICI), and a code for the three-dimensional simulation of semiconductor nanostructures (SIMNAD) coupled to a commercial drift-diffusion simulator (DESSIS_ISE).

As far as semiconductor nanofabrication is concerned, significant results have been obtained: memories consisting of an AlGaAs-GaAs HFET with a single layer and a double layer of InGaAs quantum dots have been demonstrated, with very fast write and erase times, and promising retention times. In addition, nanoscale FETs have been fabricated and characterized in which a unique signature of ballistic transport has been identified in the behavior of transconductance as a function of gate bias. A series of nanoscale devices have been fabricated that have allowed to validate and test the software tools developed within the project.

The molecular nanofabrication activity has successfully led to the demonstration of two techniques to fabricate a molecular device in which a small molecule bridges two metal electrodes separated by a gap of 1 nm. The first technique allowed to contact benzenedithiol molecules between two wires in a crossed geometry; the second technique allowed to place benzenedithiol molecules in nanogaps induced by controlled electromigration. In both cases it was possible to measure current-voltage characteristics exhibiting non-linear features close to those observed by other groups. Notwithstanding the instrinsicly poor reproducibility of molecular structures, results achieved within NANOTCAD are at the state of the art in the field.

2. Project Objectives

The importance of Computer Aided Design (CAD) tools in the development of industrial semiconductor technology is well outlined in the 1997 edition of the SIA National Technology Roadmap for Semiconductors – Technology Needs (page 6): “Modeling and simulation is the only tool available for engineers to design processes, material use, transistors, and structures; there is no viable alternative. The major challenge is getting predictive model results from atomic scale through electrical performance; to accurately model new technologies a priori resulting in development cost reduction; and faster time to market.”

In addition, during the 1990's, computational quantum chemistry has truly achieved the status of a mature technology: experimental and computational studies are applied in unison with molecular problems, while the software tools needed to perform computational studies have been commercialized and now form a mini-industry, serving academic and industrial users. This state of the art was recognized directly by the awarding of the 1998 Nobel Prize in Chemistry to Walter Kohn for his development of the density functional theory and to John Pople for his development of computational methods in quantum chemistry. Molecular CAD is routinely applied within the pharmaceutical and chemical industries, for applications like drug design, selection of molecules, and investigation of catalytic reactions.

Here we describe the main four objectives of the project from the original proposal, as modified by the updated workplan:

- **Development and the validation of a set of software tools for the simulation and the design of a wide spectrum of nanoscale devices, based both on semiconductors and on transport through single molecules**. In perspective, the set of tools developed within NANOTCAD aims at playing for the development of nanotechnology the same role as existing CAD tools have in the successful development of each new generation of microelectronic circuits and devices. However, since technologies for nanoscale devices are still at the early research stage, as opposed to the production stage of VLSI technologies, the NANOTCAD set of tools is mainly oriented at device prototyping and early evaluation of the realistic potential of a device structure. NANOTCAD should to solve the selfconsistent Schrödinger-Poisson equation in three dimensions in semiconductor structures, for open and closed systems; to compute electron densities in atoms and molecules attached to conducting electrodes; to simulate transport in molecular electron devices, and to compute the I-V characteristics both in the linear response regime and far from equilibrium. In addition, it should allow to model nanoscale structures coupled with conventional electronic devices and to explore device behavior in the temperature range from 0K to room temperature. In order to reach such a goal, significant progress was needed in modeling quantum transport in realistic nanoscale devices in the whole range of transport regimes. The NANOTCAD package had to be developed with the aim of addressing the broader possible range of nanotechnology devices and had to be made freely available to the NID community,

- **Demonstration of a procedure for the realization of prototypes of nanoscale devices based on detailed modeling**. The added value of such a procedure is represented by the possibility of detecting design flaws and problems in the early evaluation phase of a candidate device structure, and designing optimized devices structures on the basis of accurate simulations. Such procedure should therefore allow for more efficient and quicker device prototyping. This procedure was to be applied, verified and refined through the realization of two prototype classes of nanoscale devices, which are described below and represent the other two main objectives of the proposal.

- **Design, fabrication, characterization and Optimization of Molecules in which transport occurs through single molecules**. While an activity of fabrication of Mott-FETs was originally proposed, after the first year it was decided to focus on the fabrication of structures in which transport occurs through single molecules

connected to metal electrodes. To coordinate the efforts with the modeling activity, 1-3 and 1-4 benzedithiols were chosen as bridging molecules.

- **Design, Optimization, Fabrication and Characterization of Single and Double Quantum Dot HFETs**: these devices are based on ultrashort HFETs (with gate lengths between 30 and 100 nm) realized on GaAs heterostructures in which a single or a double layer of self-assembled InGaAs dots is introduced between the channel and the control gate. In collaboration with groups involved in modeling aspects, the possibility to use these devices as quasi-non-volatile flash memories had to be explored.

3. Methodologies

3.1 Simulation of quasi-equilibrium transport and ballistic field effect transistors

Nanoelectronic devices are typically characterized by strong charge confinement in at least one dimension, and by an intrinsic three-dimensional nature. For these reasons, a simulation tool aiming at addressing a broad range of devices must have the capability of solving the Poisson-Schrödinger equation in three dimensional domains. An pproach based on the envelope function approximation, and on Density Functional Theory (DFT) with local density approximation has been adopted. While the limitations of such approach are apparent [1], it still provides the best trade-off between numerical complexity and accuracy, for the vast majority of devices of interest.

A Poisson-Schrödinger solver with good scalability properties for large grids has been developed, based on a multigrid algorithm. Multigrid methods are known to solve elliptic partial differential equations discretized on N grid points in $O(N)$ operations [2], and offer several advantages with respect to the Newton-Raphson algorithm. First, multigrid methods are known to converge in a number of step smaller than any other "rapid" method (like, for example, Fourier or reduction methods [2]). In addition, they have reduced memory requirements: while the Newton-Raphson method requires the Jacobian matrix to be stored ($7N$ elements), in the multigrid method only arrays of size N have to be stored. The non-linear Poisson equation can be discretized with the box integration method on several grids of different size, from the finest (of order 10^5-10^6 points) to the coarsest (a 3x3x3 grid).

The structure of the multigrid algorithm is sketched in Fig. 1. "E" represents the exact solution on the 3x3x3 grid, the rising line "I" represents the interpolation on the next-finer grid, "S" represents the "smoothing" operation, i.e., a series of relaxation steps based on the Newton-Raphson algorithms which basically reduce the residue, the descending line "R" represents restriction on the next-coarser grid, and "L" represents smoothing plus solution of the Schrödinger equation. Without loss of generality, Fig. 1 refers to a problem with 4 different grids, where grid 1 is the finest and grid 4 the coarsest.

First, the approach consists in solving the non-linear Poisson equation with a semiclassical approximation starting from an initial solution on the coarsest grid (3x3x3 points), where the Poisson equation is a single-variable nonlinear equation. The method then consists of a fixed number of steps on different grids, called V-cycles from the recursive restriction and interpolation steps. The solution on each grid is found by adding a corrector term obtained by solving the equation on a coarser grid to

an approximate solution, obtained by means of relaxation cycles based on the Newton-Raphson algorithm. The mathematical details of the method can be found in Ref. [2].

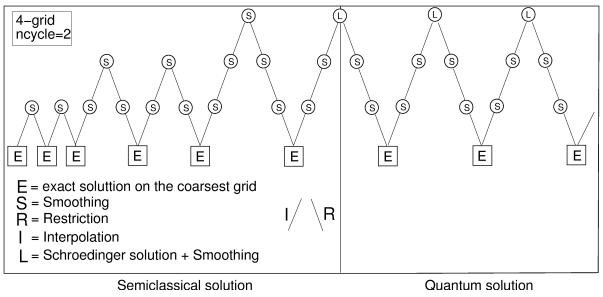

Figure 1: Structure of the Poisson-Schrödinger solver based on the multigrid algorithm. The case of four different grids is represented.

The potential obtained at the end of the semiclassical cycle is used as an initial guess of the solution of the Poisson-Schrödinger equation. Then, a new number of *V*-cycles and relaxation steps is set for the following part of the algorithm. Every time the algorithm is at the top of a *V*-cycle (i.e., on the finest grid), the Schrödinger equation is solved with DFT, and eigenfunctions are computed, restricted and stored on all grids. The *V*-cycle is then performed as already described, with the only difference that the electron density in the quantum region is computed from the stored eigenvalues.

Among several approaches to solve the Schrödinger equation (for example, [3,4]), a solver in the momentum space has been developed (*k*-space) that will allow extension to full-band simulations. The basic idea is to transfer the eigenvalue problem to the *k* space by means of Fast Fourier Transform (FFT). The problem is then solved in the *k* space and the solutions are then transferred back to the real space by the anti-transform operator. The precision of results and the efficiency of the routine strictly depend on the choice of the basis in the *k* space. If the elements of the wave vector basis are a good approximation of the single particle eigenfunctions, then a small basis is sufficient to adequately describe the solution of the Schrödinger equation, even if in the real space a larger number of points are required to accurately reproduce the potential profile. To find the lowest eigenvalues a sub matrix has to be diagonalized corresponding to the smallest wave vectors. The advantage from the point of view of memory requirements (that scale as N^2) and of computing time (that scales as N^3 for a complete diagonalization, where N is the matrix order), is evident.

Moreover, it is necessary to enforce Dirichlet boundary conditions on the eigenfunctions. In order to force the eigenfunctions to zero at domain boundaries, a basis of only sine functions for the *k* space has to be used. The sine-FFT is used to compute the eigenfunction expansion in the sine basis. By solving the sub-matrix corresponding to smaller values of *k* it is then possible to gain efficiency without losing precision of the solutions for the lowest eigenvalues [5].

As far as the simulation of nanoscale HFETs is concerned, the approach of considering ``ballistic'' electrons not just as a perturbation to a ``normal'', quasi-thermal electron distribution, but as mainstream electrons, has been adopted. As zero order approximation, fully ballistic transport has been considered.

Simulations of ballistic MOSFETs have been first performed by Natori [6] by means of an analitical model. Moreover, recent simulations based on semiclassical Monte Carlo codes [7] and on a scattering theory of MOSFETs [8] exhibit significant

differences with respect to simulations based on drift-diffusion or energy balance models.

Nanoscale MOSFETs, in particular, exhibit a significant degree of quantum confinement in the channel: indeed, in order to control short channel effects, gate oxide thickness is reduced and bulk doping is increased, which in turn cause an high electric field in the vertical direction, confining electrons at the Si/SiO_2 interface. A quantum simulation is consequently required to take into account the 2D subband splitting and the lifting of the six-fold degeneracy of silicon conduction band minima. This is especially required to reproduce the experimental MOSFET threshold voltage V_T, since semiclassical simulation may underestimate V_T by more than 100 mV [9].

Observing that quantum confinement is strong only along the direction perpendicular to the Si/SiO_2 interface, the Schrödinger equation can be decoupled into a 1D equation in the vertical direction (x) and a 1D equation in the longitudinal direction (y): the density of states in the y-direction is well approximated by the semiclassical expression, since there is no in-plane confinement, while discretized states appear in the vertical direction. Such approximation reduces has been shown to considerably the computational complexity of the problem, while introducing only a negligible error [9]. In order to obtain the I-V characteristics of the 25 nm nMOSFET, a fully ballistic model has been assumed for carrier transport. In this way, current-voltage characteristics is reduced to a simple carrier transmission problem over the channel potential, which is represented by the edge of the subbands originated by the 1D-quantum confinement.Carriers with energy larger than the subband maximum can be transmitted from source to drain by thermoionic emission, while carriers with lower energy can travel along the channel only by tunneling. Since the tunneling component is negligible even in devices with channel length of 10 nm [7,10], initially quantum tunneling of the channel barrier has not been considered. The transmission coefficient has been then taken equal to unity above the maximum of the barrier and zero below. In this way electrons with energy smaller than the subband maximum energy are in thermal equilibrium with the closest contact (source or drain), while electrons with larger energy traverse the channel without energy loss. The electron concentration is computed by assuming that the states with energy below the maximum of the potential barrier have an occupation factor determined by the source/drain Fermi energy E_{fS} and E_{fD} respectively), while states with higher energy propagating from the source (drain) have the occupation factor of the originating contact [11].

3.2 Simulation at quasi equilibrium and coupling with drift-diffusion simulation.

SIMNAD (SImulator for NanoDevices) is a quantum mechanical 3D simulator for semiconductor devices. It is based on a temperature-dependent effective mass formulation of density functional theory and applies the local density approximation.

