A short tutorial to 1D Hetero-structure Lab, simulation of a Heterojunction Field Effect Transistor.

Jean Michel Sellier
Electrical Engineering Building,
Purdue University

jsellier@purdue.edu

Introduction

The 1D Heterostructure Tool is a program for the design and simulation of 1D heterostructures. It currently implements the effective mass bandstructure model and parameters for materials belonging to GaAs substrate such as GaP, InAs, AlGaAs etc.. The user can also choose to use the semiclassical Fermi-Dirac distribution which can be faster on bigger devices. A friendly GUI has been implemented in order to easily design the heterostructure to be simulated. It is possible to define a new device in a few mouse clicks. The layers can be easily duplicated by means of "Copy and Paste" features and the heterostructure energy band can be visualized before the simulation is launched.

1D heterostructure Lab is available at the following link:

https://nanohub.org/tools/1dhetero/

The Device

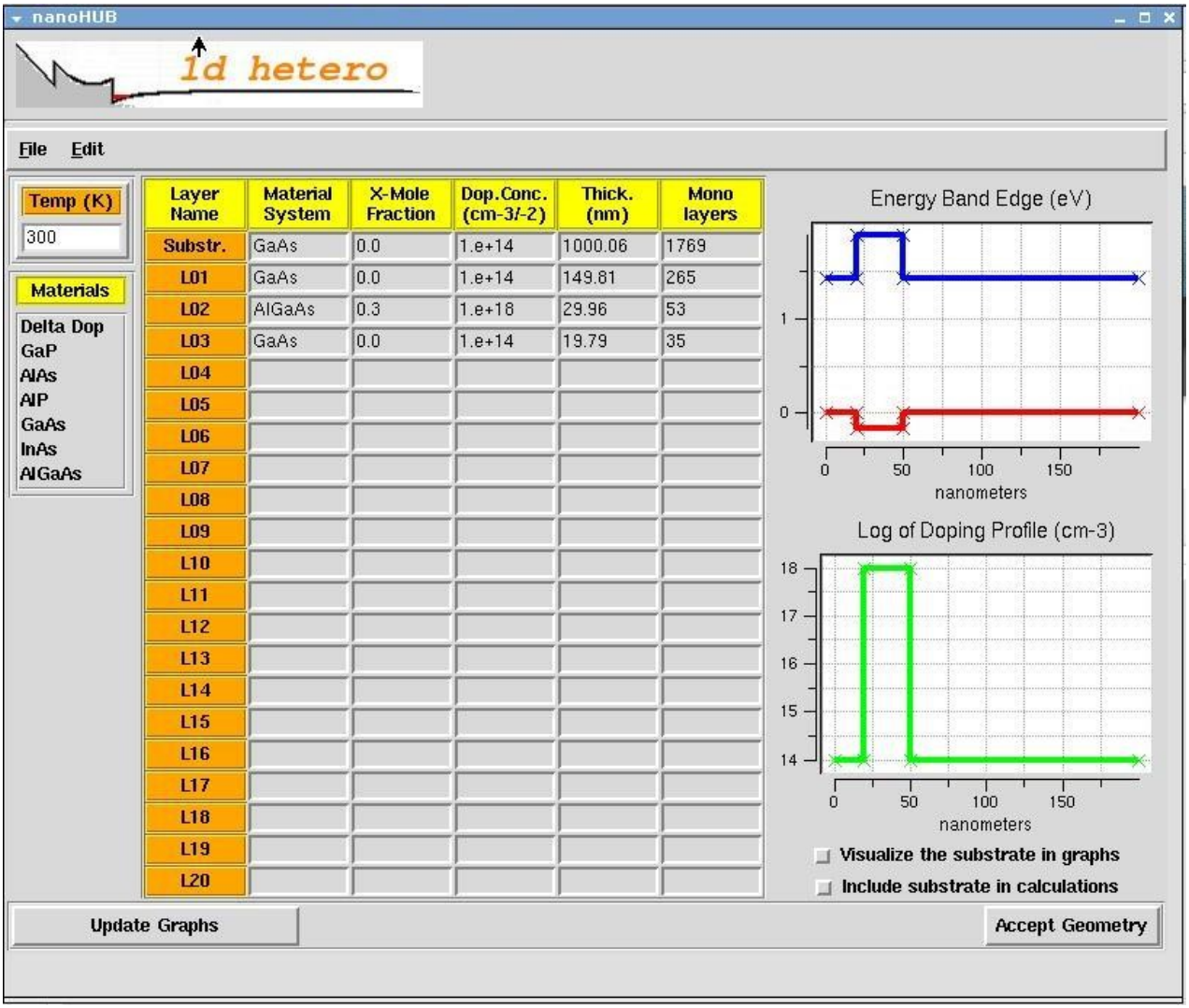
In the following, we want to simulate a Heterojunction Field Effect Transistor (HFET). An HFET is constructed by creating a junction between two materials that have differing band-gap energies, commonly referred to as a “heterojunction”. In practice, a moderately thick layer of doped AlGaAs is placed on top of a thick layer of GaAs forming a heterojunction where the layers meet. The HFET uses the wide band-gap AlGaAs layer effectively as an insulator.

