nanoscience
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ABSTRACTS
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TOWARDS REALISTIC ATOMIC-SCALE MODELING OF NANOSCALE DEVICES

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Although electronic device dimensions are rapidly approaching the nanoscale, their dimensions are still large from an atomistic perspective. Certain systems can still be studied with current state-of-the-art technology since the problems are relatively localized, such as interfaces and the effects vacancies or defects in them can have on Schottky barriers and interface resistance. For other properties, such as the influence on the transport and transistor characteristics of the electrostatic environment induced by gate electrodes, the simulation volume and atom count grows rapidly, however.

Therefore, a novel methodology is required in order to scale down current modeling techniques used within TCAD to be able to take into account atomic-scale effects. In this presentation we will present the current state-of-the-art in first-principles device modeling, as implemented in our software Atomistix ToolKit (ATK), and give an outlook to the challenges that lie ahead when scaling up the atomic-scale methods to more realistic dimensions.

We will discuss our recent progress in this area, including efficient Green's function evaluation and parallelization strategies based on block diagonalization techniques and the Krylov subspace method [1,2], the use of scattering states for improved performance of finite bias transport calculations [3], finite-element techniques coupled to first-principles calculations [4], and multi-scale models that take advantage of methods that operate on different complexity levels and length scales [4-6].

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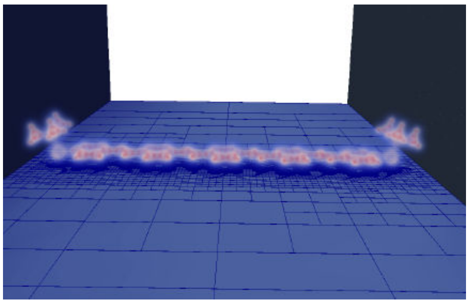

__Figure 1:__ OPV5-tBu molecule in a single electron transistor environment, colored by the effective potential. This close-up view of the molecule illustrates the extremely high level of detail in the region where the electron density is large. [4]

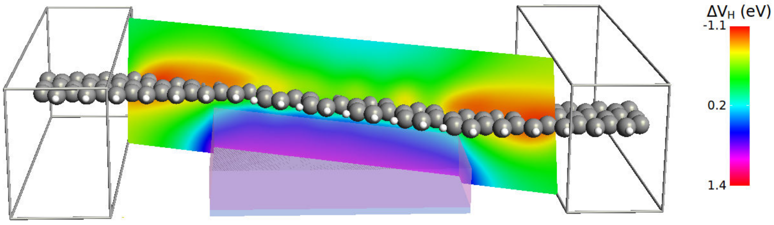

__Figure 2:__ Graphene nanotransistor consisting of two metallic zigzag nanoribbons connected by a semiconducting armchair ribbon. The nanoribbons are passivated with hydrogen, and the width of the ribbons are is 7 Å. The device is sitting on top of a dielectric and the transport is controlled by an electrostatic backgate. [6]

BIGDFT: LARGE-SCALE AB INITIO METHODS BASED ON WAVELETS

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Daubechies wavelets are a powerful systematic basis set for electronic structure calculations because they are orthogonal and localized both in real and Fourier space. We describe in detail how this basis set can be used to obtain a highly efficient and accurate method for density functional electronic structure calculations. This code, BigDFT, shows high systematic convergence properties, very good performances, and an excellent efficiency for parallel calculations alos in hybrid architectures based on CPU and graphical processing units.

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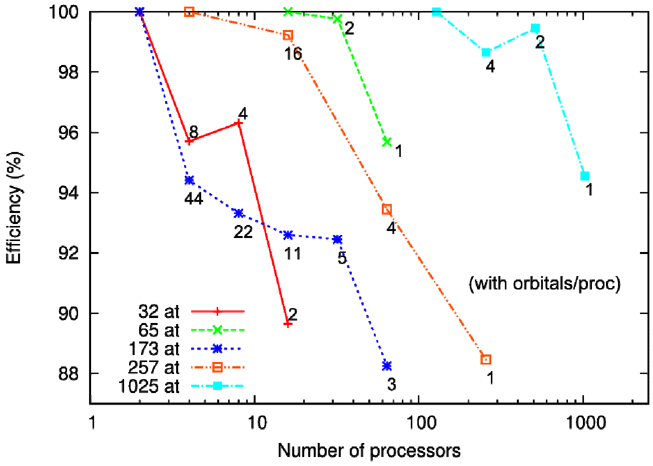

Figure 1: Efficiency of BigDFT versus the number of cores. The number near the points is the distribution of orbitals per core.

COMPRESSION OF SETS OF PRODUCTS OF ATOMIC ORBITALS, WITH APPLICATIONS TO TDDFT AND GW

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Molecular orbitals in clusters or molecules can be conveniently expressed as linear combinations of localized atomic orbitals. Products of overlapping orbitals occur in electronic densities and these, by contrast, are linearly dependent. An improved solution of this well known technical problem leads to

(i) a new solution of the Petersilka-Gossmann-Gross equation of TDDFT-
(ii) a new O(N^3) implementation, without plasmon parametrization, of Hedin's GW scheme.

Here we describe aspects of the compression algorithms we developed and their effect on the accuracy of spectra and electronic spectral functions in TDDFT and GW, respectively.

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A COMPLETE METHODOLOGY FOR THE SIMULATION OF LARGE NANOSTRUCTURES AND QUANTITATIVE ANALYSIS USING Z-CONTRAST IMAGES

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During the last few years, a complete methodology has been developed at the University of Cadiz for the simulation of High Resolution Electron Microscopy images of large nanostructures. Z-contrast imaging in scanning transmission electron microscopy (STEM) constitutes a powerful approach to investigate strained heterostructures on the nanometer scale and it has been proved to be extremely reliable for characterizing nanomaterials[1]. The proposed methodology allows the modeling and simulation of Z-contrast Electron Microscopy images of large nanostructures in reasonable time and it can be used to study materials in the presence of defects, being therefore very useful for a better knowledge of their mechanical properties and therefore of a great technological interest.

Figure 1 depicts the steps for a complete analysis of experimental and simulated HAADF images and quantitative characterization of nanostructures, and it comprises three steps, 3D nanostructure description (geometry, composition, etc.), 3D nanostructure modeling (Finite Element Modeling and/or Molecular Dynamics) and Image simulation.

A) **Geometry Description**: a commercial package (COMSOL^{TM}) is used to describe the geometry of the nanostructure (subdomains, boundaries, constraints, symmetries, etc.) and to define the local parameters (composition, initial strains, elastic constants…). The geometry of the nanostructure is usually described based on a-priori knowledge but the compositional distribution is usually extracted from experimental images by electron energy loss spectroscopy and aberration-corrected highresolution Z-contrast imaging.

B) **Nanostructure modeling**: once the geometry is fully described, an atomistic model must be generated. This goal can be accomplished by modeling the nanostructure using finite element analysis (FEA) and solving the equations of the anisotropic elastic theory to obtain the displacement field [2,3]. *SIC_Supercell* software developed at the University of Cadiz provides the corresponding 3D atomistic model from a supercell described as a sequence of (x, y, z) coordinates that have been obtained from FEA model at equilibrium, i.e. atom coordinates according to the local displacement field and occupancy or Debye-Waller factors according to the local composition. A second approach based in Molecular Dynamics is usually applied in our research group in order to obtain the 3D atomistic model [4] Molecular modeling involves theoretical and computational methods needed to model the behavior of a system at atomic scale. The collective behavior of atoms allows the understanding of how the material undergoes deformation, phase changes or other phenomena, providing links between the atomic scale to macro phenomena.