SIMNAD can be used to compute the self-consistent quantum mechanical charge density in semiconductor nano-structures, and can handle both direct gap materials (like III-V semiconductors) and materials with a silicon-like six-valley band structure and anisotropic effective mass.

SIMNAD is designed for the simulation of devices in quasi-equilibrium, e.g. single-electron transistors with infinitesimal source-drain bias. Conductances computed by SIMNAD are either tunnelling conductances (e.g. in single-electron transistors) or quantum-ballistic conductances (e.g. in quantum point contacts or ballistic MOSFETs). Users who are equipped with a coupling-enabled version of the semi-classical device simulator DESSIS can run simulations in coupled mode, i.e. SIMNAD will compute the quantum mechanical charge densities for band profiles

provided by DESSIS and will communicate this data back to DESSIS for further processing (e.g. for use in a DESSIS self-consistency iteration).

SIMNAD uses similar methods for the computation of the charge density as the code of University of Illinois at Urbana-Champaign and the code of the University of Pisa. Compared to SIMNAD, the group in Pisa uses a hierarchical multi-grid algorithm and the group in Urbana includes the effect of magnetic fields by applying local spin density approximation. These are reasonable potential extensions for SIMNAD, too. Both the group in Pisa and in Urbana-Champaign simulate Coulomb charging in the T=0 K limit, which eliminates the need to evaluate the free energy of the various N-particle states contained in the grand-canonical ground state but neglects the thermal broadening of the Coulomb staircase. The latter can be correctly simulated with SIMNAD based on a Monte-Carlo method that allows the computation of the Gibbs distribution function and the free energies at arbitrary electron numbers with moderate computational effort.

SIMNAD can calculate the full 3D wave function in MOSFET channels and SET leads based on the scattering matrix method with open boundary conditions (``Quantum Transmitting Boundary Method''). This can be used to compute the tunnel probabilities in SETs. The group in Urbana-Champaign applies the adiabatic 2D+1D decomposition of the Schrödinger equation; which reduces the task of the computation of transmission probabilities to a one-dimensional transfer-matrix calculation. The group in Pisa has been approaching the same problem without decomposition by means of recursive Green's functions. Recently, an improved scattering matrix solver capable of including inter-subband coupling has been developed at the university of Pisa.

SIMNAD uses a conductance model for Coulomb blockade devices based on the description by Beenakker (sequential tunneling). SIMNAD can also compute the coherent resonant tunneling current based on a modified Landauer-Büttiker formula. Currents through individual quantum point contacts can be obtained from a simplified ballistic tunneling model. The transport model by the group in Urbana-Champaign treats coherent transport by means of a modified Landauer Büttiker formula: the energy at which the transmission is evaluated is altered in order to account for single electron charging. The formula succeeds in producing conductance peaks; yet quantitative agreement with experimental data is poor.

SIMNAD can be coupled to the commercial device simulator DESSIS (drift-diffusion transport). This enables the simultaneous modeling of a (3D) quantum-mechanical charge distribution in a sub-region of a larger device, which is under full operation. Such a methodology is unique and no other comparable simulation package is known. So far, only a non-self-consistent version is available, but the self-consistent version is being developed and tested. In the non-self-consistent version of the coupling scheme, the quantum-mechanical charge density from SIMNAD is frozen-in for a subsequent DESSIS solve without any feedback. In the self-consistent version, the Poisson solver of SIMNAD is deactivated and the quantum-mechanical charge density is computed with the fixed potential obtained in a DESSIS run with the previous quantum-mechanical charge. The iteration is continued until convergence. The two simulators communicate via semaphor files, where DESSIS requests an update of the quantum-mechanical charge if required.

3.3 Quantum Monte Carlo modeling

The workpackage on Quantum Monte Carlo aims at the modeling of quantum transport in far from equilibrium conditions in the presence of dissipative processes.

The most comprehensive theory which can be used for this purpose is based on the non-equilibrium Green's functions. Next to it is the Wigner function formalism which utilizes one time variable less than the Green's function. The Wigner formalism has been recognized as a convenient approach, that combines a rigorous treatment on a quantum-kinetic level with the classical concepts of phase space and open boundary conditions.

In presence of dissipation processes due to interaction with the lattice, the generalized Wigner equation depends on the electron coordinates and on an infinite number of phonon coordinates. Aiming at finding a numerically treatable formulation of the problem, a hierarchy of transport models accounting for quantum effects at different levels of approximation has been derived from the equation. A closed equation for the reduced electron Wigner function has been obtained, which is viewed as a main result of the approach. Further approximations in this equation recover basic semiconductor transport models. In the homogeneous case the equation reduces to the Levinson equation. The classical limit in the electron-phonon (e-p) interaction leads to the Wigner-Boltzmann equation which, to our knowledge, up to now has been introduced only phenomenologically. The hierarchy which ends with the well known Boltzmann equation is a novel systematic theoretical result which gives insight in the introduced assumptions and simplifications associated to each transport model.

The Levinson equation has been investigated during the first period of the project. A backward stochastic method for simulation of e-p interaction in the homogeneous case of an applied electric field has been developed [12]. The approach utilizes the numerical theory of the Monte Carlo method applied to the integral form of the equation. Techniques for variance reduction such as importance sampling and randomization are introduced. The dimensionality of the equation has been reduced by an appropriate transform in the wave vector space. Another transform in the time domain has been used to fix the simulation domain which otherwise extends to infinity with the increase of the evolution time. Simulations reveal the effects of collision broadening, collision retardation due to the memory character of the integral kernel and the intra-collisional field effect in the quantum solution. These effects have been observed in the time domain, up to an evolution time of few hundred femtoseconds for GaAs. Since in the long time limit the Boltzmann equation is recovered, these effects are expected to become negligible at higher times. Despite the progress in the numerical treatment of the equation, for increasing evolution times an exact simulation of the problem remains a hard numerical task. Approximate models of quantum electron-phonon interaction must be introduced.

Consequently the stationary Wigner-Boltzmann equation has been chosen as a basic quantum transport model, which is more suitable for numerical treatment. A Quantum Monte Carlo (MC) method has been developed and successfully used to simulate realistic nanoelectronic devices.

The methodology for deriving the method is summarized in the following. The integral form of the Wigner-Boltzmann equation has been used as a starting point for deriving the method. The kernel of the adjoint equation has been decomposed into a linear combination of conditional probability densities. These densities are used to form a transition density used, in accordance with the Monte Carlo theory, for construction of numerical trajectories. The peculiarities of the selected transition density allow a particle picture to be introduced. In this picture dissipation and interference phenomena are taken into account by two alternative processes involving quasi-particles. Dissipation caused by interaction with phonons is accounted for by drift and scattering processes corresponding to the semi-classical Boltzmann transport

picture. Interference effects due to the Wigner potential are associated with generation of pairs of particles having statistical weight ±1.

The classical force term is separated from the Wigner potential and included in the Liouville operator. With this modification, the developed model corresponds to a Boltzmann equation augmented by a generation term. The challenge of employing such method is to handle the avalanche of numerical particles properly. The problem has been solved for stationary conditions: particles of opposite weight and a sufficiently small distance in phase space are continuously removed in the course of a simulation. The cancellation is due to the fact that such particles have a common probabilistic future but opposite contribution to the statistics.

The MC method has been integrated into a device simulator called VMC (Vienna Monte Carlo code). A description of the utilized concepts, features and input-output decks of the VMC simulator are presented in a user's guide. Experience about the features of the MC method has been collected during simulations of different types of resonant tunneling diodes. The properties of the method with respect to complexity for implementation, physical relevance and scope of applicability are discussed below. Phonons can play an important role in the behavior of nanoelectronic devices. In resonant-tunneling devices phonon scattering can lead to an increase in the valley current and a resonance voltage shift.

Comparison with alternative Methodologies

The advantage of the Monte Carlo approach is that phonon scattering is rigorously considered as a 3D process. All kinds of phonons are considered, including acoustic deformation potential and polar optical phonons. In comparison, deterministic approaches meet difficulties in accounting for phonon scattering. The majority of models consider the wave vector space as one-dimensional, while the phonon interaction involves all tree dimensions. Then the phonon interaction is approximated by a damping parameter determined by the relaxation time. An exception is the NEMO-1D simulator, based on non-equilibrium Green's functions [13], where initially phonons of Einstein and Debye type were included [14]. Einstein phonons correspond to dispersion-less deformation potential optical phonons. The polar optical phonon has been included later in the comprehensive model [15]. The VMC program has been compared with the solver NEMO--1D. A benchmark RTD from the literature has been used and common physical models are assumed. The simulation results obtained by the two methods for both coherent and non-coherent transport have been critically compared. It is concluded that the VMC simulator provides a reliable description of stationary carrier transport in nanostructures. Effects of tunneling and dissipation are found to be in a good agreement.

Beyond the scope of applicability of the MC method remain conditions where the physical quantities vary several orders of magnitude. The required resolution in the simulation results is unattainable for the proposed approach. The numerical noise of the stochastic approach poses a natural limit for the resolution of the simulated averages.

State of the art

An alternative particle model for simulation of quantum transport has been proposed by Shifren and Ferry [16]. The model has been initially devised for the solution of the coherent case Wigner equation. Particles cross the device by collisionless drift over classical trajectories. The information about the Wigner equation is retained as a new property of the particles called affinity. The affinity depends on the local value of the

quantum potential and thus remains bounded during the simulation. The method requires a large number of particles to be kept simultaneously in memory. Recently the method has been combined with the Ensemble Monte Carlo technique in order to account for phonon scattering. Quantum effects are incorporated which account for the finite collision duration and the intra-collisional field effect.
It can be concluded that the Wigner-Boltzmann equation has come into the focus of other research groups. It is recognized that the Monte Carlo approach to solving the equation has many advantages when phonon scattering has to be considered.

3.4 Semiconductor Nanofabrication

In order to achieve the project objectives of utilizing semiconductor nanofabrication to realize single quantum dot flash memories, nanotechnologies including the growth of modulation doped heterostructures and self-assembled quantum dots by molecular beam epitaxy and electron beam lithography have been combined and improved. In close cooperation with NANOTCAD simulation tools a new layout with in-situ fabricated side-gates has been proposed. The gate layout allows the control of narrow sections with widths down to 30 nm in GaAs/AlGaAs heterostructures containing only a few quantum dots. In addition the employment of single quantum dots as floating gates and basic units of flash memories has been challenging as depending on the number of charges localized in the quantum dots the resistance of a nearby read-out channel should be changed significantly. Thus different geometries have been tested with variable distances between the conducting channel, the side-gates, and the quantum dots. Since quantum dots have been proposed as nanoscaled memory devices several different approaches have been realized to utilize the three dimensional confinement for the robust storage of electrons. However, most of the publications related to QD memory devices have studied concepts involving several hundreds of quantum dots such as Si-nanocrystals [17-19]. So far, only a very limited number of publications were reported on memories with feature sizes only a few self assembled quantum dots [20,21]. Within the project the principle operation of a single QDFM memory has been demonstrated. Room temperature memory functionality was reached when exploring a coherent growth mode of 2 nearby quantum dots.

Ballistic field effect transistors were realized based on a short metallic gate evaporated on top of a GaAs/AlGaAs modulation doped heterostructure with a highly mobile electron gas beneath the surface. Gate lengths down to 20 nm were reached with widths exceeding several tens of micrometers. This specific layout allowed to observe an new transport feature due to the ballistic motion of electrons in the non-linear transport regime. Detailed simulation with NANOTCAD tools demonstrated that this transport feature is universal for ballistic FETs.

3.5 Molecular Modeling

An approach similar in spirit to the scattering boundary conditions applied to single particle distribution functions is the time irreversible boundary conditions for the Wigner distribution function [22]. First the approach is presented for a one-dimensional self-consistent Schr\"odinger equation, and it will be shown how to extend the boundary conditions for correlated electrons in three-dimensional space. The boundary conditions are formulated in terms of the Wigner transform of the density matrix $\rho(x', x) = \psi^*(x')\psi(x)$, given by

$$f(q, p) = \int dr \rho(q + \frac{1}{2}r; q - \frac{1}{2}r) \exp(-ipr), \qquad (1)$$

with the change of variable $q = 1/2(x + x')$ and $r = x - x'$. The Wigner distribution function $f(q,p)$ has the advantage of echoing the properties of a classical distribution function (aside for the requirement of strictly positive probabilities). Time irreversible boundary conditions are applied to a domain $0 < x, x' < L$ by requiring $f(0, p > 0)$ and $f(L,p < 0)$ be constrained to their (local) equilibrium values. The device region is allowed to find a steady state by allowing the values of the Wigner function for $f(0, p < 0)$ and $f(L, p > 0)$ to vary. In this way, the properties of the reservoirs as ideal emitters and absorbers for particles, depending on the direction of their flow, is enforced. In essence, the single particle scattering conditions are applied through the Wigner variables q and p, respectively, which have as their *classical* limit the physical position and momentum.