Fig.1 – Simplified plot of a HFET

The simulation

In order to launch a simulation, click on the above link and then on the following button:

As one can see, once the tool is launched, the default device to be simulated is the HFET.

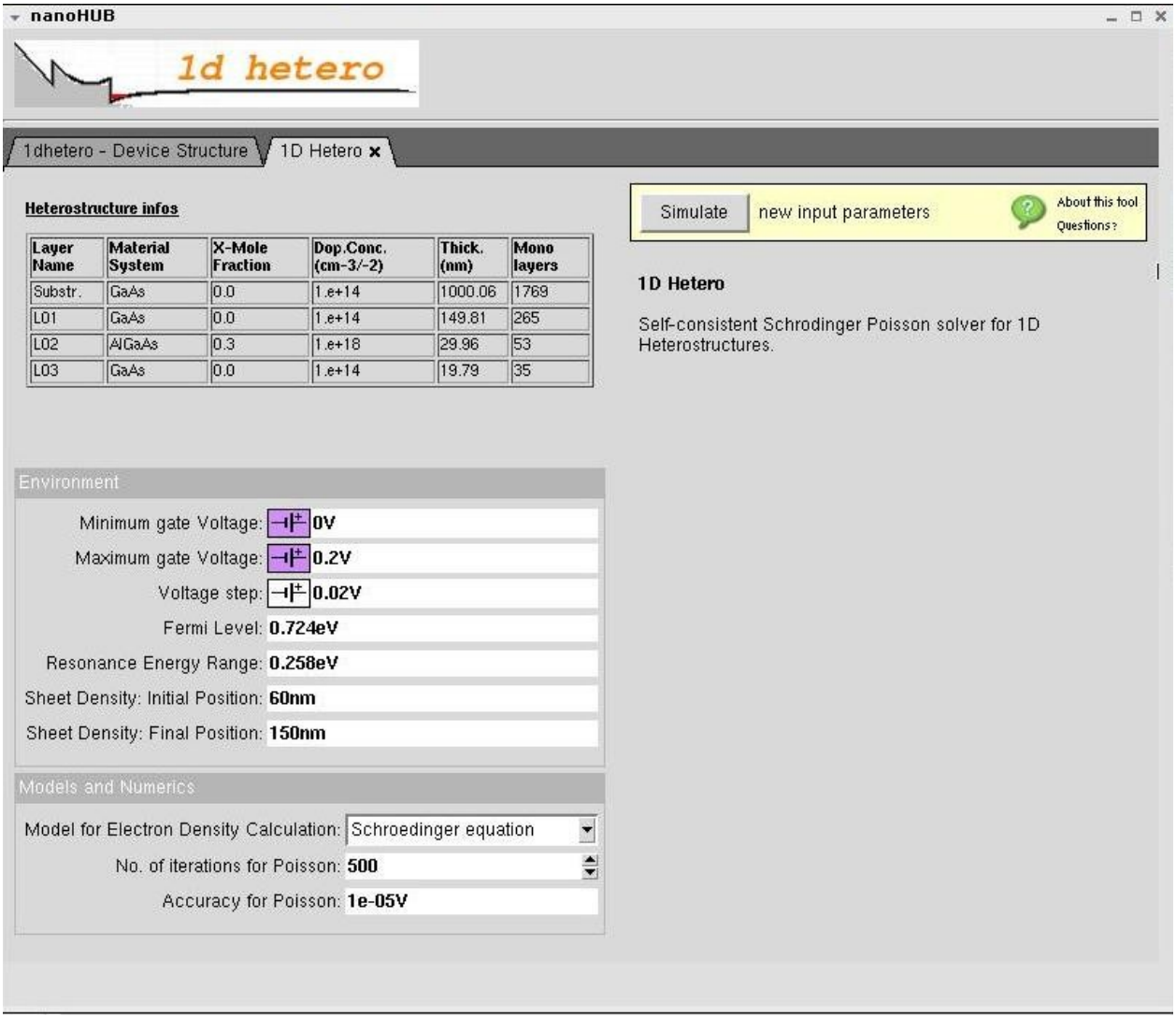


The first GUI that appears deals with the definition of the heterostructure to be simulated. By a simple click, it is possible to define a new layer in the structure. The most important values the user has to specify in order to define a new layer are the material name, the doping concentration and the thickness. Eventually, one can specify the thickness in number of monolayers instead of nanometers. The X-mole fraction has to be specified only if the material is an alloy, otherwise it will be ignored.

To specify a new layer one can click on a layer label (like “L01”, “L02”, etc) and then on a material in the Material List in the left side of the table. Alternatively, it is possible to specify the material by typing it in the related entry.