The resulting strain obtained by any of these two techniques may be compared with that obtained directly from experimental images applying a strain mapping technique. Using high-resolution electron microscopy images and under some limitations we may assume there exists a constant spatial relationship between the intensity maxima and the location of atomic columns in the studied material [5]. This relationship appears in the form of a spatial shift of the intensity maxima positions with respect to atomic columns. *Peak Pairs Analysis* is a strain mapping technique developed at the University of Cadiz [6] and implemented in a Digital Micrograph plug-in. It is distributed by HREM Research [7] and improves both, the speed of computation, and memory requirements with respect to other strain mapping approaches.

C) **Image simulation**: STEM image simulation of a few unit cells can take hours and the simulation of medium-size nanostructures, where millions of atoms are involved, is unfeasible in the state of the art personal computers. To overcome this problem, a parallel HAADF-STEM simulation software has been developed [8].The software runs in the University of Cadiz cluster, having 320 nodes and 3.8 Tflops and it is capable to simulate images from nanostructures represented by about 1 million atoms in a couple of days. The software can generate one dimensional line scans, two dimensional images and focal series and its results has been successfully compared with WinHREM [4,8] software.

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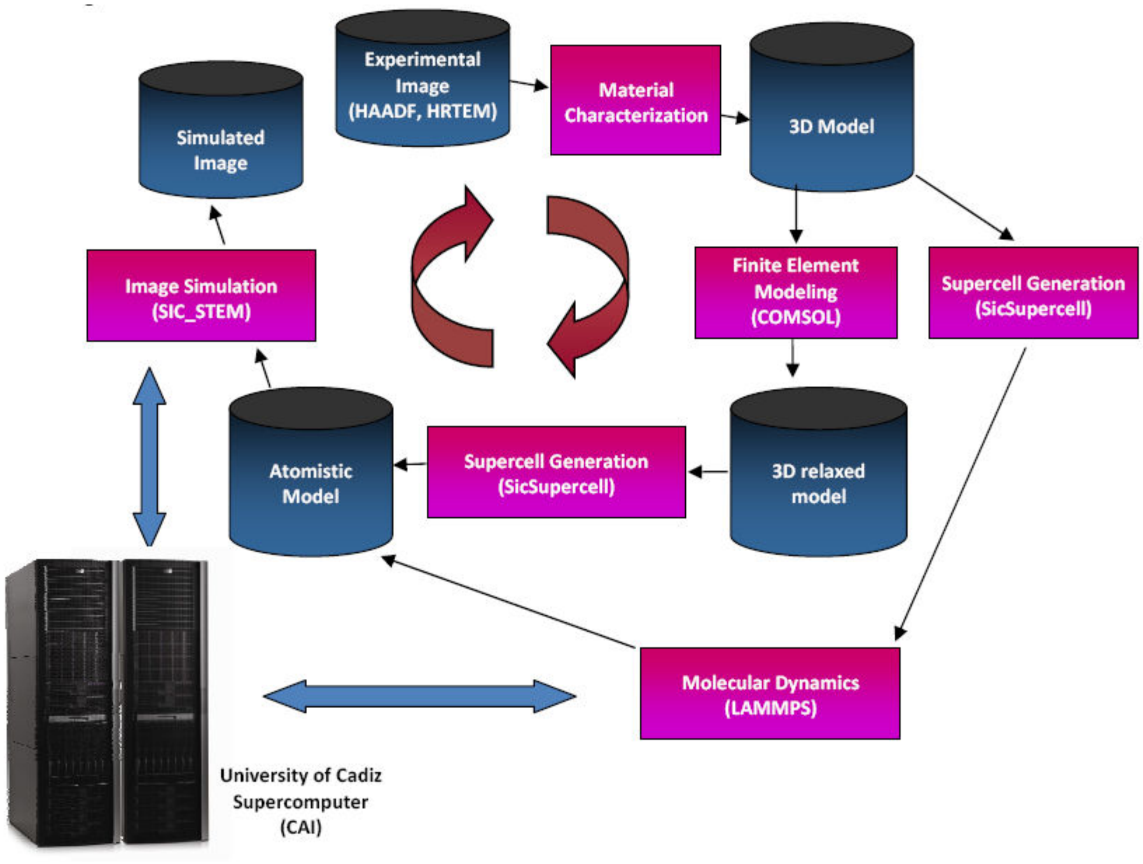

Experimental Image (HAADF, HRTEM)
Material Characterization
3D Model
Simulated Image
Image Simulation (SIC_STEM)
Finite Element Modeling (COMSOL)
Supercell Generation (SicSupercell)
Atomistic Model
Supercell Generation (SicSupercell)
3D relaxed model
Molecular Dynamics (LAMMPS)
University of Cadiz Supercomputer (CAI)

Figure 1: *Schematic diagram of the nanostructure modeling methodology developed at the University of Cadiz*

MONTE CARLO CONFIGURATION INTERACTION FOR MOLECULES AND NANOSTRUCTURES

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Wave function methods such as configuration interaction and coupled cluster theory provide systematic treatments of electron correlations in nanoscale systems and provide accurate prediction for photoexcitation spectra in finite quantum systems. Arbitrarily accurate solutions to the many-body Schrödinger equation are possible through a brute force expansion of the wave function in determinants or spin coupled sums of determinants (‘configuration state functions’), the so called configuration interaction (CI) or superposition of configurations method. Due to the length required for a complete many-body expansion, the brute force approach becomes computationally intractable except for few-electron problems.

A Monte Carlo technique for sampling configurations and evaluating their contribution to the energy or their weight in the many-electron wave function is designed to find only the most import configurations in many-electron wave functions [1,2] and has been applied to a variety of molecular problems. Recently using this Monte Carlo configuration interaction (MCCI) method, singlet and triplet electronic excitation energies have been calculated for few electron molecules for systems with single and multi-reference 0th order wave functions. We find that vertical photoexcitation energies can be predicted to within a few tens of meV (to within an accuracy of < 1%) of full CI (FCI, or complete many-body basis sets) limits using expansions consisting of only a few thousand configuration state functions as compared to the $O(10^{10})$ to $O(10^{12})$ configurations occurring in the corresponding FCI expansions [3]. The method thus represents the state-of-that art for predicting electronic excitations in few-electron systems with accuracy comparable to the equation-of-motion coupled cluster method with the inclusion of full triple excitations.

Interactions between localized molecular bound states and a continuum of states such as occurring for molecules bonded between electrodes in nanoscale tunnel junctions can be modeled by using an (energy-dependent) self-energy, or approximately through use of a complex potential. We discuss the relation between the two approaches and give a prescription for using the self-energy to construct an energy-independent complex potential [4] that generalizes single-electron electrode self-energies for use with many-electron wave functions. This allows for a treatment of molecular correlations on a nanoscale sub-system while 'opening' the system to allow interaction with larger systems such as electrodes, coupling to bulk bands for localized defect states, or for molecules-surface interactions.