The quantum many-body transport problem is formulated by making the following Ansatz: the appropriate many-body wave function in the device region minimizes the device energy $E_D = \langle \Psi | H | \Psi \rangle_D / \langle \Psi | \Psi \rangle_D$ while simultaneously satisfying appropriate open system boundary conditions (note H and Ψ are the full n-particle Hamiltonian and correlated many body wave function over the device region). In addition, boundary conditions on the many-body wave function in the absence of correlation are required to reduce to the time irreversible boundary conditions formulated for the one-particle density matrix. To achieve this requirement, the one-particle reduced density matrix

$$\rho(\mathbf{r};\mathbf{r}') = \int \Pi_{i=2}^{n} d\mathbf{r_i} \Psi^*(\mathbf{r}', \mathbf{r_2}, \ldots, \mathbf{r_n}) \Psi(\mathbf{r}, \mathbf{r_2}, \ldots, \mathbf{r_n}) \tag{2}$$

is introduced. The Wigner transform of this function is introduced over the spatial co-ordinate (taken to be the x-direction) of the net current flow across the device region. The net inward flow of Wigner momentum p at the reservoir boundaries q=0, p>0 and q=L, p<0 is determined by summing over each reservoir/device interface. This is equivalent to impose the reservoir properties after integration of the one particle reduced density matrix over planes normal to the net current flow

$$\bar{\rho}(x;x') = \int dydz \rho(x', y, z; x, y, z) \tag{3}$$

and applying the Wigner transform to $\bar{\rho}(x, x')$. The energy E_D is minimized in the presence of these time irreversible boundary conditions. By summing the Wigner momentum over the reservoir interfaces, the effect of the net inward equilibrium flow is constrained, and the planar momentum distribution at reservoir interface is allowed to vary within this constraint. This allows to the local distribution near the device to deviate from the equilibrium distribution maintained deep with the contacts, while maintaining the net inward equilibrium flow from the contacts.

Numerical Implementation

To implement the described procedure, the many particle wave function for the system is first expanded in terms of many-body expansion functions (spin-projected determinants)

$$\Psi(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_n}) = \sum_{\mu} c_\mu \Psi_\mu(\mathbf{r_1}, \mathbf{r_2}, \ldots, \mathbf{r_n}). \tag{4}$$

A one-body operator $\mathbf{F}^i$ whose expectation value in Ψ projects out the Wigner function at a given point in Wigner phase space (q^i,p^i) is defined:

$$f_0(q^i, p^i) = \left\langle \Psi_0 \,|\, \mathbf{F^i} \,|\, \Psi \right\rangle, \tag{5}$$

where Ψ_0 denotes the zero (equilibrium) current wave function for the system, i.e. the solution without applied voltage bias, and f_0 denotes the corresponding equilibrium Wigner function. A set of $f_0^{i'}$s at the reservoir boundaries $\{q = L, p^i < 0\}$ and $\{q = 0, p^i > 0\}$ are chosen and defined as constraints for the minimization of E_D, in addition to the constraint on particle number within the device region. To each constraint, a Lagrangian multiplier $\{\lambda_i, \mu\}$ is introduced and the following expression is minimized

$$\vec{c} * \mathbf{H}\vec{c} + \sum \lambda_i \vec{c} * \mathbf{F^i}\vec{c} - \mu \vec{c} * \mathbf{S}\vec{c} = \min \tag{6}$$

Applying standard methods to the constrained minimization problem leads to a many-body wavefunction defined on the device region miminumizing the energy and respecting the imposed boundary conditions. Varying the applied external electric field and calculation of the current allows for the determination of current-voltage characteristics across the device region.

State of the art

There has been substantial interest in recent years in extending the machinery of electronic structure theory, largely developed to study closed or periodic systems, to incorporate open system boundary conditions. A primary motivation for this work is the study of electronic transport for nanoscale systems and more specifically, to the study of molecular electronics [23,24]. Early approaches have combined elements of tight binding methods with non-equilibrium Green's functions or by solving a one-body Schrödinger equation for transmission coefficients, combined with an application of the Landauer Büttiker formula. However, it is well-known that electron correlation plays a crucial role in the study of molecular systems, and recent approaches have introduced density functional theory (DFT) methods to scattering or non-equilibrium Green's function methods. Notwithstanding this effort, the prediction of current as a function of applied voltage in molecular scale systems [26-33] remains one to three orders of magnitude larger than measured currents [23,25].

Central to the study of electronic transport is the concept of two reservoirs locally in equilibrium, but driven away from equilibrium with respect to one another. The resulting chemical potential imbalance is interpreted as the voltage driving a current across a device interacting with both reservoirs (reservoir-reservoir interactions are taken to be absent). Typically, scattering boundary conditions are introduced to define the properties of the electron reservoirs. One reservoir is associated with the emission of particles with left moving particles with fixed energy distribution, and is capable of absorbing right moving particles at any energy. Similary, the second reservior may completely absorb any distribution of left moving particles, but emits right moving particles with a fixed energy distribution. Implementing scattering boundary conditions to a system of fermions within a single particle approximation is straightforward. Fermi-Dirac statistics are applied to the reservoirs and a voltage is introduced as the difference in chemical potential between the left and right reservoir distributions. If this approach is applied with commonly used DFT calculations, several problems arise. First, the exchange-correlation functional is current dependent, a fact not explored to date within molecular electronic studies. Recently it has been pointed out that the currents theoretically predicted with DFT methods can vary by over an order of magnitude simply due to the choice of

exchange-correlation functional [33]. Even if practical exchange correlation functionals are developed, calculating scattering coefficients the system is driven away from the ground state, where the Hohenburg-Kohn theorem is simply not valid (i.e. there is no expectation that density functional theory will provide a correct answer). Another drawback is that application of a single particle distribution function to the Kohn-Sham eigenvalues is an ambiguous procedure, at best. Also, from this starting point, the path to obtain the classical limit yielding the Boltzmann transport equation remains unclear. Finally, for scattering approaches, a Schrödinger equation is solved to calculate transmission and reflection coefficients, and the application of the Landuaer-Büttiker formalism is made. This introduces a level of approximation difficult to control beyond the linear response regime; and indeed in most experiments the systems are driven far from equilibrium to study conductance properties over a wide range of voltages.

Non-equilibrium Green's function formalisms may be applied to the electronic transport problem, but these methods suffer too from drawbacks when applied to electronic transport on the nanoscale. In practice, their applications is hampered by the need for higher order Green's functions to handle highly correlated systems. Furthermore, issues for reservoir-device decoupling for the calculation of self-energies is difficult for realistic system Hamiltonians within Green's function formalisms.

In the approach to the electronic transport problem adoped within NANOTCAD, these issues are sidestepped by miminizing the energy of a region within a many-body basis (configuration interaction) with appropriate open system boundary conditions. Contact is made to the time irreversible boundary conditions advocated by Frensley [22] by re-formulating these boundary conditions in a manner appropriate to the case of correlated many-body wave functions. Application of the method leads to first calculation of current-voltage characteristics for a commonly studied system, the benzene di-thiol molecule bridging two gold contacts, within the same order of magnitude as experimental observations.

3.6 Molecular Nanofabrication

The methods used so far by various research groups for electrical contacting a small number of (or even individual) molecules fall into four main categories:

Mechanically controlled break junction. 1,4-Benzenedithiol molecules were self-assembled into a mechanically created gap within a gold wire [23]. Although this approach has provided evidence for electrical transport through single molecules, it is based upon an unstable mechanical structure which can not be electronically integrated. It further does not allow the implementation of a third terminal (gate electrode), nor to realise a four-probe configuration (which is necessary to separate transport through a molecule from the series resistance). Moreover, the cross-section of the gap structure is not small enough to allow a high yield of single-molecule contacts.

Electromigration break junction. Single-C_{60} transistors [34] or transistors incorporating individual molecular complexes [35,36] were fabricated by breaking thin gold wires via electromigration. To achieve that the corresponding molecules were self-assembled onto the wire surface prior to breaking. In addition to signatures of electrical transport through molecular states, electrostatic gating effects could be observed. Thus, transistor action was achieved for the first time in a structure which active component is a single molecule.

"Classical" sandwich configuration. A series of different small phenylene-based conjugated molecules has been investigated, as an active part of three terminal devices, with respect to gate action and reproducibility [25]. In this study, the top electrode was evaporated on top of the molecular monolayer self-assembled onto the bottom electrode. A sizeable fraction of the junctions showed short-circuits, and with some molecules the yield of intact junctions was even zero. Despite the close vicinity of the gate electrode (few nm separation), it was impossible to modulate current of the molecular junction by the gate potential. This result demonstrates one serious intrinsic problem related to the small size of phenylene molecules, *i.e.* electrostatic shielding from nearby electrodes suppresses the gate-induced field. Furthermore, the transport properties were found to considerably vary from sample to sample, reflecting a low reproducibility of the contact configuration.

Crossed-wire sandwich configuration. This contact configuration was realised by depositing pre-made palladium nanowires on top of the molecular monolayer self-assembled onto the surface of lithographically patterned bottom wires made of gold [37]. Since no metal evaporation is required for the deposition of the top contact, the formation of shorts was avoided, which allowed for a systematic investigation of memory effects using molecular wires with a three-benzene-ring structure.

Within WP6, two of the above techniques for contacting of molecules have been used. During the course of NANOTCAD, certain steps were further developed, which has led to several improvements in the application of these techniques.

(i) In case of the first contacting technique, the fabrication of crossed-wire sandwich junctions, assembly of the molecules was performed by a method which had not been used for that purpose before. Specifically, benzenedithiols were electrochemically deposited onto the bottom AuPd nanowire patterned by electron beam lithography. It is an important property of the electrochemical approach that the thickness of the deposited layer can be effectively controlled. This opens the possibility to determine the minimum thickness required to obtain a high yield of non-shorted junctions. It is known that evaporated metal atoms principally penetrate into an organic film up to a certain depth; accordingly, the minimum thickness of the film corresponds to the situation that the *effective* thickness of the (metal/organic film/metal) sandwich amounts to just one monolayer. At the same time the compact, thicker molecular film created by electro-deposition contains a much smaller density of defects (pin holes) as compared to a monolayer. These advantages largely simplify the fabrication scheme because evaporation at low temperature and ultra-small rates are not required. In effect, almost 100% yield of non-shorted samples could be achieved in this manner. The crossed-wire configuration allows for four-terminal electrical measurements, whereby any series resistance can be eliminated. On the other hand, one drawback of these structures lies in the fact that the molecules are completely shielded by electrodes, which severely limits the possibility of gate control over conductance.

(ii) Within the second contacting technique, employing nano-gaps produced by electromigration-induced breaking, the above described electrochemical deposition method proved also very useful. For that task, very thin (6nm height) and narrow (~15nm width) AuPd nanowires were used as starting

basis. Importantly, since the wire dimensions are smaller than those used in earlier works, the AuPd wires can be broken at voltages of only ~1.5V, which is small enough to ensure that the incorporated molecule is not damaged by the high electric field across the nano-gap. Electrochemical coating of the AuPd wires before breaking enabled effective trapping of phenylene-based molecules (benzenedithiols) during gap formation. Noteworthy, these dithiols are smaller than the molecules contacted before by other groups using the same technique.

