# Towards ab-initio simulations of nanowire field-effect transistors

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**Introduction** The dimensions of transistors, the active components of integrated circuits, have nowadays reached a point where quantum mechanical effects strongly affect their behavior. To accurately simulate always smaller devices and predict their performance prior to fabrication, the usage of a quantum transport (QT) approach is no more an option, but a must. In this context, several QT simulators have recently started to emerge, based either on continuous methods (effective mass approximation and k·p) or on atomistic models (tight-binding or pseudo-potentials).

The required material-dependent input parameters represent the major drawback of all these approaches. For example, the effective mass values must either be taken from bulk experiments (no quantization effects) or from higher order models such as tight-binding. In turn, the tight-binding parameters are derived from experimental values too or from bulk density-functional theory (DFT) calculations. In both cases surface and interface effects are not captured. Furthermore, parameters are not necessarily available for all possible materials or material combinations.

The parameterization issue can be overcome by using an "ab-initio" method as quantum transport basis. The original idea was proposed more than 10 years ago [1], but so far only relatively small atomic structures such as molecules, carbon nanotubes, or graphene nanoribbons have been simulated due to the heavy computational burden. Here, we present the first results of a new DFT-based quantum transport simulator capable of handling more than $10,000$ atoms. The tool combines the Quickstep module of the CP2K program package [2] and an existing tight-binding QT solver [3]. By leveraging the capabilities of both codes, Si nanowire field-effect transistors (NWFETs) with realistic dimensions can be investigated [4].

**Simulation approach** The device simulations are accomplished in two steps. First, CP2K performs a self-consistent DFT calculation in a 3SP contracted Gaussian basis (3 $s$ and 9 $p$ orbitals per atom) with GTH pseudo-potentials [5] and LDA as exchange-correlation functional. Periodic boundary conditions (PBC) are applied along the transport direction to fill the valence band states. Although the selected basis set is quite localized, connections up to the seventh nearest-neighbor are still taken into account.

As a next step, the PBC blocks are removed from the Hamiltonian $H$ and overlap $S$ matrices produced by CP2K. Then $H$ and $S$ are imported into a quantum transport environment. A Wave Function (WF) equation $\left(E \cdot S - H - \Sigma^{R,B}\right) \cdot C = Inj$ is solved for all the conduction band electron energies $E$ with a parallel sparse linear solver such as MUMPS [6]. In 3-D ballistic transport simulations computing the expansion coefficients $C$ is more than $10\times$ faster than solving the standard Non-equilibrium Green's Function (NEGF) equations [3]. The open boundary conditions ($\Sigma^{R,B}$ and $Inj$) are obtained through an extension of the high-performance FEAST algorithm [7]. The Poisson equation is formulated on a finite element grid and accounts only for the charge coming from the conduction band since the influence of the valence band electrons has already been considered in CP2K.

**Results** As an application, the $n$-type Si NWFET shown in Fig. 1 is simulated. It has a diameter of 2.2 nm and a total length of 35 nm. Its atomic structure consists of 64 unit cells for a total of 10,560 atoms. In comparison to tight-binding, DFT underestimates the nanowire band gap by about 0.4 eV, but in the absence of tunneling, the consequences on the device behavior remain minimal. It is worthwhile noting that a $sp^3d^5s^*$ tight-binding calculation of the same NWFET as DFT leads to a very similar bandstructure.

Figure 2 depicts the average electron density and electrostatic potential energy of the Si NWFET in Fig. 1 at different gate voltages. The electron density close to the source and drain contacts is equal to the doping concentration because charge neutrality is imposed in these regions through the boundary conditions of the Poisson equation. In Fig. 3(a) the transmission probability through the same Si NWFET as before is shown at $V_{gs}$=0.0, 0.2, and 0.4 V while the $I_d$-$V_{gs}$ characteristics at $V_{ds}$=0.6 V are plotted in Fig. 3(b) and compared to tight-binding calculations. For the simulated device with an ideal atomic structure, the DTF and tight-binding results match very well, but they might strongly differ when surface reconstruction effects and discrete doping atoms are introduced.

**Conclusion** In this paper, it has been demonstrated that ab-initio simulations of realistic systems of the size of 10,000 atoms and more is possible through the development of advanced algorithms and a massive parallelization of the work load. These capabilities will open new perspectives to carefully design next-generation nano-devices.