The use of MCCI to the study of the charged nitrogen-vacancy (NV-) center in diamond [5] is presented; interest in the center is motivated by its potential use as a qubit. Within these calculations 116 electrons are correlated using 130 orbitals/260 spin orbitals. Use of the MCCI method allows for a study of the symmetry and spin of the electronic excitations needed to understand the mechanism for spin relaxation and hence lifetimes of the excited states. Our study suggested that the assumed ordering is unlikely to be correct and this theoretical prediction is consistent with recent experimental studies [6].

We will also report on recent results for porting the method to the IBM Blue Gene and discuss scaling of the algorithm in massively parallel environments. Recently several new methods that adaptively construct and refine a many-electron wave function have been reported using quantum Monte Carlo in a determinant space, coupled cluster theory, CI methods and the density matrix renormalization group theory. An overview of the common elements of these recent approaches is highlighted.

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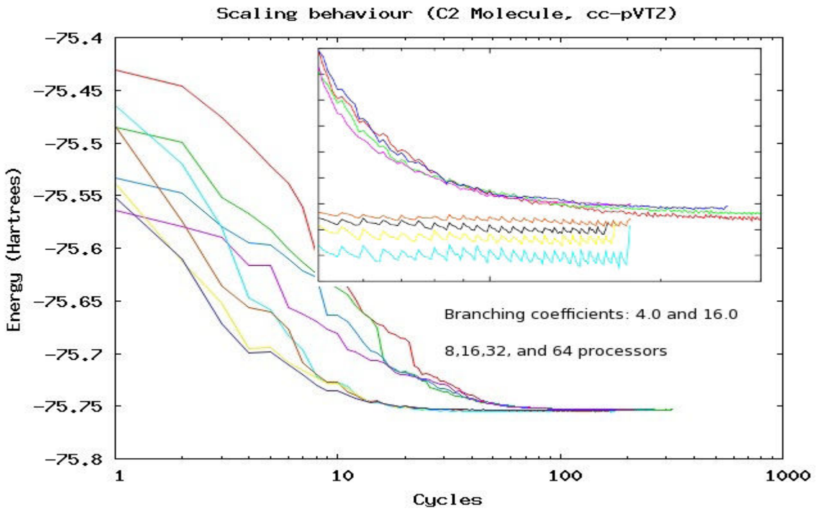
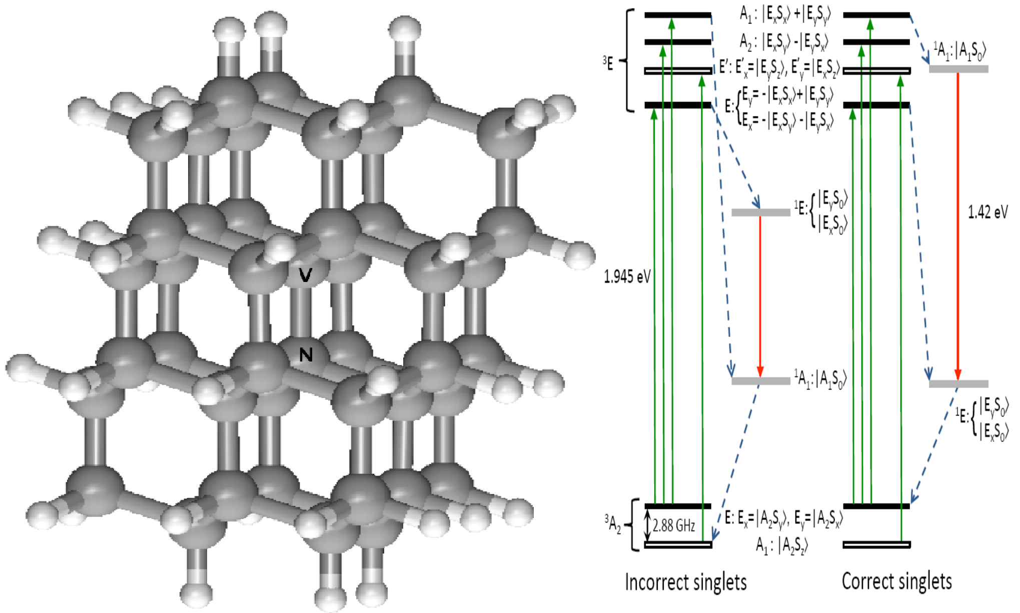


Figure 1: *Convergence behavior for the MCCI algorithm for the C_2 molecule in a correlation consistent polarized valence quadruple-ζ (cc-pVQZ) basis set. The inset reveals that with different sampling conditions, the final total electronic energy agree within a few milli-electron Volt or approximately 1 part in 10^4 In the correlation energy.*



V
N
^3E
$A_1 : |E_xS_x\rangle + |E_yS_y\rangle$
$A_2 : |E_xS_y\rangle - |E_yS_x\rangle$
$E' : E'_x = |E_yS_z\rangle, E'_y = |E_xS_z\rangle$
$E : E_y = -|E_xS_x\rangle + |E_yS_y\rangle, E_x = -|E_xS_y\rangle - |E_yS_x\rangle$
$^1A_1 : |A_1S_0\rangle$
$^1E : |E_yS_0\rangle, |E_xS_0\rangle$
1.945 eV
1.42 eV
$^1A_1 : |A_1S_0\rangle$
$^1E : |E_yS_0\rangle, |E_xS_0\rangle$
$^3A_2$
2.88 GHz
$E : E_x = |A_2S_y\rangle, E_y = |A_2S_x\rangle$
$A_1 : |A_2S_z\rangle$
Incorrect singlets
Correct singlets

Figure 2: *Convergence Cluster model of the NV- center in diamond. MCCI spectra suggests that the ordering assumed for the singlet A_1 and degenerate E state should be reversed, with the singlet A_1 state lying higher in energy.*

INTEGRATED HPC APPLICATION SERVICES FOR MULTISCALE MATERIALS MODELING

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Computational materials science is essential for development of products with novel properties (examples: catalysis, semiconductors, and alloys). Nevertheless, next generation materials, especially nano-structured materials, exhibit pronounced complexity and multiscale behavior. Also "classical" systems like the biological cell and its building blocks include structures on many length scales. Thus, the physical models and the simulation protocols employ many different well established methods and different codes to treat the steps in these protocols. However, the lack of integration of these individual codes, the increasing complexity of models and the high demand for distributed HPC resources reduces industrial usability of the methods. In addition, joint effort of groups providing expertise for all different methods is needed. These aspects are treated within the project MMM@HPC [1] which brings together scientists from industry and academia into a unified community which is able to use the e-infrastructure to solve modern real-life problems.

We will give an overview of our methodology to provide adequate solutions for the following requirements:

Reusable interfaces and workflows. To this end, we adopted GridBeans [2] which is a modern technology to create application interfaces for use in grid middleware, such as UNICORE 6 [3] or Globus. Every GridBean provides a graphical user interface and can be readily included into different workflows without further modifications. Moreover, the workflows created for one specific task can be reused in other simulations with minor parametric modifications.