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4. Main results and Achievements

Overview of main project results

No	Self-descriptive title of the result	Category A, B or C*	Partner(s) owning the result(s)
1	Development and release of NANOTCAD1D, NANOTCAD2D and NANOTCAD3D simulation programs for nanoscale semiconductor devices	A	DII-IET PISA
2	Development and release of a code for the simulation of transport through single molecules	A	NMRC CORK
3	Development and release of the SIMNAD code and coupling with standard semiconductor simulation codes (DESSIS).	A	ETHZ Zürich
4	Development and release of VMC: a code for Monte Carlo simulation of quantum transport.	A	TUV Vienna
5	Fabrication and characterization of Flash Memories with a single and a double layer of quantum dots.	A	UWUERZ Würzburg
6	Fabrication of two-terminal molecular devices and assessment of techniques for contacting single molecules	A	MPG Stuttgart
7	Characterization and demonstration of a universal signature of ballistic transport in nanoscale field effect transistors.	B	UWUERZ Würzburg DII-IET Pisa
8	Dissemination of tools developed within the project outside the project consortium and support to external users	A	DII-IET Pisa TUV ETHZ NMRC

* A: results usable outside the consortium / B: results usable within the consortium / C: non usable results

Result 1: Development and release of NANOTCAD1D, NANOTCAD2D and NANOTCAD3D simulation programs for nanoscale semiconductor devices

Three programs have been developed for the simulation of semiconductor nanostructures in quasi-equilibrium conditions in one-, two-, and three-dimensional domains (NANOTCAD1D, NANOTCAD2D, NANOTCAD3D, respectively). All codes are based on the solution of the many-body Schrödinger equation with density functional theory, local density approximation, and allow subdivide the domain in several regions with different types of quantum confinement, providing a reasonable level of flexibility. In addition, NANOTCAD2D also allows to simulate ballistic FET both in the III-V and in the Si-SiO2 material system.

During the project duration such codes have allowed to simulate several nanoelectronic devices fabricated within and outside the project, and to gain important insights into the transport mechanisms of such devices.

Particularly interesting results have been obtained in the simulation of quantum dot flash memories, both in the silicon-silicon oxide and in the AlGaAs-InGaAs material systems, of single electron transistors, of silicon-germanium quantum wires and of ballistic field effect transistors. To provide some examples, Fig. 2 shows the typical structure of a silicon nanocrystal flash memories considered in a simulation and the relevant results as far as the stationary electrical properties of the device are concerned, i.e. chemical potentials and electron density in the channel as a function of the gate bias and of the number of electrons stored in the dots; Fig. 3 shows results from the simulation of a so-called "well tempered" MOSFET with channel length of 25 nm, used as a benchmark structure for comparison of different simulation methods.

With respect to initial project objectives, several additional results have been obtained. Indeed, the simulation of nanoscale field effect transistors was not present among original objectives, but was included in the course of the project since after the first year it was very clear that the formalism and the tools developed for other ballistic devices such as quantum point contacts could be easily extended to include FETs. In addition, a model for mesoscopic transport in the presence of decoherence, that was not an original objective of the project, was developed in order to obtain a better agreement with experiments as far as the simulation of transport in coherent or quasi-coherent devices is concerned. On the other hand, the three-dimensional codes are not as fast as initially expected. This aspect actually limits the possibility of using them as a design tool, since it makes a detailed exploration of the design space unpractical.

Sinergy with other european and national projects has been very fruitful for access to experimental data, in particular with the EU project ADAMANT, aimed at the development of silicon nanocrystal memories, and mainly focused on large scale fabrication and reliability aspects, and with the Italian Ministry of Research project "Single Electron Devices".

If nanotechnology will acquire industrial and economic relevance, it will strongly depend for its development on reliable Computer Aided Design tools, in the same way as Microelectronics relies upon TCAD tools. In that case, a broad basis of expertise in the development of CAD tools for nanotechnology - firmly established in Europe - would represent a real competitive advantage, with significant impact in terms of economic development and employment. NANOTCAD codes are tools for research and prototyping, but we believe their development has helped creating the necessary expertise on which a possible industrially oriented successor of the NANOTCAD project could be based.

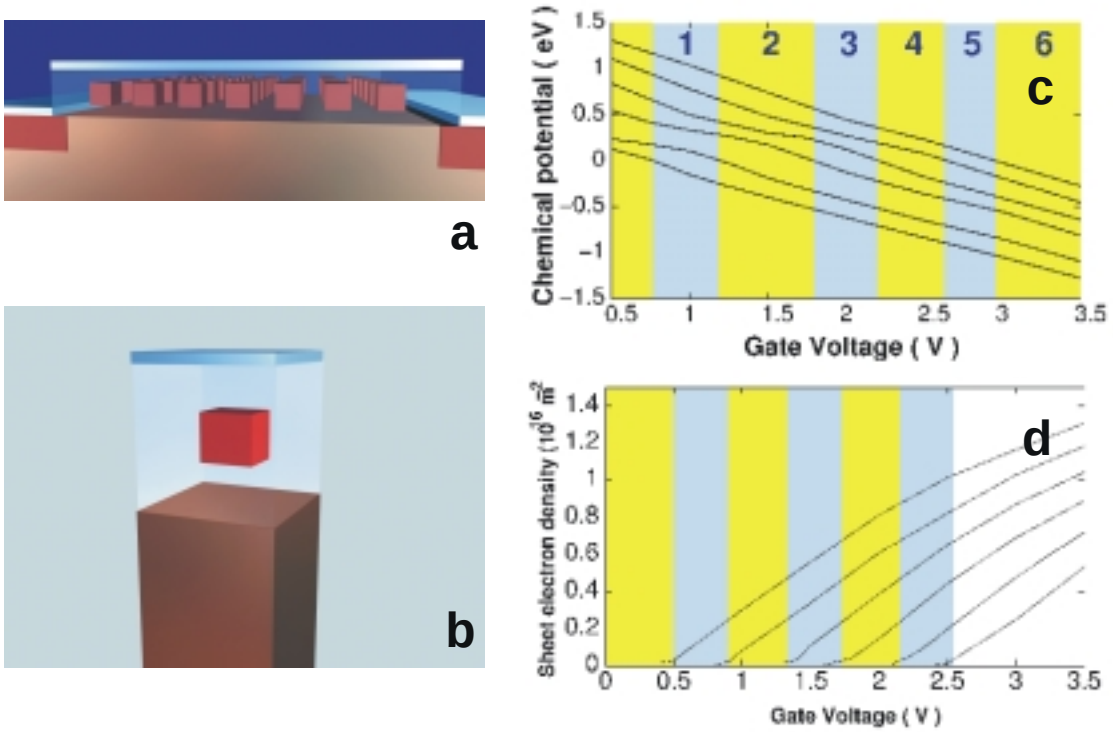

Figure 2: Simulation of silicon nanocrystal memories with NANOTCAD3D: a) simplified structure of a nanocrystal memories, in which disorder in nanocrystal size and density has been removed; b) elementary periodic cell considered in the 3D simulation; c) chemical potential of the dot as a function of the voltage applied to the top gate for number of electrons in the dot ranging from 1 to 6; d) two-dimensional electron density at the Si-SiO2 interface as function of the gate voltage for an increasing number of electrons in the dot, from 0 to 5.

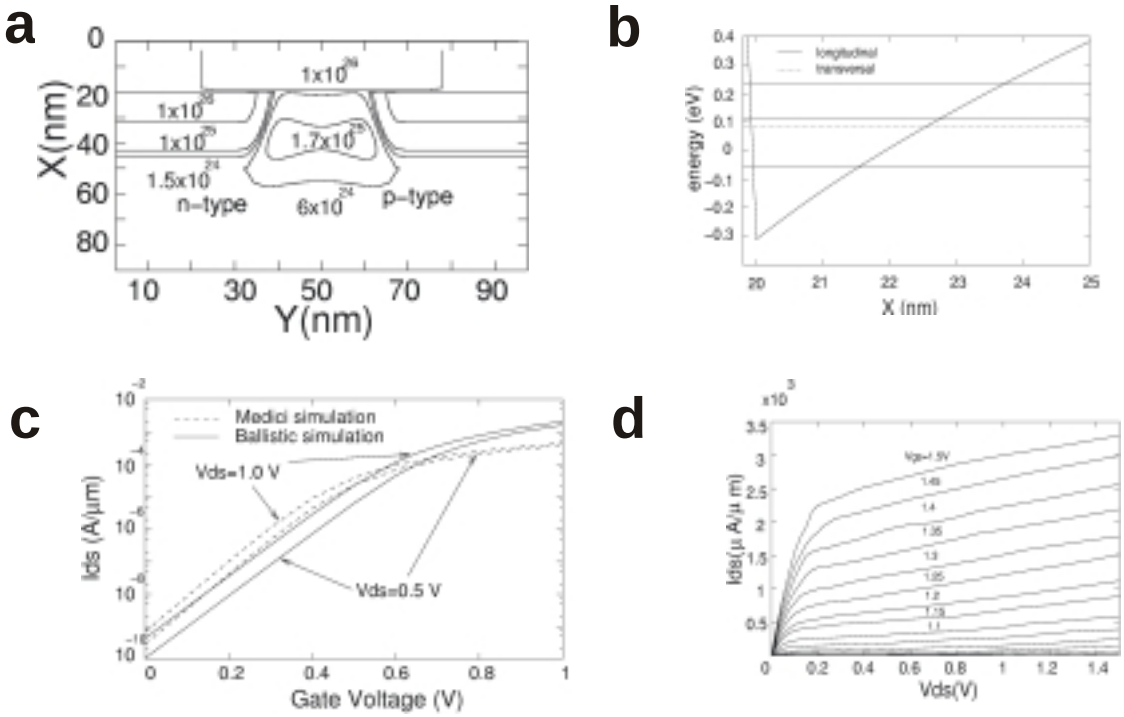

Figure 3: Results from the simulation of the 25 nm "well tempered" MOSFET: a) doping profile of the device; b) conduction band profile and energy levels of the two-dimensional subbands in the middle of the channel, from which the very strong quantum confinement is apparent; c) comparison between the transfer characteristics computed with the ballistic code and those obtained from simulations with the commercial simulator Medici; d) output characteristics of the device.

Result 2: Development and release of a code for the simulation of transport through single molecules

A physical formalism has been constructed and implemented in the computer code package `VICI` which provides the capability to simulate two and three temrmineal molecular devices. The name `VICI` stands for *Voltage Current (I) in Configuration Interaction*. The two programs in the package are: `analytic_integrals`, a prerequisite integral generation code; and `iv_Wigner_lm_penalty_function`, the two- and three-terminal device simulator.

These codes are complex in internal operation but are based on a simple underlying physical formalism which minimises the number of adjustable parameters. What is most singular about these codes is that they operate genuinely at the *many-body* level: they do not rely on Density Functional Theory (DFT), an exchange-correlation functional, a Hartree potential or any Poisson-Schrodinger self-consistent cycle. They deal with *N*-electron many-body wavefunctions Ψ, and calculate matrix elements and expectation values of many-body operators exactly. The reason for the decision to attempt to implement a many-body formalism is that, since the beginning of the NANOTCAD project, the state-of-the-art in molecular transport calculations has evolved considerably from a simple tight-binding approach to an *ab initio* DFT-based method: the two most well-known methods are by M. Di Ventra et al. [Phys. Rev. Lett. **84** 979 (2000)] and K. Stockbro et al. [Comp. Mat. Sci. **27** p. 151 (2003)]. To produce a third usable code at this level would have been a significant achievement by itself, but the fact of the matter is that even with these state-of-the-art approaches, there are large (2--3 orders of magnitude) discrepancies between theoretical predictions and experimental measurements of IV characteristics of single molecules (see mentioned paper by Di Ventra), and substantial disagreement even between these leading single-electron theoretical approaches. This motivated the decision to go substantially beyond all present formalisms and do a proper, first principles, treatment of the electronic motion of a current-carrying molecule. Even the very first runs of version 1 of the many-body code, in contrast, obtained the correct order of magnitude of the electric current flowing through the well-studied molecule benzene-1,4-dithiol.

The two programs developed within NANOTCAD require three preliminary calculations, two at the Density Functional Theory/Hartree Fock level (DFT/HF) and one at the Configuration Interaction (CI) level. An initial DFT/HF run is a standard requirement for all popular accurate many-body methods like CI or Quantum Monte Carlo (QMC), and there are many experienced research groups throughout the world who can perform such a calculation. Because the transport code is based on the CI formalism, the user would be well advised to spend some time learning the fundamentals of this approach to many-body theory. Once this is done, running the third preliminary calculation using the CI code `mcci` should not be too difficult.

Both the `VICI` codes are governed by user-friendly control files: in the case of `analytic_integrals` this can be simply one line in length. The transport code proper `iv_Wigner_lm_penalty_function` has a control file with more options, relating to the range of the applied bias, the gate field magnitude and direction, the number and position of the Wigner function constraints which capture the scattering boundary conditions, and some minimisation parameters for solving the central non-linear constrained optimisation problem. Compared to the typical number of parameters needed in running a DFT/HF calculation using a program suite like `TURBOMOLE` [R. Ahlrichs et al. Chem. Phys. Lett. **162** pp. 165-169 (1989)], this control file is very short, showing the simplicity of the underlying physical scheme.