**References** [1] M. Brandbyge et al., Phys. Rev. B **65**, 165401 (2002). [2] J. VandeVondele et al., Comput. Phys. Commun. **167**, 103 (2005). [3] M. Luisier et al., Phys. Rev. B **74**, 205323 (2006). [4] S. D. Suk et al., Proc. of IEDM 2007, 891 (2007). [5] S. Goedecker et al., Phys. Rev. B **54**, 1703 (1996). [6] P. R. Amestoy et al., Comput. Methods in Appl. Mech. Eng. **184** 501 (200). [7] E. Polizzi, Phys. Rev. B **79**, 115112 (2009).

ISBN 978-2-9547858-0-6

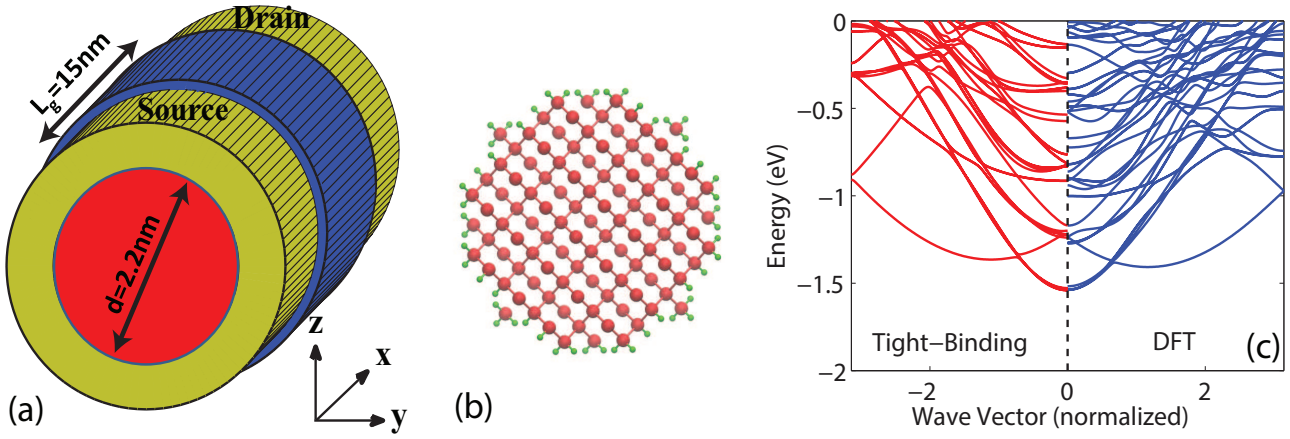


Fig. 1. (a) Schematic of the Si nanowire field-effect transistor (NWFET) considered in this work: it is composed of a $L_g$=15 nm long channel with a diameter $d$=2.2 nm, the source and drain extensions measure 10 nm each and are doped with $N_D$=1e20 cm$^{-3}$. The surrounding oxide layer has an equivalent oxide thickness EOT=1 nm made of $SiO_2$ Transport occurs along the <100> crystal axis. (b) Cross section of the selected Si NWFET. It contains 165 atoms (Si: 113 in red, H: 52 in green) with 12 orbitals per atom. The Si nanowire includes 64 such unit cells for a total of 10,560 atoms. (c) Conduction bandstructure corresponding to the cross section in sub-plot (b). Tight-binding ($E_g$=1.863 eV) and DFT ($E_g$=1.489 eV) results are shown.