Robust tools and standards for data exchange between individual codes. In the field of materials modeling a variety of data formats are used and virtually every individual code has its own non-standard input and output formats. Thus, we aim to enhance data interoperability of individual GridBeans employing the Chemical Markup Language (CML) standard and work together with experienced developers from other projects, currently from UNICORE and OpenMolGrid [4, 5].

Solutions for licensing issues. Unfortunately, many of the codes used in the community are provided under non-free (proprietary) licenses. To treat this aspect we are working on a solution based on the Virtual Organization Membership Service (VOMS) and UNICORE.

Security and reliability. Industrial applications need secure handling (communication, storage) of simulation data. Moreover, the storage, the connection and the processes must be error-tolerant and thus reliable. All these are implemented properties of the underlying generic e-infrastructures and they are reused in our approach.

Capacity (high throughput) and capability (high performance) computing. The applications addressed in the community are particularly demanding with regard to computing and storage resources. This is why the scalable deployment of the application services requires linking to HPC and distributed resources, e.g. such as those provided in the projects EGI and PRACE.

All these user requirements pose a great challenge for both code developers and providers of e-infrastructures. These aspects are addressed in the EU project MMM@HPC. The application protocols are mapped onto scientific workflows and the application interfaces are able to ex-change input/output data using data formats like CML. The platform of our choice is the UNICORE middleware that is broadly and productively deployed in different grid infrastructures such as D-Grid, DEISA and PRACE.

As an example, we present in Figure 1 a model of an Organic Light Emitting Diode (OLED) that requires treatment on different size scales using different code types – quantum mechanics, molecular mechanics, kinetic Monte Carlo (coarse-grained method) and finite element analysis (continuous method). Two of the interfaces are shown on the figure. We aim genericity of the developed workflow so that we consider several different codes that can perform one specific step in the simulation protocol. For example, an electronics structure calculation can be carried out employing two or more alternative programs. Our code selection criteria are maturity, open accessibility, high parallel performance, and availability of expertise by partners.

To demonstrate the functionalities of the developed tools we consider key applications, including de-novo modeling and simulation of whole devices, such as organic electronics, molecular electronics, carbon nano-device and Li-Ion batteries.

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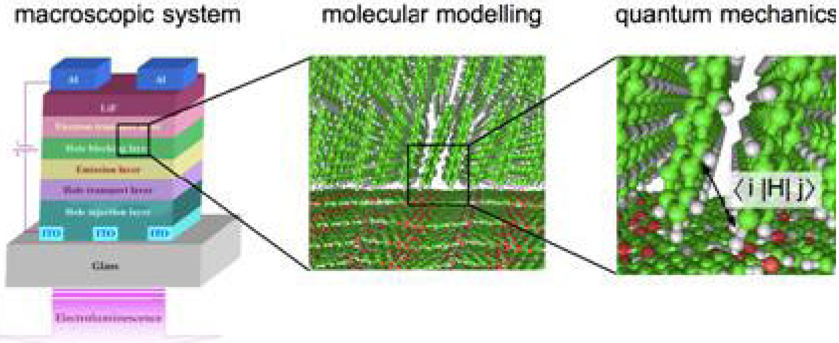

Figure 1: *Multiscale modeling of an Organic Light Emitting Diode (OLED).*

AN O(N^3) IMPLEMENTATION OF HEDIN'S GW APPROXIMATION FOR MOLECULES

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The knowledge of excitation properties of molecules is crucial in developing organic semiconductor devices. Many-body perturbation theory is one of the most promising theories for characterization of excitations in electronic systems. In particular, Hedin's GW approximation for one-electron Green's function is capable of calculating lumo and homo of molecules with O(N^3) computational complexity like TDDFT.

In this work [1], we implement the Hedin's GW approximation on top of DFT calculations performed with SIESTA [2] code. We apply a dominant product technique [3] to span the space of orbital products and to reduce the dimensionality of dielectric matrix. Moreover, to describe the frequency/time dependence of necessary correlators, we use their spectral functions. The spectral function techniques avoids otherwise necessary analytical continuations and allow for Fast Fourier techniques to be applied in our method. As examples of application, we discuss several results for ionization potentials and electron affinities of large molecules, revealing strengths and limitations of our implementation.

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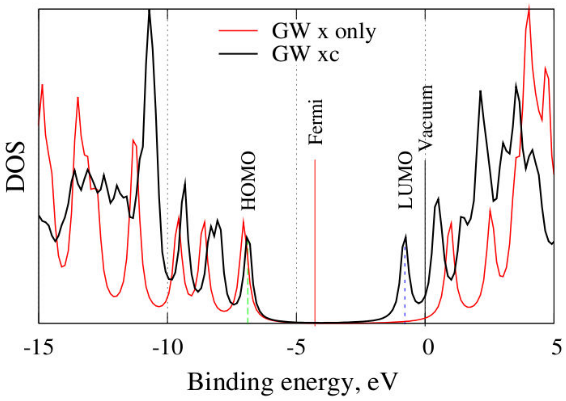

***Figure 1:** The density of states of anthracene molecule computed in two approximations: "GW x-only" – only instantaneous part of self-energy is taken into account, while "GW xc" – the correlation effects due to dynamical screening are taken into account. Please, note that it is the correlation effects make our theoretical anthracene an aceptor, while exchange-only self-energy wrongly predicts our anthracene being donor.*

TAILORING THE ATOMIC AND ELECTRONIC STRUCTURE OF TWO-DIMENSIONAL CARBON AND BORON-NITRIDE SYSTEMS WITH ELECTRON AND ION BEAMS

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Recent experiments (see Refs. [1,2] for an overview) on ion and electron bombardment of nanostructures demonstrate that irradiation can have beneficial effects on such targets and that electron or ion beams can serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of various nanostructured materials.

We systematically study irradiation effects in nanomaterilas, including two-dimensional (2D) systems like graphene and hexagonal boron-nitride (h-BN) sheets. By employing various atomistic models ranging from empirical potentials to time-dependent density functional theory we simulate collisions of energetic particles with 2D nanostructures and calculate the properties of the systems with the irradiation-induced defect. In this talk, our latest theoretical results on the response of graphene and h-BN to irradiation will be presented, combined with the experimental results obtained in collaboration with several groups [3,4]. The electronic structure of defected graphene sheets with adsorbed transition metal atoms will be discussed [5], and possible avenues for tailoring the electronic and magnetic structure of graphene by irradiation-induced defects and impurities will be introduced [4,6]. The effects of ion and electron irradiation on boron-nitride sheets and nanotubes will also be touched upon. Finally, we will discuss how electron irradiation and electron beam-assisted deposition can be used for engineering hybrid BN-C nanosystems by substituting B and N atoms with carbon with high spatial resolution.

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GRAPHENE EDGE MAGNETISM FOR SPINTRONICS APPLICATIONS: DREAM OR REALITY?

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We critically discuss the stability of edge states and edge magnetism in zigzag edge graphene nanoribbons (ZGNRs). We point out that magnetic edge states might not exist in real systems, and show that there are at least three very natural mechanisms - edge reconstruction, edge passivation, and edge closure - which dramatically reduce the effect of edge states in ZGNRs or even totally eliminate them. Even if systems with magnetic edge states could be made, the intrinsic magnetism would not be stable at room temperature. Charge doping and the presence of edge defects further destabilize the intrinsic magnetism of such systems. We conclude that edge magnetism within graphenes ZGNRs is much too weak to be of practical significance, in particular for spintronics applications. We further discuss the influence of nonmagnetic edges on the electron transport through ZGNRs.