Both the applied bias and the gate field are included exactly in the quantum mechanical many-body Hamiltonian, and the electric current is calculated exactly using the probability current density operator. What makes `VICI` code singular, as mentioned above, is that the exact matrix elements of the hard part of the Schrodinger equation-the electron-electron Coulomb repulsion- are included. Thus, it is possible, in principle, to find the *exact* solution of the Schrodinger equation for a molecular system: this is the main strength of CI, and therefore of the `VICI` package which is built on the CI formalism.

The code has been tested on a 38 atom gold cluster-benzenedithiol-gold cluster test system that has been well studied in the literature, of overall length 1.8 nm, obtaining on the very first runs currents of the same order of magnitude as experiment, and scaling up of the code in future versions is planned, so that larger systems can be studied. The main aim here is to simulate, atomically and with many-body accuracy, devices of the size of the commercial transistors of 5-10 years time, when the minimum feature size of the transistor should reach a few tens of nanometers or less. As already the exact Hamiltonian is included in the problem, there are no extensive changes to the code required in order to study Coulomb blockade, dopant fluctuations, or any other of the quantum effects that semiconductor companies are currently concerned about.

The deliverable codes are modular in form, use dynamically allocated arrays, and are written in Fortran 90. Therefore, it will be easy to update the code, adding new features or improvements to the optimisation engine: for example, in addition to the present conjugate gradients method, it is planned to include a limited memory Broyden-Fletcher-Goldfarb-Shanno quasi-Newton minimisation algorithm for improved efficiency in the unconstrained minimisation that takes most of the total CPU time. These codes are also extensively commented, and because they use dynamically allocated arrays, have fewer user-specified parameters and make efficient use of system memory. They are also simple to use, and it is easy to graph both the final results and various intermediate quantities like the Wigner function so as to ascertain that the constrained optimisation routine is indeed finding the constraint-obeying minimum of the energy. They are optimised so that operator data that depend only on a particular molecular structure are calculated once in the initial run on this geometry, and then written to disk as files. Subsequent IV characteristic calculations of the same molecular system then simply read in these operator ingredients from the files, thus speeding up the calculation to the maximum extent possible and increasing usability and convenience for the user. Consistency and error checks in some detail are made on the quantities read in from the control files and from the data files from the preliminary calculations, so that user errors are more likely to be spotted and reported by the program.

Comparision to original planned work

The original plan for the molecular electronic transport work was to to generate a Hückel (tight bonding) model for electronic transport. To extend the state-of-the-art at the time, external electric field gating would be included into the tranpsort code by including parametrized matrix elements. However, the development of transport simulators saw significant development during the early years of the NANOTCAD project.

The most notable developments was the inclusion of more advanced treatment of electronic structure into then newly written transport codes in the form of density functional theory. However, this seemingly more fundamental treatment still do not

improve the theoretical prediction of current-voltage characteristics as compared to experiment. This led to an analysis of the methods being applied, and to the identification of many approximations being made that were either uncontrollable or poorly justified. Therefore it was dediced to backtrack and propose a much more fundamental approach to the electronic transport problem, really on as few approximations as possible.

This led to a revision of the original work, where the original electronic structure methods to include in the transport code would be based on direct solutions of the Schrödinger equation - the configuration interaction method. The advantage of this approach was the ability to control approximations to the electronic structure, independent of the transport issues.

The original goals of developing two- and three- terminals were retained, but the intent of the new revisions were to allow us to better the state-of-the-art in terms of the accuracy of predicting transport properties.

Relationship to other projects

Molecular electronic transport predicition is a goal for many Future and Emerging Technologies projects within the Nanoscale Information Devices inititive, including BIOAND, NICE and related projects in Quantum Information Processing and Communication initiative, such as QIPDDF and ROSES.

Furthermore, the ability to predict electronic transport on the nanoscale is relavant to IST projects concerned with the development of Ultimate CMOS technologies, whereby accurate quantum mechanical simulation is required for device design.

Implications for EU Policies and Standards, Benefits to Society

Currently, theory and experiment for molecular electronic transport are difficult to reproduce. This statement applies to the repeatability of measurements, agreement between different theoretical treatments, and as well the agreement between theory and experiment. By producing a theoretical treatment that is parameter and approximation free, it will be possible to define repeatable and stable measurements of currents for atomic scale devices. This will lead to the establishment of standards for the relationship of molecular and atomistic structure on electrical (current voltage) characteristics.

Once these standards are established, and a firm understanding of device design on atomic scale dimensions is established, future technology generations extending beyond ultimate CMOS limits will be enabled. This will help to establish information and communication technologies extending past Moore's law, allowing for continued development of ICT for the Networked Society, and bring the societal benefits associated with this continued development.

Result 3: Development and release of the SIMNAD code and coupling with standard semiconductor simulation codes (DESSIS).

Comparison to original objectives

The original objectives were stated as follows: The objective is the integration within the NANOTCAD framework of the ability to simulate hybrid devices consisting of conventional MOSFETs and single-electron transistors (SET). A common simulation environment for both drift-diffusion (DD) based devices (MOSFET) and single-electron tunneling devices would significantly enhance the modeling capabilities of standard TCAD tools in the nano range, which has up to now been out of scope for

DD simulators. At the same time this would help in advancing new device principles as single-electron tunneling and in selecting the most promising designs for further applications.

With the substantial enhancements of the capabilities of the SET simulator SIMNAD and the coupling to the commercial device Simulator DESSIS$_{-ISE}$ this goal has been reached. SIMNAD (SImulator for NanoDevices) is a quantum mechanical 3D simulator for semiconductor devices based on a temperature-dependent effective mass formulation of density functional theory. It can be used to compute the self-consistent quantum mechanical charge density in semiconductor nano-structures, and can handle both direct gap materials (like III-V semiconductors) and materials with a silicon-like six-valley band structure and anisotro-pic effective mass. SIMNAD can calculate the full 3D wave function in MOSFET channels and SET leads based on the scattering matrix method with open boundary conditions. This can be used to compute the tunnel probabilities in SETs. Conductances computed by SIMNAD are either tunnelling conductances (e.g. in single-electron transistors) or quantum-ballistic conductances (e.g. in quantum point contacts or ballistic MOSFETs). SIMNAD uses a conductance model for Coulomb blockade devices based on the description by Beenakker (sequential tunneling). SIMNAD can also compute the coherent resonant tunneling current based on a modified Landauer-Büttiker formula. Currents through individual quantum point contacts can be obtained from a simplified ballistic tunneling model.

With a coupling-enabled version of the semi-classical device simulator DESSIS one can run simulations in coupled mode, i.e. SIMNAD will compute the quantum mechanical charge densities for band profiles provided by DESSIS$_{-ISE}$ and will communicate this data back to DESSIS$_{-ISE}$ for further processing (e.g. for use in a DESSIS$_{-ISE}$ self-consistency iteration). This enables the simultaneous modeling of a (3D) quantum-mechanical charge distribution in a sub-region of a larger device, which is under full operation. Such a methodology is unique and no other comparable simulation package is known. So far, only a non-self-consistent version is available, but the self-consistent version is being developed and tested. In the non-self-consistent version of the coupling scheme, the quantum-mechanical charge density from SIMNAD is frozen-in for a subsequent DESSIS$_{-ISE}$ solve without any feedback. In the self-consistent version, the Poisson solver of SIMNAD is deactivated and the quantum-mechanical charge density is computed with the fixed potential obtained in a DESSIS$_{-ISE}$ run with the previous quantum-mechanical charge. The iteration is continued until convergence. The two simulators communicate via semaphor files, where DESSIS$_{-ISE}$ requests an update of the quantum-mechanical charge if required.

Benefits to society

Semiconductor based single-electron nano devices both from III-V materials and from silicon represent a field of growing interest and a challenge in technology development. TCAD (Technology Computer Aided Design) is expected to become an increasingly valuable tool because of the immense difficulties (and costs) in producing nano-scaled devices with well-defined functionality. The following table from the Technology Roadmap for Nanoelectronics shows the expected development for SET (Single Electron Transistor) logic.

Year	2006	2012
Lithography	100 nm	50 nm
Feature Size	10 nm	< 10nm
Switching time	500 ns	100 ns
ft	~ 1MHz	~ 10 MHz
Gain	1	~ 1
Power dissipation	10 pW	~ 1 pW
Number of electrons	< 100	< 20

The SIMNAD-DESSIS$_{-ISE}$ coupling might lead to a commercial software product in the future, provided that solid-state based nano-electronics will reach an industrial level. On the other hand, the acquired knowledge of modeling quantization and coherent transport effects as well as of numerical techniques will have a strong impact on the development of the commercial device simulator DESSIS$_{-ISE}$ of ISE AG, in particular in the field of ultra-small MOSFETs, where certain quantum effects show up as unwanted features. DESSIS$_{-ISE}$ contains tools for the TCAD-oriented modeling of quantum effects. A great deal of the commercial success of DESSIS$_{-ISE}$ in recent years is founded on these new features. Main criteria for a commercial device simulator are flexibility, numerical robustness, and CPU time efficiency. However, a market analysis has revealed a saturation of consumer demand for the approximate quantum modeling tools. For the future it is of utmost importance to find new extensions and improvements of DESSIS$_{-ISE}$ that are on one hand compatible with the demands of electronics industry and, on the other hand significantly raise the market value of DESSIS$_{-ISE}$. Since the so far available quantum modeling tools in DESSIS$_{-ISE}$ provide only an approximate description of deep sub-micron devices, and because certain relevant questions about future CMOS cannot be answered at all with these models, the integrated SIMNAD-DESSIS$_{-ISE}$ package is of strategic importance. The necessity to model quantum effects on a sound physical basis is also given by the foreseen development in CMOS technology: SOI devices with ultra-thin silicon layers and ultra-short channels, which exhibit a truly three-dimensional distribution of charge density, potential, and current density, will become dominant soon. Customers will demand for 'first-principle' quantum transport models, since they will mistrust the above-mentioned approximate methods available today. This need for a physics-based simulation of quantum effects in advanced devices is further illustrated by the articles "Quantum Transport Simulation in Nanoscale and Double-Gate MOSFETs" and "Density Gradient Transport Approach to 3D FinFET", both to be found in the ISE News from December 2002.

Result 4: Development and release of VMC: a code for Monte Carlo simulation of quantum transport

A novel MC method for the solution of the Wigner-Boltzmann equation has been integrated in the one-dimensional device simulator VMC (Vienna Monte Carlo code). The concepts and features of the simulator, input deck and out files are described in a user's guide. The basic input quantity is the profile of the conduction band edge in the device. This profile can either be specified analytically in the input deck, or, for the purpose of a self-consistent simulation, be read from an input file, which is typically generated by a Schroedinger-Poisson solver. The simulator VMC is released by the Institute for Microelectronics, see http://www.iue.tuwien.ac.at. The simulator can also be accessed on the phantoms simulation hub.

The Wigner-Boltzmann equation for electrons in semiconductor devices is solved numerically by means of a novel Monte Carlo method. This equation describes both quantum interference and dissipation effects due to carrier scattering. The methodology for deriving the method is summarized in the following. The integral form of the Wigner-Boltzmann equation is used as a starting point for. The kernel of the adjoint equation has been decomposed into a linear combination of conditional probability densities. These densities representthe transition density used for the construction of numerical trajectories. The properties of the transition density employed allows a particle picture to be introduced. In this picture dissipation and interference phenomena are taken into account by two alternative processes involving quasi-particles. Dissipation caused by interaction with phonons and other scattering sources is accounted for by drift and scattering processes corresponding to the semi-classical Boltzmann transport picture. Interference effects due to the Wigner potential are associated with generation of pairs of particles having statistical weight ±1. The classical force term is separated from the Wigner potential and included in the Liouville operator. With this modification, the developed model corresponds to a Boltzmann equation augmented by a generation term. The challenge of employing such method is to handle the avalanche of numerical particles properly. The problem has been solved for stationary conditions: Particles of opposite weight and a sufficiently small distance in phase space are continuously removed in the course of a simulation. The cancellation is due to the fact that such particles have a common probabilistic future but opposite contribution to the statistics.

Comparison to the original project objectives:
The simulator has been developed in accordance with the project objectives. More efforts than anticipated have been put in the development of suitable a variance reduction technique. Such technique turned out to be indispensable since the so-called negative sign problem would lead to an exponential increase in variance as function of time. Various techniques have been devised and tested.

The novel MC method has been validated by comparison with NEMO-1D, a well-known simulator based on the non-equilibrium Green's function technique and developed in the US. Different types of resonant tunneling diodes have been used as benchmark devices. In some cases phonons scattering is found to play an important role, as predicted by both simulators. Simulation results are also compared with measurements of a RTD fabricated and characterized within this project by UWUERZ. Reasonable agreement is found for the resonance voltage and peak current density.