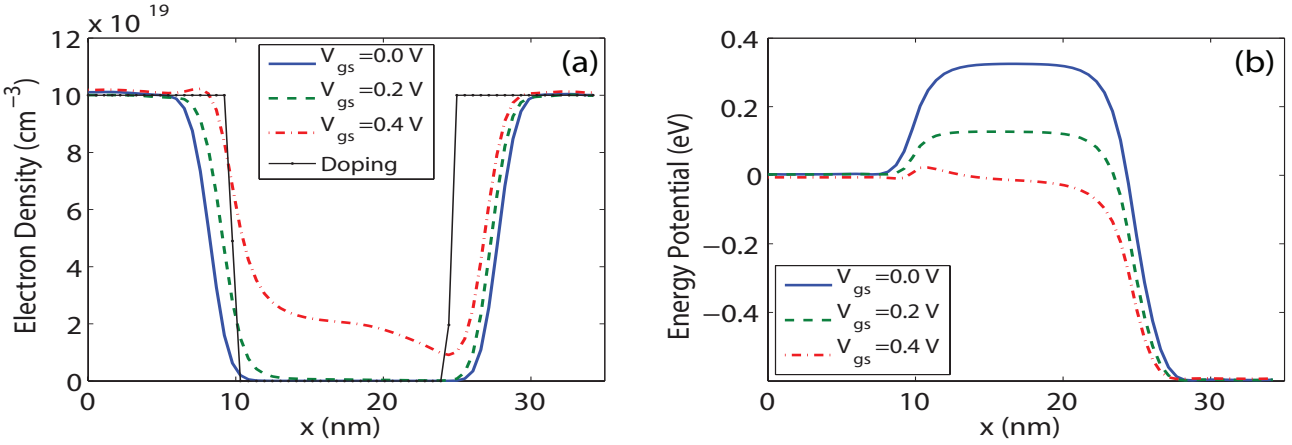


Fig. 2. (a) Electron concentration per unit cell (in cm$^{-3}$) and (b) averaged electrostatic potential energy in the Si NWFET of Fig. 1 at different $V_{gs}$ and $V_{ds}$=0.6 V. The solid blue lines refer to $V_{gs}$=0.0 V, the dashed green lines to $V_{gs}$=0.2 V, and the dashed-dotted red lines to $V_{gs}$=0.4 V.

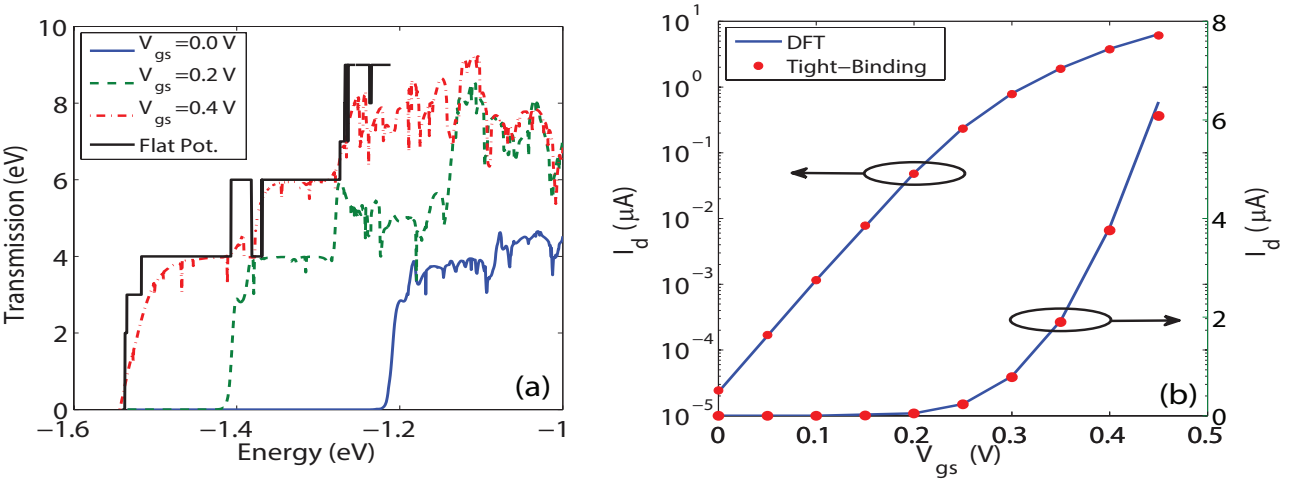


Fig. 3. (a) Transmission through the Si NWFET in Fig. 1 under different bias conditions. The same plotting conventions as in Fig. 2 are used. Furthermore, the transmission through a nanowire with a homogeneous flat potential is reported (black solid line). (b) Transfer characteristics $I_d$-$V_{gs}$ at $V_{ds}$=0.6 V of the same NWFET as before. Both DFT (blue lines) and tight-binding (red dots) currents are plotted on a logarithmic and linear scale.