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SIMULATION OF SCANNED PROBE SPECTROSCOPY: A CHALLENGING NUMERICAL PROBLEM

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Scanned probe spectroscopy is an interesting technique developed a few years ago [1,2] for the direct investigation of the flow of electrons and of the position of impurities in nanoscale devices based on a 2- dimensional electron gas. Initial applications [1,2] were to the electron gas obtained by modulation doping in a GaAs/AlGaAs heterostructure and, more recently, to that in a graphene sheet [3]. The basic concept of scanned probe spectroscopy consists in measuring the effect on the device conductance of the potential perturbation due to a negatively biased probe that is scanned over the region of interest of the device. By creating a map of the conductance values in correspondence with the probe positions, interesting information about current paths and impurity scattering can be obtained.

We have been interested in the numerical simulations of these experiments, in order to develop a tool providing a better understanding of what is actually measured in such experiments and a reliable estimate of the achievable resolution. Our initial work was focused on GaAs/AlGaAs heterostructures and, in the last year, we got interested in the simulation of scanned probe spectroscopy experiments performed on graphene flakes [3].

Simulation of this type of experiments requires indeed a significant computational effort, because in principle the conductance across the device has to be re-computed for each probe position. The conductance can be evaluated, via the Landauer-Buettiker formula, from the knowledge of the transmission through the device for a range of energies around the Fermi level. Transmission can be obtained, for example, by means of the recursive Green’s function technique or the recursive scattering matrix technique. All of these methods include a first step in which the device is subdivided into slices, within each of which the potential is assumed to be longitudinally constant. Calculation of the transmission is in itself a computationally intensive task, if, at least in some regions, a large number of transverse modes are propagating; then this has to be repeated for a number of times corresponding to the possible positions of the scanning probe. Without some form of optimization, such a calculation would definitely be unfeasible. We have looked into several forms of optimization, starting from preventing the repeated calculation of the transverse wave functions of the sections: the transverse Schroedinger equation is solved again, at each step in the probe position, only for the slices which are directly affected by the probe potential. Furthermore, one could compute the Green’s function matrix from each end of the device to any of the intermediate slices (in the absence of the probe), keep this information in memory, and reuse most of it at each scanning step (thereby computing from scratch only the Green’s function matrices of the region whose potential is altered by the probe). There is clearly a trade-off in terms of memory occupancy vs. speed, because if we want to keep all of this information, quite significant an amount of memory will be needed. With such an approach we can obtain plots of the results of scanned probe spectroscopy of quantum point contacts (Fig. 1) or of mesoscopic cavities (Fig. 2) with a computational effort of the order of a CPU-day.

Further improvements could be achieved by treating the potential of the probe as a perturbation and recomputing the overall Green’s function matrix via the Dyson equation. This has been done with success in Ref. [4], where the effect of the probe was assumed to be localized in a single grid-point. In principle, this approach can be extended to the case of a probe creating a generic perturbation of the potential at the 2DEG level (usually assumed to be a Lorentzian), but the speedup is reduced and, depending on the size of the area affected by the potential perturbation, may not be convenient.

We are currently working on the implementation of scanned probe spectroscopy simulations of grapheme flakes: such simulations pose a very challenging computational problem, since experiments are performed on flakes with a width of the order of 1 micron, which makes approaches based on the atomistic methods usually applied to graphene (such as tight-binding) unfeasible. Therefore we have chosen a continuum approach consisting in the solution of the Dirac equation in each transverse section (which corresponds to the equation for the envelope functions in the vicinity of the band degeneration points). The numerical solution of such an equation is, however, a very challenging problem in itself, due to the difficulties in finding a proper, consistent discretization. By extending the solution to a domain that is twice the width of the original domain, the boundary conditions become more standard and an efficient algorithm for the numerical solution can be implemented.

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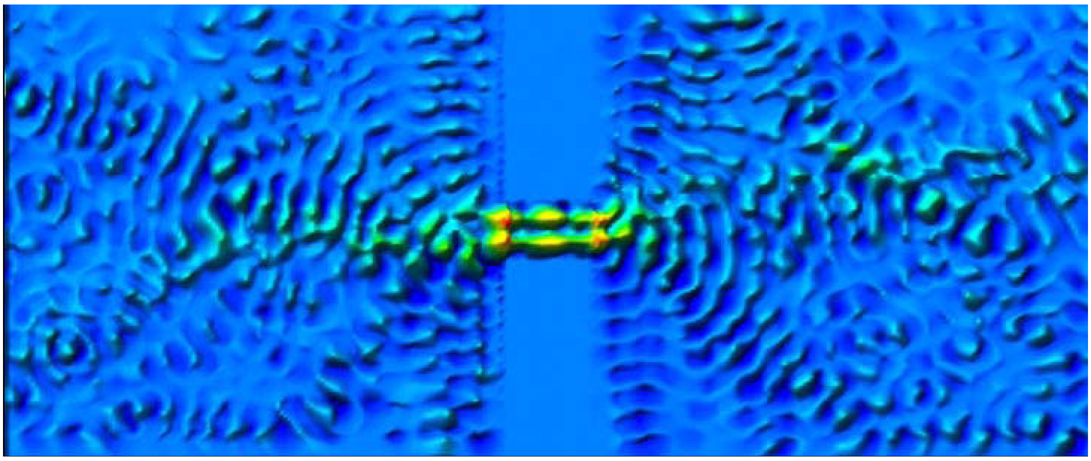

Figure 1: *Results for the scanned probe spectroscopy of a quantum point contact in the presence of a random potential due to dopants.*

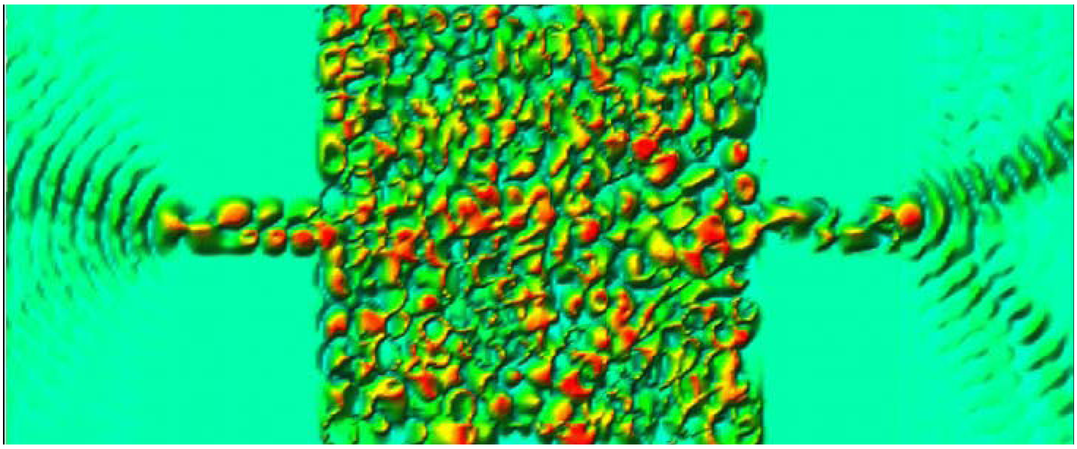

Figure 2: *Results for the scanned probe spectroscopy for a mesoscopic cavity, in the presence of the potential due to randomly located dopants.*