Support the future growth of European industry:
Software developed in the US and funded by national US agencies is often not available outside the US. Especially NEMO-1D, which has been specificly developed for the design of high performance RTDs, is protected intellectual property and cannot be obtained outside the US. The tools developed in NANOTCAD are therefore a valuable design aid to be used by European industry and research institutions.

Result 5: Fabrication and characterization of Flash Memories with a single and a double layer of quantum dots

Not yet publicly available. Material under consideration for publication.

Results 6: Fabrication of two-terminal molecular devices and assessment of techniques for contacting single molecules

Not yet publicly available. Material under consideration for publication.

Result 7: Characterization and demonstration of a universal signature of ballistic transport in nanoscale field effect transistors

Not yet publicly available. Material under consideration for publication.

Result 8: Dissemination of tools developed within the project outside the project consortium and support to external users

The NANOTCAD package has been developed as a hierarchical set of tools. All tools have been prepared and freely delivered to the nanoelectronics community through the PHANTOMS Simulation Hub (www.phantomshub.com) or, in the case of one code using proprietary routines (SIMNAD), are freely available to those institutions with a licence of ISE-TCAD. Comprehensive manuals have been prepared for all tools and available for download on the project site (nanotcad.iet.unipi.it) and on the PHANTOMS hub. In addition, a tutorial session on tools developed within NANOTCAD will be organized during the NID Workshop in Cork, and a presentation with a tutorial part on NANOTCAD tools will be given at the International School MIGAS ``Towards Nanoelectronics" held in Autrans 14-20 June 2003.

In addition, a series of collaborations have been established with experimental groups not participating to the present project, in order to validate the tools with a broader set of experimental data and to make the results available to the nanoelectronics community already before the end of project.

The structure of the NANOTCAD package is shown in Fig. 10:

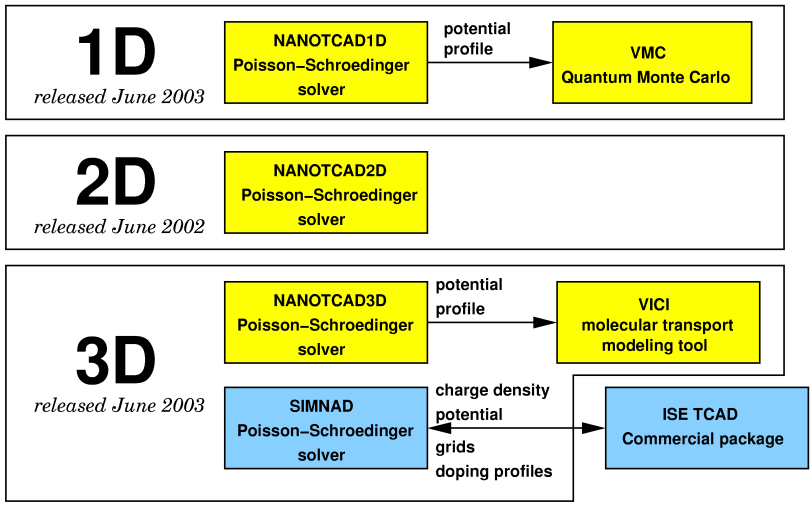

Figure 10 Structure of the NANOTCAD set of tools

1D
One dimensional simulations may be performed with the Poisson-Schrödinger (PS) solver NANOTCAD1D and with the quantum Monte Carlo code VMC (Vienna Monte Carlo). NANOTCAD1D computes the self-consistent potential, charge density profiles, and the current through one or more barrier layers. VMC reads the potential profile from the PS solver and computes the terminal current and distributed quantities such as charge density, mean energy, and mean velocity, by taking into account phonon scattering. Typical run time of NANOTCAD1D is in the order of few minutes, while the much more physically detailed VMC has simulation times ranging from hours to a few days.

2D
Two dimensional simulation of the Poisson-Schrödinger equation and of the continuity equation for the ballistic current in 2 dimensions can be performed with NANOTCAD2D. It can be used for the simulation of quantum wires and of ballistic field effect transistors.

3D:
Available tools for the three-dimensional simulations of semiconductor structures are NANOTCAD3D, which is available to the general public through the PHANTOMS hub, and SIMNAD, that will be made freely available to institutions with a license of the ISE-TCAD package. NANOTCAD3D is a 3D Poisson-Schrödinger solver, in which several regions with different degrees of confinement can be defined, and structures described in the present and the preceding report can be simulated (QD memories, SETs, FETs, etc..). SIMNAD is a 3D PS solver which can be coupled to a commercial drift-diffusion simulator, and allows to simulate devices containing both quantum confined regions (e.g. quantum dots) and regions in which transport is described by the drift-diffusion model. Simulation of transport through a single molecule for a given contact-molecule-contact system is performed with the newly developed VICI program. VICI relies on physical model that can treat electron-electron interaction to an arbitrary accuracy, and goes beyond linear response allowing the investigation of transport in far from equilibrium conditions.

5. Complete table of Deliverables

COMPLETE TABLE OF DELIVERABLES

Project Number: **IST-1999-10828**

Project Acronym: **NANOTCAD**

Title: **NANOTechnology Computer Aided Design**

Del. No.	WP	Title	Type[1]	Classification[2]	Due Date	Issue Date
D1	**4**	Split gate double quantum dot available for measurements	**D**	**IST**	**6**	**6**
D2	**1**	Report on exposed surface states and on quantization in GaAs-based heterostructures and on their numerical treatment.	**R**	**IST**	**12**	**12**
D3	**3**	Algorithms for complete set of transport equations	**R**	**IST**	**12**	**12**
D4	**2**	Quasi-equilibrium simulator of Si-based SETs including two-terminal linear-response transport modeling capabilities. Example library for various kinds of device structures fabricated outside NANOTCAD.	**D**	**IST**	**12**	**12**
D5	**2**	Simulation interface formulation and implementation	**R**	**IST**	**12**	**12**
D24	**10**	Dissemination and use plan	**R**	**IST**	**6**	**6**
D27	**10**	Project Presentation	**R**	**Pub.**	**3**	**3**
D28	**10**	Project web site	**R**	**Pub**	**6**	**6**
D29	**8**	Three dimensional simulation of quantum dots, fabricated within other projects in MELARI or NID	**R**	**Pub.**	**6**	**6**
D8	**1**	Design of a QD-HFET based on detailed simulations	**R**	**IST**	**18**	**18**
D15	**1-3**	Simulation of a GaAs resonant tunneling diodes with a 1D Poisson Schroedinger solver	**R**	**IST**	**24**	**24**
D32	**2**	Simulation of a single electron structure on the AlGaAs/GaAs heterostructure.	**R**	**IST**	**24**	**24**
D33	**2**	Simulation of a silicon single electron structure fabricated in other projects.	**R**	**IST**	**24**	**24**
D14	**3**	Full test and evaluation of the algorithms. Simulation of resonant tunneling diodes fabricated in Würzburg and comparison with the simulations performed in Pisa.	**R**	**IST**	**24**	**24**
D9	**4**	Short channel (30 nm gate length) HFET	**R**	**IST**	**18**	**18**
D34	**4**	Resonant tunneling diodes fabricated and characterized.	**R**	**IST**	**21**	**21**
D13	**4**	Report on quantum dot flash memory technology and measurements	**R**	**IST**	**24**	**24**
D7	**5**	Simulator of a molecular device immersed in a scalar potential defined on a three-dimensional grid. First results.	**R**	**IST**	**24**	**24**
D31	**6**	First electrical transport characteristics of single molecules in ultrasmall gap (< 2 nm)	**R**	**IST**	**24**	**24**
D10	**7**	Definition of common description format and of a database of material parameters.	**R**	**IST**	**18**	**18**

D30	**8**	Simulation of molecular devices fabricated in other projects within MELARI or NID	**R**	**Pub**	**18**	**18**
D25	**9**	Dissemination of a first release of the NANOTCAD package with full documentation	**D**	**Pub**	**24**	**24**
D11	**1**	Design of a 2QD-HFET based on detailed simulations.	**R**	**IST**	**38**	**38**
D23	**2**	Release of the code including coupling with Drift-diffusion codes and of the full documentation	**R**	**IST**	**38**	**38**
D21	**3**	Monte Carlo module integrated in device simulator, documentation, and results.	**R**	**IST**	**38**	**38**
D19	**4**	Fabrication of 2QD-HFETs and characterization in terms of program, erase and retention times – report.	**R**	**IST**	**38**	**38**
D16	**5**	Refined simulator of molecular devices. Simulation of molecular structures (fabricated within WP6 or taken from the literature) and comparison with the experiments.	**R**	**IST**	**38**	**38**
D17	**5**	Three terminal molecular device simulator	**R**	**IST**	**38**	**38**
D18	**6**	Device properties of molecular nanostructures and single molecules: gate dependence, stability, and reproducibility.	**R**	**IST**	**38**	**38**
D20	**6**	Fabrication and characterization of second generation of structures with single molecule in ultrasmall gap	**R**	**IST**	**38**	**38**
D22	**7**	Complete NANOTCAD package delivered.	**R**	**IST**	**38**	**38**
D26	**8**	Dissemination of the final release of the NANOTCAD pac with full documentation	**R**	**IST**	**38**	**38**

1 *R: Report; D: Demonstrator; S: Software; W: Workshop; O: Other – Specify in footnote*

2 *Int.: Internal circulation within project (and Commission Project Officer + reviewers if requested)*
Rest.: Restricted circulation list (specify in footnote) and Commission SO + reviewers only
IST: Circulation within IST Programme participants
FP5: Circulation within Framework Programme participants

Pub.: Public document

6. Short description of the main deliverables

The main deliverables, highlighted in light grey in the above table, are briefly described.

D2: Report on exposed surface states and on quantization in GaAs-based heterostructures and on their numerical treatment

The accurate simulation of devices defined by split gates on AlGaAs/GaAs heterostructures requires the use of physical models in which surface states are taken into account, because of the proximity of the two-dimensional electron gas to the exposed surface. We propose to describe these states with a simple model based on two parameters: an "effective" surface work function and a uniform density of surface states per unit area per unit energy.
As a first step, we have extracted the values of those parameters from a set of test heterostructures purposely fabricated by the group in Würzburg within WP1. Then, we have included the model for surface states in our three-dimensional Poisson-Schrödinger simulator and have simulated a few split gate quantum point contacts (QPCs) fabricated and characterized in Würzburg on AlGaAs/GaAs heterostructures. Once the confining potential in the two-dimensional electron gas is computed, the conductance of a QPC is evaluated by means of a method based on recursive Green's functions. The agreement between experiments and simulations is very good, in

particular as far as the pinch-off voltages of the quantum point contacts are concerned, and represents a significant validation for our model of surface states. Finally, we have evaluated from a quantitative point of view the dispersion of pinch-off voltages due to the discrete distribution of impurities in the doped layer and of surface states. We have simulated an ensemble of QPCs with identical geometry and doping, but different "actual" distributions of impurities and surface states, obtained with a Monte Carlo algorithm. In such a way, we have obtained a standard deviation of the threshold voltage which is about a half of the experimental value, meaning tha the we have discarded other important sources of dispersion, such as, for example, tolerances on gate definition

D4 Quasi-equilibrium simulator of Si-based SETs including two-terminal linear-response transport modeling capabilities. Example library for various kinds of device structures fabricated outside NANOTCAD

The SET (single-electron transistor) simulator *SIMNAD* of ETH Zurich has been advanced and extended to silicon devices and geometrically defined confinements. Three Schrödinger equations for each pair of valleys are solved. The crystal orientation has to be <100> with respect to the SET transport direction. The level spectrum, charging curves, and the charge densities of silicon quantum dots can be calculated. To obtain the tunneling rates for the evanescent modes in the insulating barrier material, a simplified path integral method was developed. A small examples library of nano-scale devices manufactured outside the NANOTCAD project has been set up. It contains five devices, which have been meshed and simulated. (i) A GaAs/AlGaAs heterostructure with Schottky gates, where special attention was paid to the influence of the Schottky barrier under the gates and the Fermi-level pinning at exposed surfaces. (ii) A SiGe SET with a Ti/Al top gate confining electrons electrostatically within a 10 nm thick silicon layer. (iii) A part of a SOI silicon double dot with side gate. (iv) A SOI MOSFET with a silicon wire surrounded at three sides by a short poly gate. (v) A quantum dot FLASH EPROM with a nano-scale floating gate, which serves as test device for derivable 5. Results for these devices were presented in form of level spectra, conductance characteristics, charge density plots, charging curves, and capacities. Temperatures are in the range from mK to 300 K

D29: Three dimensional simulation of quantum dots, fabricated within other projects in MELARI or NID (month 6)

As far as quantum dot are concerned, we have used the three-dimensional Poisson-Schrödinger code developed within the project to simulate Silicon nanocrystal memories, which have recently attracted the interest of researchers in both academic and industrial laboratories. Nanocrystal memories consist of metal-oxide-semiconductor field-effect-transistors (MOSFETs) with an array of silicon nanocrystals (with diameter of 3-5 nm) embedded in the gate dielectric. Information is encoded in the MOSFET threshold voltage, which depends on the amount of charge stored in the nanocrystal layer. Nanocrystals are charged through direct tunneling of electrons from the channel. Such memories are promising in terms of shorter write-erase times, larger cyclability, and lower power consumption with respect to conventional non-volatile memories. We have shown results obtained from the self-consistent solution of the Poisson-Schrödinger equation on a three-dimensional grid, focusing on the charging process and on the effect of charge stored in the nanocrystals on the threshold voltage

D32: Simulation of a single electron structure on the AlGaAs/GaAs heterostructure (month 24)

A single electron structure on an AlGaAs/GaAs heterostructure fabricated and characterized by the group in Würzburg was simulated with the SET simulation package *SIMNAD* of ETHZ and compared with simulation results obtained by the group in PisaBecause of the possibly large numbers of electrons and single particle orbitals involved in GaAs devices, a Monte Carlo integration scheme for the free energies and Gibbs probabilities was developed and implemented in order to handle the computational expense for the explicit evaluation of the phase space average. The calibration of the surface pinning energy to a value, that yields the experimental conductance through the source/drain QPCs turned out to be crucial for a good simulation of the SET structure. The QPC was treated with a 2DEG-1DEG-2DEG quantization model, the floating gates being eliminated from the grid. The pinning energy was fixed in such a way that only one transverse mode remained in transmission. This value then was used for the SET simulation, where the full 2DEG-1DEG-0DEG-1DEG-2DEG domain decomposition was applied for the computation of charge densities, charging curves, and gate-to-dot capacities. From the derivative of the electron number in the dot with respect to the Fermi potential a gate-to-dot capacitance of 3.2 aF was extracted which exactly corresponds to the measured distance of the first two conductance peaks. It was found that the threshold voltage is very sensitive to the value of the surface pinning energy: 2 mV will change the electron number by 1 and, correspondingly, the threshold voltage by about 10 mV. Convergence at 300 mK turned out to be extremely poor, but rapidly improves with increasing temperature

D 33: Simulation of a silicon single electron structure fabricated in other projects

The SOI single electron transistor fabricated in Tübingen within the MEL-ARI FASEM project (APL 76, 2065 (2000)) was simulated with the SET simulation package *SIMNAD* of ETHZ and compared with simulation results obtained by the group in Pisa. Information on the structure orthogonal to the transport plane could only be inferred from the process description (e.g. stress limited oxidation) and the conductance characteristics. Different geometries were built (prismatic or semispherical dot geometry with half-cylindrical constriction regions) and their impact on the device characteristics was studied. An automatic construction scheme for 3D transfer Hamiltonians (in the spirit of Bardeen's transfer Hamiltonian) was developed and implemented to overcome spurious states localized in the artificial potential well between the tunneling barrier delimiting the active quantum dot volume and the hard-wall potential used for Dirichlet boundary conditions. This scheme searches for a saddle point in a quantum-mechanically modified potential which includes the transverse kinetic energy contribution of a localized electron. An improved connection condition in the overlap region between wire and quantum dot region was also implemented. The free energy computation was changed from an old version (Stopa et al., orthodox theory) to the actual free energy of the quantum dot with explicit calculation of the entropy. The linear response conductance of the SOI SET was simulated with constant tunneling rates assuming complete ionization of dopants. Extracted gate-to-dot capacities are in good agreement both with the measured values and the simulation results by the Pisa group. Both simulators also yield the same position of the first conductance peak, if the same ionization model is used.

D14:Full test and evaluation of the algorithms. Simulation of resonant tunneling diodes fabricated in Würzburg and comparison with the simulations performed in Pisa (month 24)

A Monte Carlo algorithm for the solution of the stationary Wigner equation augmented by the Boltzmann scattering term has been developed, implemented and evaluated. As opposed to semiclassical transport, where all particles have positive weight and the number of particles is conserved, in quantum transport particle weights are subjected to sign changes, and either the magnitude of the particle weight or the number of numerical particles grows exponentially with time. This so-called "negative sign problem" gives rise to very large variance in the Monte Carlo estimators. The evaluation of a plain quantum Monte Carlo algorithm revealed that the variance gets prohibitively large even for rather simple structures. As a consequence of this evaluation various variance reduction techniques have been implemented and evaluated. A new method based on trajectory splitting turned out to be successful. The Monte Carlo method has been developed to a mature state which permits simulation of realistic RTD structures. Results from the Monte Carlo method and the simpler Schrödinger-Poisson model from Pisa are compared. Effects visible in the first and neglected in the second method are the finite resistivity of the collector and emitter regions and the quantization in the accumulation region. The considered structure is a RTD fabricated and characterized in Würzburg. The I-V data near the first resonance has been simulated by both a coherent Monte Carlo and non-coherent Monte Carlo model, which includes inelastic scattering by phonons

D9: Short channel (30 nm gate length) HFET

In order to allow detailed modeling of field effect transistors (HFETS), we have fabricated HFETs with gate lengths varying from 200 down to 20 nm by high resolution electron lithography and mask techniques on GaAs/AlGaAs modulation doped heterostructures. Special emphasis was taken to realize extremely short gates covering a width of the HEMT structure along a length of 150 μm with width to length aspect ratios exceeding a factor of 6000. Thus the influence of gating by interconnects can be disregarded. The gate length is orders below the elastic free mean path of electrons in the 2DEG (~10 μm). The HFETs have been characterized regarding I-V traces, conductance and transconductance. We have been able to control the conductivity of the nanoelectronic HFETs by the short gates with a length of 20 nm. Pinch-off by ultrashort gates is demonstrated. Special care was taken to investigate a new feature of ballistic HFETs observed in the transconductance and related to a non local, ballistic resistance not observed before.

D13: Report on quantum dot flash memory technology and measurements

Regarding semiconductor nanofabrication within NANOTCAD the quantum dot HFET devices play a key role. Technology aspects starting from optimization of growth parameters, e.g., time sequences of temperature ramps in the effusion cells and substrates or composition of materials, as well as the gate layout, e.g., side gate technology, were discussed coherently with our theoretical partners and analyzed with NANOTCAD tools. Measurements of the QD HFETs were done in terms of characterization of the structural quality of the devices, e.g., luminescence, X-ray diffraction and electron microscopy, and determination of transport properties, e.g., current versus voltage characteristics. Within the second year quantum dots with one layer of self assembled InGaAs close to the conducting 2DEG were investigated. Depending on the charging state of the quantum dots the I-V traces were found to vary

drastically. Memory functionality related to a shift in the pinch off of 2DEG conductivity with nearby quantum dots with respect to the gate voltage sweep was demonstrated. Depending on the number of electrons confined in the InGaAs dots, the pinch off voltage is shifted up to 2 V compared to uncharged dots. A flash mechanism was demonstrated, which allows to charge and discharge the dots without illumination of the samples by controlled leakage of electrons from monolithically fabricated side gates into the dots and back. The report informs about: structure layout, fabrication details, transport investigations, characteristic times for write, erase and retention.

D31: First electrical transport characteristics of single molecules in ultra-small gaps (deliverable date: month 24).

A method was developed to fabricate crossed-wire sandwich junctions of ultra-small active area (~15x15nm^2), based upon the etching mask approach to nanowires which had been established during the first year of the project. First junctions incorporating a self-assembled monolayer of 1,4-benzenedithiol between two metal (AuPd) wires were obtained. The corresponding electrical transport data revealed a resistance of the order of 25kΩ at room temperature, which turned out to be due to shorts formed between the bottom and top metal contacts.

D25 Dissemination of a first release of the NANOTCAD package – month 24

A first release of the NANOTCAD package, consisting of a 2D Poisson-Schroedinger solver of semiconductor nanostructures, with a self-consistent solver of the continuity equation for ballistic current, has been put on the PHANTOMS simulation HUB. In this way, it is available to anybody connected to the InternetThe codes runs on a server located at the University of Pisa, and can be used with a simple browser, once the perspetive user freely registers to the website. A tutorial and a few examples are available at the NANOTCAD 2D page on the PHANTOMS simulation HUBTwo classes of devices may be simulated

1. Quantum wires, whose structure is completely determined by the cross section (i.e., structures with a translational symmetry). Parallel quantum wires, and regions in which different degrees of quantum confinement are present, can also be simulated.
2. Ballistic HFETs and MOSFETs, in which transport occurs along one of the axis represented in the 2D domain. The structure must have translational invariance along a dimension orthogonal to the current flux

D23 Release of the code including coupling with Drift-diffusion codes and of the full documentation – month 38

An interface between the commercial drift-diffusion (energy-balance) simulator *DESSIS*$_{\text{-ISE}}$ and the DFT-based SET simulator *SIMNAD* was implemented and the coupled simulation of a single-electron memory (SEM) with a quantum-dot floating gate embedded in a classical MOSFET was demonstrated. The quantum-mechanical (QM) charge density obtained from the solution of the 3D Kohn-Sham equations is passed to *DESSIS*$_{\text{-ISE}}$ for a full solve of the current continuity equations. Data sets of the two simulators are exchanged via interpolation on different grids in order to keep the advantages of the specific mesh. *DESSIS*$_{\text{-ISE}}$ in its latest release version was extended by several features, which facilitate the coupling to *SIMNAD.* In a non-self-consistent version of the coupling scheme, the QM charge density from *SIMNAD* is frozen-in for a subsequent *DESSIS*$_{\text{-ISE}}$ solve without any feedback. In the self-consistent version, the Poisson solver of *SIMNAD* is deactivated and the QM charge

density in the SEM dot is computed with the fixed potential obtained in a *DESSIS*$_{\text{-ISE}}$ run with the previous QM dot charge. The iteration is continued until convergence. The two simulators communicate via semaphor files, where *DESSIS*$_{\text{-ISE}}$ requests an update of the QM charge if required. A comprehensive manual of *SIMNAD* containing parts on the coupling to *DESSIS*$_{\text{-ISE}}$ is available

D21: Monte Carlo module integrated in device simulator, documentation, and results.

An optimized version of the quantum Monte Carlo (MC) algorithm has been integrated in the device simulator VMC (Vienna Monte Carlo code). A user's manual has been prepared, introducing the basic theoretical, physical and numerical concepts utilized in the simulator. The format of the input deck and the output quantities is described and examples are given. The basic input quantity is the potential profile of a device. This profile can either be either specified analytically in the input deck, or, for the purpose of a self-consistent simulation, be read from an input file. In this case the basic output quantity is the carrier density which can be used from a Poisson solver to recalculate the potential profile of the device. Experience about the features of the MC method has been collected by extensive simulations of different types of resonant tunneling devices (RTDs). The properties of the method regarding complexity, physical relevance and scope of applicability are analyzed. A comparison of the method with alternative quantum transport solvers such as NEMO-1D has been performed by joint simulations of benchmark RTDs. Simulation results are compared with measurements of a RTD fabricated and characterized within this project by UWUERZ. Good agreement is found for the resonance voltage and peak current density.

D19: Fabrication of 2QD-HFETs and characterization in terms of program, erase and retention times – report

Modulation doped GaAs/AlGaAs heterostructures with two layers of self-assembled InGaAs quantum dots imbedded in the undoped spacer were grown by molecular beam epitaxy. The samples were further processed by electron beam lithography and etching techniques to realize short channels with widths down to 50 nm. The design of the structure was composed in close cooperation with DIIEIT. Transport spectroscopy was performed to characterize double quantum dot flash memories. A large memory window with hysteresis exceeding several volts for gate voltage sweeps has been observed. Time resolved I-V traces were recorded for determination of characteristic time scales of the nanoscaled memory devices. Load and erase times down to a few microseconds were observed. At room temperature hold times larger than one hour were found.