ELECTRONIC AND TRANSPORT PROPERTIES OF CHEMICALLY FUNCTIONALIZED NANOGRAPHENES

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Recent advancements in production techniques have allowed the synthesis and characterization of novel nanostructured materials based on graphene.[1] Particularly, recent research efforts have been targeted to the investigations of low-dimensional nanographenes, such as graphene quantum-dots (GQDs) and nanoribbons (GNRs). Here, the dimensional confinement at the nanoscale allows the tuning of the intrinsic electronic properties of graphene, which can potentially be exploited for the production of next-generation nanostructured electronic devices. Nevertheless, limitations in current experimental methodologies hinder both the controlled synthesis of nanographenes, with well-defined electronic properties, and large-scale production. To overcome these issues, the chemical modification of graphenes has been spotted as a viable route to produce materials with controlled and well-defined properties with potential use in applications. However, despite recent theoretical and experimental efforts, [2,3] a comprehensive understanding of the relationships between chemical structure and electronic properties in nanostructured graphenes is still missing. This concern is particularly critical in relation to the electron transport properties of chemically-modified graphenes, in view of their use in nanoelectronics.

In this work, we analyze, by means of density functional theory and non-equilibrium Green's function calculations, the electronic and transport properties of low-dimensional graphene nanostructures subjected to chemical functionalization. Our calculations concern models based on GQDs, GNRs and functionalized nanostructures thereof, targeting systems of interest in recent experiments, focused on oxidization and edge-functionalization of nanographenes.[4] In particular, we demonstrate how the remarkably versatile chemistry of sp^2 carbon and the use of traditional organic chemistry concepts [5,6] provide a reliable guide to rationalize the properties of chemically functionalized graphenes. The application of rigorous concepts in the definition of model systems and the use of high-performance computing platforms constitute crucial prerequisites for realistic simulations of low-dimensional carbon nanostructures aimed at the development of novel materials with potential application in nanoelectronics.

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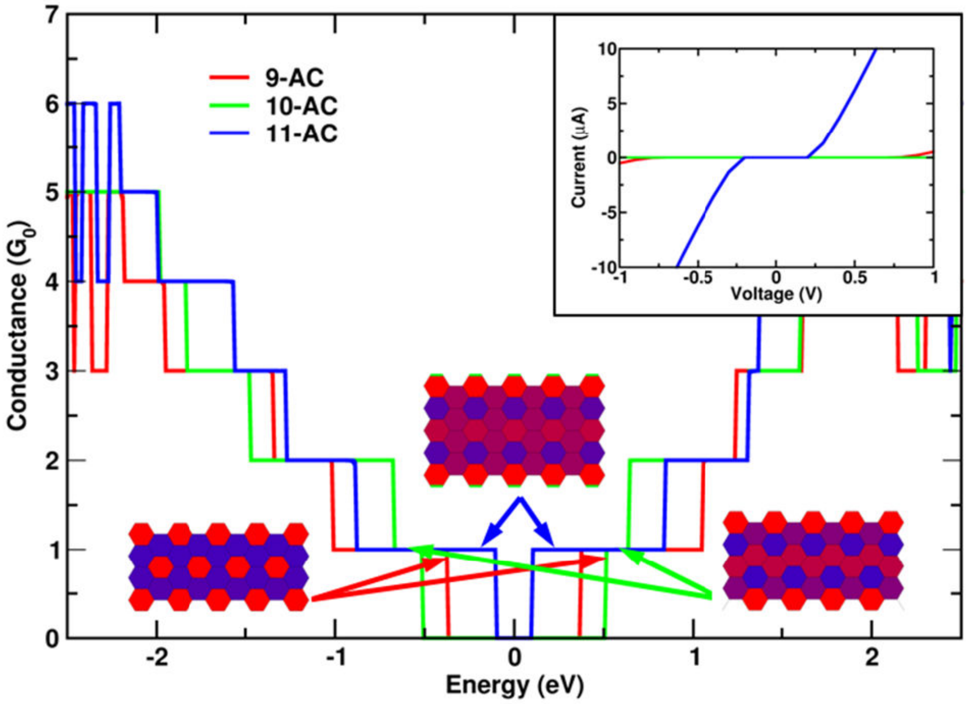

Figure 1: *Transmission spectra and I(V) characteristics (inset) of armchair-edge 9-AC (red lines), 10-AC (green lines) and 11-AC (blue lines) GNRs. Optimized structures, color-coded according to their mean bond length (average of the six C-C bond lengths for each six-term ring), are also depicted above the corresponding transmission plateau.*

MASSIVE COMPUTATION FOR NON-EQUILIBRIUM PHENOMENA IN NANOCARBONS

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In this presentation, I will introduce you computational scheme of extremely strong optical electric field (E-field) generated by compressed laser pulse (femtosecond laser pulse). Since the optical E-field is over 1 V/Å and the pulse has very short time-range (less than 40 fs), the conventional perturbation theory does not work so direct numerical simulation solving electrons' real-time dynamics under time-varying E-field should be solved. For that purpose, we have applied the time-dependent density functional theory combined with molecular dynamics.

As examples of applications we will provide our result for graphene exfoliation from graphite surface [1] and molecular photochemical reaction inside nanotubes [2]. We will also discuss future possible applications of non-equilibrium phenomena on nano-carbons which has high melting temperatures and difficult to deal with conventional thermal processes.

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EXPLORING THE REAL NANO-WORLD USING HPC BEYOND THE AB-INITIO APPROACH

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The advances in the predictive power, speed and reliability of ab-initio methods has occurred in the last few decades at a very fast pace. Simultaneously, the computing power available through HPC facilities has continued growing exponentially. This combination has brought the paradigm of ab-initio simulations as an invaluable tool to understand and predict the behavior of matter at the nanoscale. However, enormous challenges are still ahead of us, to be able to extend the range of practical applicability of these methods to the sizes and time scales which are relevant to most of the practical problems in nanotechnology. In this talk, I will talk about some of these challenges, and discuss strategies to use the information extracted from ab-initio simulations to tackle problems in the length and time scales which are really relevant for practical uses of nanotechnology. In particular, I will describe approaches to study electronic transport properties in nano-to-meso scale devices (see Figure 1) [1], and the interaction of large proteins with inorganic nanostructures. The role of HPC facilities and the interaction between these and the development of simulation tools will also be discussed [2].

Acknowledgements:

Work done in collaboration with Carlos F. Sanz-Navarro (CIN2-ICN), Stephan Roche (CIN2-ICN), Alberto García (ICMAB-CSIC), and Jose M. Cela (BSC). Financial support from Spanish MICINN grants CSD2007-00050 (Supercomputing and e-Science), and FIS2009-12721-C04 are fully acknowledged.

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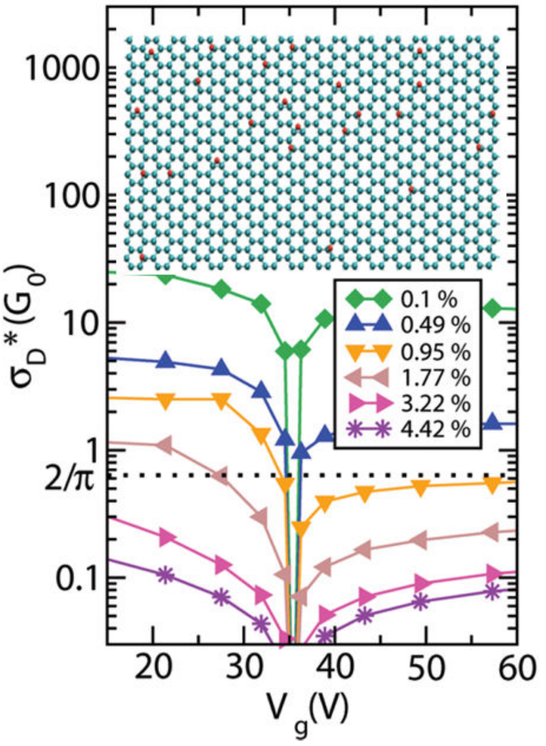

***Figure 1**: Drude conductivity of samples of graphene functionalized with different concentrations of oxygen, in the configuration of epoxide groups, as a function of gate voltage. The inset shows a section of one of the samples. Adapted from Ref. [1]*

BITLLES: A QUANTUM-TRAJECTORY SIMULATION TOOL FOR ELECTRON TRANSPORT IN LARGE ELECTRONIC STRUCTURES

G. Albareda, A. Alarcón, F. L. Traversa, A. Benali, A. Padró, and **X. Oriols**

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With the aim of manufacturing smaller and faster devices, the electronic industry is today entering the nano and picosecond scales. In such particular scenarios, electron dynamics becomes affected by strongly correlated quantum dynamics, both in space and time. Thus, in order to provide an enough accurate description of the electron-electron correlations, quantum transport simulators must consider a reasonable approach to the many-particle problem. Anyway the big deal concerns the solution of the many-particle Schrödinger equation nowadays solvable only for very few degrees of freedom.

In this work we present a general purpose time-dependent 3D quantum electron transport simulator based on Bohmian trajectories that we call **BITLLES** [1-3]**.** It is based on a recently published algorithm [1] that, on the grounds of Bohmian Mechanics [2], solves the many-particle Schrödinger equation for hundreds of electrons in terms of multiple single-particle pseudo-Schrödinger equations without losing the explicit Coulomb and exchange correlations among electrons (at a level comparable to the Time Dependent Density Functional Theory) [1-4].

The code of the **BITLLES** simulator is currently made up of more than 15000 FORTRAN lines (see the algorithm in Fig.1). It has also a 3000 C++ lines for a (Windows, MAC and Linux compatible) user friendly environment to design an verify the simulated electronic structures (see Fig. 2). The computational burden associated with the solution of the self-consistent many-particle 3D Poisson-Schrödinger loops involves large simulation times. For example, one week for the complete I-V curve (DC, AC and noise) with a cluster of 24 Intel Xeon CPUs at 2.7GHz.

Same examples of the numerical viability of the **BITLLES** simulations are provided below for a Resonant Tunneling Diode (RTD). Its characteristic I-V curve with Coulomb correlations introduced at different approximation levels is plotted in Fig. 3 [3,5]. Many-particle tunneling phenomena are reveled in the (super-Poissonian) behavior of the Fano factor shown in Fig. 4 [2]. Finally, in Figs. 5 and 6 we show the transient (time-dependent) current response and its Fourier transform respectively, when a voltage step is applied in the negative differential conductance region.

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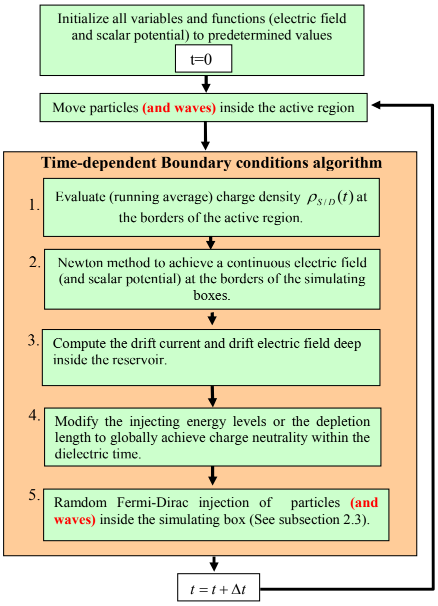
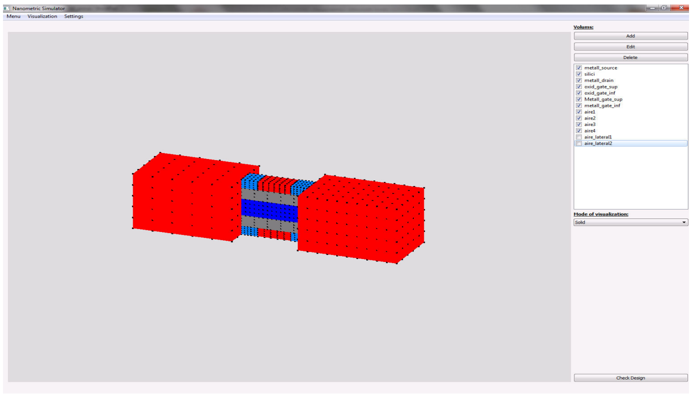

Initialize all variables and functions (electric field and scalar potential) to predetermined values
t=0
Move particles (and waves) inside the active region
Time-dependent Boundary conditions algorithm
1. Evaluate (running average) charge density $\rho_{S/D}(t)$ at the borders of the active region.
2. Newton method to achieve a continuous electric field (and scalar potential) at the borders of the simulating boxes.
3. Compute the drift current and drift electric field deep inside the reservoir.
4. Modify the injecting energy levels or the depletion length to globally achieve charge neutrality within the dielectric time.
5. Ramdom Fermi-Dirac injection of particles (and waves) inside the simulating box (See subsection 2.3).
$t = t + \Delta t$

Figure 1: *General algorithm describing the fundamental routines defining the BITLLES simulator.*


Nanometric Simulator
Menu
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Volums:

- ☑ metall_source
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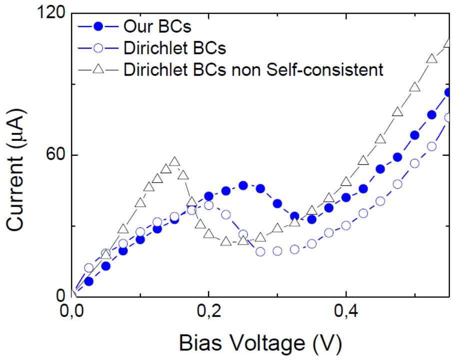
- ☑ metall_drain
- ☑ oxid_gate_sup
- ☑ oxid_gate_inf
- ☑ Metall_gate_sup
- ☑ metall_gate_inf
- ☑ aire1
- ☑ aire2
- ☑ aire3
- ☑ aire4
- ☐ aire_lateral1
- ☐ aire_lateral2