D16: Refined simulator of molecular devices. Simulation of molecular structures (fabricated within WP6 or taken from the literature) and comparison with the experiments

We have written a many-body quantum mechanical transport code for calculating current-voltage characteristics of a given contact-molecule-contact system. Responding to developments in the state-of-the-art in transport calculations, we have attempted and achieved the development of a physical method and corresponding transport code which can treat the electron-electron interaction to an arbitrary accuracy (hence going beyond Hartree-Fock and Density Functional Theory) and which does not rely on the Landauer formalism (hence going beyond linear response). Our tests of this code on the well-studied system of the molecule benzenedithiol sited between two

gold electrodes has given us electrical currents which are within an order of magnitude of the experimental data, and which are two to three orders of magnitude more accurate than other widely cited theoretical calculations.

D18: Device properties of molecular nanostructures and single molecules: gate dependence, stability, and reproducibility (deliverable date: month 38).

The yield of non-shorted sandwich junctions, incorporating 1,3- or 1,4-benzenedithiol, could be improved via two different approaches. In the first case, the aromatic dithiol was embedded in a matrix of an aliphatic dithiol, which stabilizes the mono-molecular layer and helps to dilute the "active" (aromatic) molecules. The second method employed electrochemistry to deposit a molecular film of controlled thickness onto the bottom wire prior to attaching the top contact. This process allows to form multi-molecular layers of dithiols without altering the chemical nature of each molecule. Sandwich junctions prepared by either approach revealed a low-bias resistance of the order of 1GΩ at room temperature, and their low-temperature I/V characteristics displayed pronounced steps and/or kinks, which may be associated with tunneling through discrete molecular states. As a major complication, the voltage position of these features was found to vary from sample to sample. Moreover, the maximum gap width (~0.4V) seems too small to be in accord with typical HOMO-LUMO gaps in small organic molecules. For a given sample, on the other hand, the I/V traces proved to be quite stable, sustaining electric fields of up to ~10^7V/cm, as well as at least one temperature cycle (room temperature(RT)→2K→RT). Importantly, for all junctions under study, no gate effect could be detected (a back gate separated by 100nm of SiO_2 was used). This is attributed to strong electrostatic shielding, which constitutes an inherent problem of the contact configuration.

D20: Fabrication and characterisation of second generation of structures with single molecule in ultra-small gap (deliverable date: month 38).

Although ultra-small gaps (≤1nm) were made available within the first year of the project through electromigration-induced breaking of nanowires, the incorporation of benzenedithiol molecules into gap remained a serious hurdle. Within the third year, this limitation was overcome by using an electrochemical method to coat the nanowire with a dithiol multi-layer prior to breaking (the same electrochemical technique as was employed for coating the bottom wire within the sandwich junction approach). The I/V traces obtained at low temperatures after breaking the 1,3-benzenedithiol-coated wire exhibited step-like features which may be a signature of tunneling through molecular states. However, the width of the gap around zero bias was found to be surprisingly small (50meV). Identical to the case of the sandwich junctions, no gate effect on conductance was observed.

D22:Complete NANOTCAD package delivered

All simulation codes constituting the NANOTCAD package have been fully developed and delivered. As already discussed last year, the package is not a unique tool, but a hierarchical set of tools with different level of complexities and physical accuracy. In order to ensure broad dissemination of the NANOTCAD package, all codes, except SIMNAD, are freely available to the nanoelectronics community through the PHANTOMS simulation hub (www.phantomshub.com). SIMNAD is freely available to users with a license of the ISE-TCAD package. For each code, a comprehensive manual has been prepared, including the physical background, a description of the code capabilities and limitations, instructions on how to use it, and a

set of pre-prepared simulation examples.A tutorial course has been prepared and will be given during on June 24, during the NID workshop in Cork.

7. List of publications

7.1. Papers in peer reviewed journals

[1] P. Coli, G. Iannaccone, "Evaluation of performance and perspectives of nanocrystal Flash memories based on 3D quantum modeling", First IEEE Conference on Nanotechnology, vol. -, 140, Maui, Hawaii, USA 2001.

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Submitted papers

- G. Curatola, G. Fiori, G. Iannaccone, “Modeling and simulation challenges for devices at the end of the Roadmap”, submitted to Solid-State Electronics, 2003.
- G. Curatola, G. Iannaccone, “Two-dimensional modeling of etched strained-silicon quantum wires”, submitted to J. Appl. Phys., 2003.
- A. Schliemann, L. Worschech, A. Forchel, G. Curatola, G. Iannaccone, “Universal signature of ballistic transport in nanoscale field effect transistors”, submitted to Phys. Rev. Letters, 2003.
- X. Wang, J. J. Lee, G. Iannaccone, W. Bai, D. L. Kwong, “Demonstration of superiority of HfO2 high-k gate dielectric to SiO2 in Si nanocrystal flash memory devices using a 3D quantum simulation”, submitted to IEEE Electron Device Letters.

7.2. Proceedings of International conferences

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8. Future Prospects

8.1 Modeling of semiconductor nanodevices in the linear and in the ballistic regime

In the short term, two lines of research are foreseen. One consists in improving the physical models and the numerical aspects in order to fully include energy relaxation and dephasing without increasing the computational requirements, and make the code a real design tool, at least for well controlled technologies, characterized by quantitative reproducibility of the results and tight control of the process. The second line of research is represented by focusing on particular problems related to electron transport that can benefit from the use and/or customization of NANOTCAD tools. A partial list of these problems include understanding of mobility improvement in SiGe devices and of mobility degradation in MOSFETs with high-K dielectrics; definition of an architecture for MOSFETs capable of reaching the end of the Roadmap, control of phase coherence in semiconductor implementation of quantum computing, the 0.7 conductance anomaly in transport through quantum point contacts.

Collaborations with TCAD and semiconductor companies will be established in order to transfer some of the research results to industry.

8.2 Modeling of semiconductor nanostructures and coupling with DD codes

Continuing work on full coupling of DESSIS$_{-ISE}$ and SIMNAD, coupled simulation of QD FLASH EPROM:

In the self-consistent coupling version, the solution of the Poisson equation is completely deactivated in SIMNAD - only the computation of the charge density is active. Potential and density are read-in from files. With the given potential, SIMNAD computes the quantum-mechanical charge density in the quantum region. The two programs are linked via semaphor files, where the drift-diffusion simulator DESSIS requests an update of the quantum mechanical density if required. The iteration proceeds as long as convergence on the DESSIS side is achieved with the self-consistent SIMNAD charge.

The implementation of the self-consistent coupling version has to be finished and tested. Efficient test examples have to be defined, as well as samples with strong self-consistency effect.

Implementation of continuum strain model for Si-based QDs and SETs:

Recently, there has been great interest in devices making use of strained silicon, mainly in conjunction with silicon-germanium compound material, but also in nano-scale silicon-on-insulator (SOI) devices. Material strain is known to alter the band structure by introducing a valley-dependent energy shift. This can cause a redistribution of electrons between the different valleys, and - due to the different tunneling masses associated with different valleys - might have a pronounced effect on the conductance. The inhomogeneous strain field due to the lattice mismatch between Si-nc and SiO_2 will be computed according to the continuum strain model by minimizing the elastic energy of the system. It has to be shown how the effect of the Si-nc orientation compares with the strain effect on a Si-nc with (100) orientation.

Inclusion of multiple sub-bands and non-parabolicity:
Currently only the lowest transverse sub-band inside channel regions adjacent to a quantum dot participates in the conductance computation. While this seems adequate for III-V semiconductors, which exhibit a single valley band-structure, it is not suited for silicon-based devices with its six-valley band-structure: due to the different orientations of the anisotropic effective mass tensor for different conduction band minima, the lowest sub-bands associated with different mass orientations may cross as the channel cross-section varies along the transport direction. Thus, a 'lowest sub-band' cannot be uniquely defined, and any choice of a 'dominant' sub-band is arbitrary. Different valleys will typically see different resonance energies, and the 'lowest lying' sub-band is not necessarily the one that dominates transport, since it may be off-resonance. In the case of strong geometrical confinement, the splitting of the lowest sub-band from the bottom of the conduction band may be so large that the assumption of parabolic bands can produce a large error. The standard non-parabolicity model is thus expected to improve the modelling.

Magnetic field effects:
SIMNAD is a software project under continuous development. A straightforward extension is the implementation of LSDA (Local Spin Density Approximation). Based on this implemen-tation, the spin polarization effect on the conductance spectrum of III-V-based quantum dots should be demonstrated.

8.3. Quantum Monte Carlo Modeling of nanoscale devices

At present, the simulator VMC can be used as is in education and research. Not only does it give integral quantities such as the terminal current, but also insight in distributed quantities within a quantum device.

RTDs are good test devices to study the capabilities of the novel quantum MC method. However, the function of an RTD is dominated by quantum interference effects, such that in many cases other methods than the MC method are more suitable and computationally efficient, for instance, a Schrödinger-Poisson solver or a Green's function solver.

A wide field of application for the MC solver is the quasi-ballistic transport regime occurring in down-scaled devices. This regime is rarely investigated in the literature, mainly because of a lack of proper numerical methods. Instead, nowadays it has become very popular to study the ballistic limit of various devices using a Schroedinger solver. Such study can give an estimate for the upper limit of device performance, but can be very poor in predicting the actual device performance. Since the novel MC method describes quantum effects and scattering effects with equal accuracy it is believed to be a predictive tool whenever some kind of quasi-ballistic

conditions are present. Both limits, namely the scattering dominated classical case and the pure quantum case are treated properly. Typical applications are MOSFET in the scaling limit, where source to drain tunneling starts to contribute to the current, bipolar devices with very thin base barriers, or tunneling through hetero-barriers and dielectric barriers. A future prospect of quantum MC modeling is therefore likely to be in classical device modeling, where with ongoing down-scaling more and more quantum effects have to be taken into account.

8.4. Semiconductor Nanofabrication

Due to the progress in nanofabrication technologies of semiconductors complex shaped structures with features sizes smaller than characteristic scattering lengths, we will be allowed to enter the regime of ballistic effects at room temperature. Thus, we believe that ballistic non-linear transport properties including switching, amplification and rectification represent the basics for novel concepts of nanoelectronic devices with a higher integrated functionality.

8.5. Modeling of transport through molecules

The development of a bottom up approach simulation approach for technolgy design allows for the understanding and virtual prototyping of new electronic device concepts. The molecular scale simulators need to be scaled from the approximately 1 nanometer range up to approximately 10 nanometer to 20 nanometer range where ultimate CMOS devices will reach their final limits, or at least their anticipated final limits. Once this overlap between end-of-the-roadmap device technologies and molecular scale simulation is achieved, truly novel new device architectures and circuits may be explored.

8.6. Molecular nanofabrication

The two methods employed for single-molecule contacting (crossed-wire sandwich junctions comprising electrochemically deposited molecules; molecules trapped into ultra-small gap structures by electromigration-induced breaking of electrochemically coated nanowires) are certainly worth to be applied also to larger molecules. The benzenedithiols used within this project have a length of less than 5Å and are thus much harder to contact in a controlled manner, as compared to spatially more extended molecules such as C60 with a diameter of ≈ 1nm [H. Park *et al*, Nature **407**, 57 (2000)], or oligo(phenylene-ethynylenes) [J.G. Kushmerick *et al.*, PRL **89,** art.no.086802 (2002)] with a length of approximately 1nm. The electrical characterization of this type of molecules would provide data urgently needed to independently test the reproducibility of the results obtained by other groups.
Moreover, it is of strong interest to further evaluate the application potential of the electrochemical method that has been optimized to deposit ultra-thin molecular films onto metallic nanowires. Our very recent studies have shown that, in addition to the dithiols, also aromatic rings bearing two amino-groups can be electrochemically deposited. Although in the latter case, the molecules become slightly modified (primary amino groups are converted into secondary amino groups), they offer the advantage that the amino groups (when protonated) are well-suited to attach negatively charged counter ions which could add additional functionality (e.g. magnetic properties) to the junctions. Thus, the formed film could be an ideal matrix to incorporate a wider range chemical species that cannot be assembled into the ultra-small gaps by other means.

With respect to the impossibility of controlling the conductance by an applied gate potential, as experienced within this project as well as in the recent work of other groups [J.-O. Lee at al., Nano Letters 3 (2003), 113], it is hard to imagine real improvements. This is due to the problem of extensive electrostatic shielding which principally occurs when tiny molecular objects are placed between closely spaced metal electrodes. Thus, alternative concepts of switching are required – one possibility is to rely upon a conformational switch of the molecule, which may be induced by an applied electric field or photo-irradiation. The methods developed within this project should provide a viable route to electrical contacting of molecules of such capability.