Mode of visualization: Solid

Figure 2: *Very recently BITLLES has been provided with a user friendly interface.*



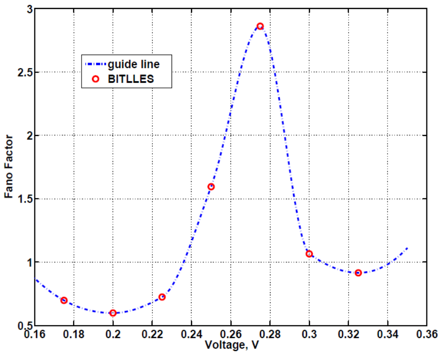
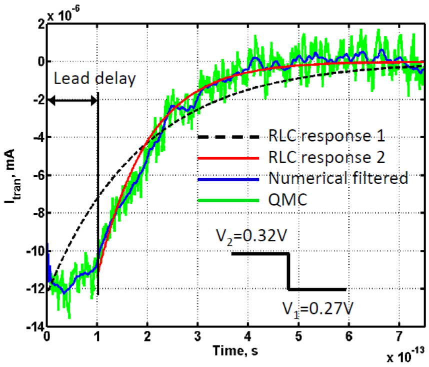


Figure 3: *DC Current for a RTD with Coulomb correlations introduced at different levels of accuracy.*

Figure 4: *Fano Factor computed for the RTD of Fig. 1 computed directly from the (time-dependent) current fluctuations.*



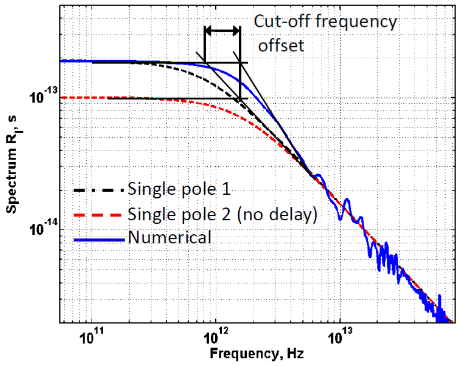


Figure 5: *Current response of the RTD to a step input voltage. Self-consistent boundary conditions including the leads are used*

Figure 6: *Spectrum of the current response of Fig. 5. Cut off frequency and its offset due to the lead delay are pointed out.*

MODELING PHOTO-INDUCED DYNAMICAL PROCESSES IN MASSIVE PARALLEL ARCHITECTURES

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There has been much progress in the synthesis and characterization of nanostructures however; there remain immense challenges in understanding their properties and interactions with external probes in order to realize their tremendous potential for applications (molecular electronics, nanoscale opto-electronic devices, light harvesting and emitting nanostructures). In this talk we will review the recent advances within density-functional based schemes to describe spectroscopic properties of those complex systems. Special emphasis will be made in modeling new materials and simulate new time and spatially resolved spectroscopies. We will address both linear and non-linear response regimes to study the optical absorption and luminescence of bio-chromophores, one-dimensional polymers and nanotubes and layered materials. Moreover, we will illustrate how an optimal control theory can be implemented such that we could have control of the quantum state of a molecular structure.

Within the goal of spanning larger time-scales and more complex structures, we will describe a new method to mimic the electron-ion dynamics within the Ehrenfest scheme where no explicit orthogonalization is necessary and we can increase of the time step while keeping the system close to the Born-Oppenheimer surface. The method is easily implemented and scales very well with the system size. Applications to the excited state dynamics in some organic molecules will be used as text cases to illustrate the performance of the approach. We will present the dynamical processes in organic/inorganic charge-transfer systems and biological complexes. In particular we will show the effect of electron-hole attraction in those systems. Pros and cons of present functionals will be highlighted and provide insight in how to overcome those limitations by merging concepts from many-body perturbation theory and time-dependent density functional theory.

All those developments constitute a basic ingredient for the realization of the European Theoretical Spectroscopy Facility (ETSF, http://etsf.eu) as a top-level scientific infrastructure. We implemented all those ideas in the open source computer code OCTOPUS (http://www.tddft.org). This program released in 2002 simulates the dynamics of electrons and nuclei under the influence of arbitrary time-dependent fields. his code is very versatile and can handle diverse physical situations (molecules, solids, 2D quantum dots, etc.) making it an extremely powerful tool for spectroscopy. Thanks to its current parallel capabilities, OCTOPUS was chosen as a benchmark code for the Partnership for Advanced Computing in Europe1 (PRACE) initiative that aims to provide European scientists with world-class leadership supercomputing infrastructures.

References:

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TUNABLE BANDGAPS AND EXCITONS IN DOPED SEMICONDUCTING CARBON NANOTUBES MADE POSSIBLE BY ACOUSTIC PLASMONS

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Doping of semiconductors is essential in modern electronic and photonic devices. While doping is well understood in bulk semiconductors, the advent of carbon nanotubes and nanowires for nanoelectronic and nanophotonic applications raises some key questions about the role and impact of doping at low dimensionality. Here we show that for semiconducting carbon nanotubes, bandgaps and exciton binding energies can be dramatically reduced upon experimentally relevant doping, and can be tuned gradually over a broad range of energies in contrast to higher dimensional systems. The later feature, made possible by a novel mechanism involving acoustic plasmons, establishes new paradigms for the understanding and design of nanoelectronic and nanophotonic devices.

ELECTRON TRANSPORT OF NANO-CARBON MATERIALS

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We have investigated electron transport of nano-carbon materials at finite temperatures through the large scale simulation using high-end supercomputers. For our purpose, we have developed an electron transport simulation model, based on a non-equilibrium finite temperature Green's function. The advanced tight-binding, Hamiltonian and molecular dynamical approaches enable us to consider phonon mode effect on electron transport at finite temperatures.

Through oder (N) approach, we are able to simulate meso-scale transport phenomena with several ten thousands of carbon atoms. In addition to calculating fundamental transport coefficient, our method is able to give atomistic electron current for all atomic positions. From the atomistic point of view, we can more clearly understand the interesting behavior of electron transport as nanoscale carbon materials. Our results show that electron current properties of nano-carbon materials strongly depend on a way of attachment of electrodes to such materials. Moreover, a choice of carbon orbital, pi or sigma, which is connected to electrodes, has crucial influence on electron transport behaviors. As for carbon nanotube, grahene, and Macky crystal, we will introduce our progress of researches and our large-scale simulation experiences.

COMPUTATIONAL STUDIES OF DIRAC FERMION MATERIALS AND NANOSTRUCTURES

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Graphene and topological insulators are among the most remarkable scientific discoveries of the past decade. High-performance computing plays important role in exploring various aspects of the physics of these novel materials and derived nanostructures. In my talk, I will cover our recent studies in the field of Dirac fermion materials which involve computational methods of various complexities: model Hamiltonian approaches applied to large nanostructures, density functional theory and many-body perturbation theory techniques. In particular, I will focus on the electronic properties of chiral graphene nanoribbons and on the electronic transport in polycrystalline graphene. Finally, I will discuss our recent investigations of the bismuth-based bulk topological insulators.