Once the user has specified the heterostructure, the GUI is ready to simulate it.

In our particular case, the HFET is the first default example. It consists of a substrate (1000.06 nm), a GaAs layer (149.81 nm), a AlGaAs layer (29.96 nm, X-mole 0.3), and finally a GaAs layer (19.79 nm).



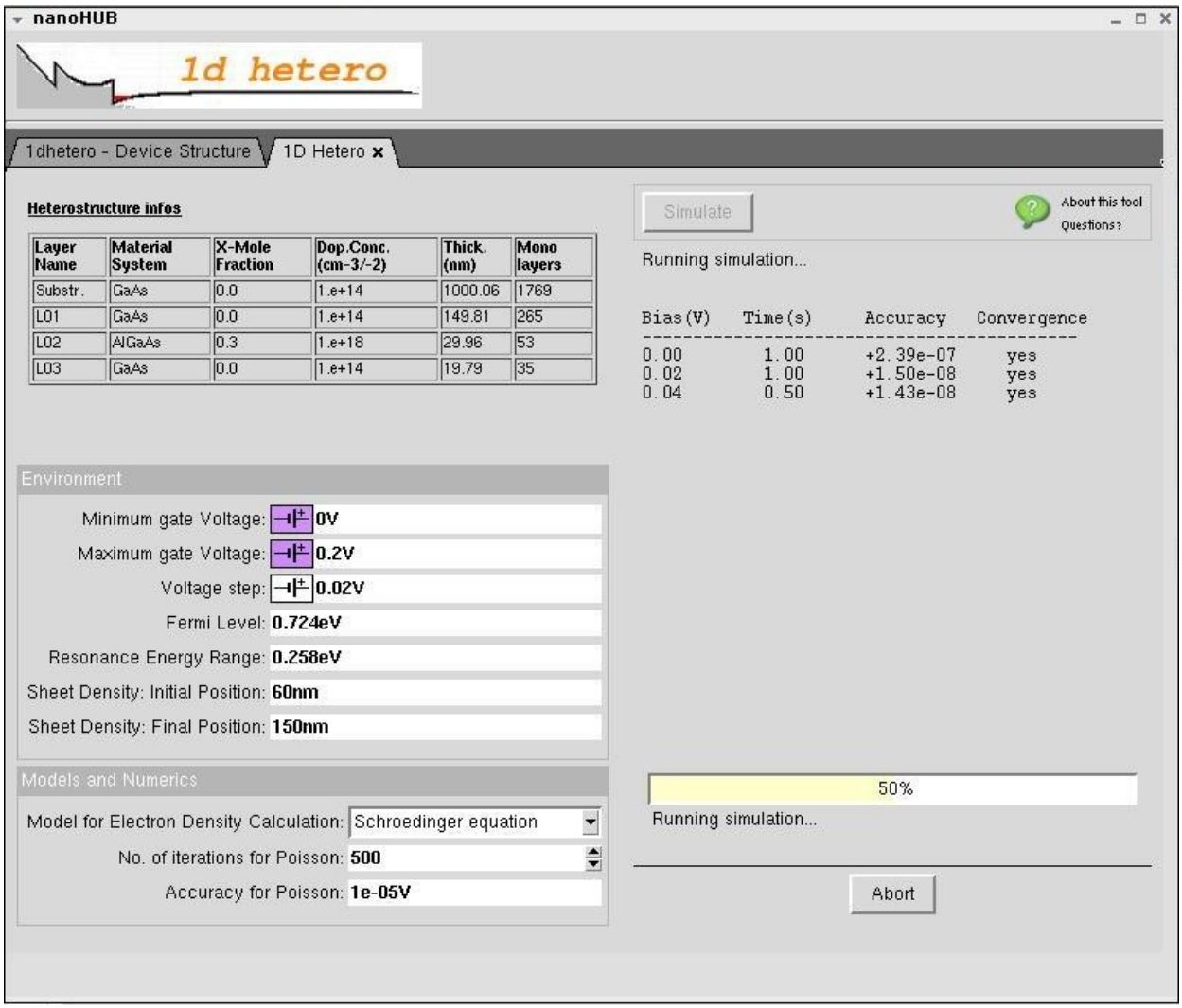
In the bottom right part of the first GUI, one finds the “Accept Geometry” button. Clicking on this button, the user basically launch a second GUI which defines some other simulation variables.

The second GUI that appears after clicking “Accept Geometry” is a classical Rappture GUI asking for further informations about the numerical methods one wants to use. The most important are the Fermi Level, the Resonance Energy Range and the model for Electron Density calculations.

The Fermi level, *Ef*, is specified in eV and is kept fixed during the simulation.

The Resonance Energy range, *RE*, specify the energy interval in which the algorithm is looking for resonances. The interval is specified as *[Ef-RE,Ef+RE]*.

The models for electron density calculations can be one of the following two:
- Schroedinger, quantum tight binding model with orbitals *s1*
- Thomas-Fermi, semiclassical model

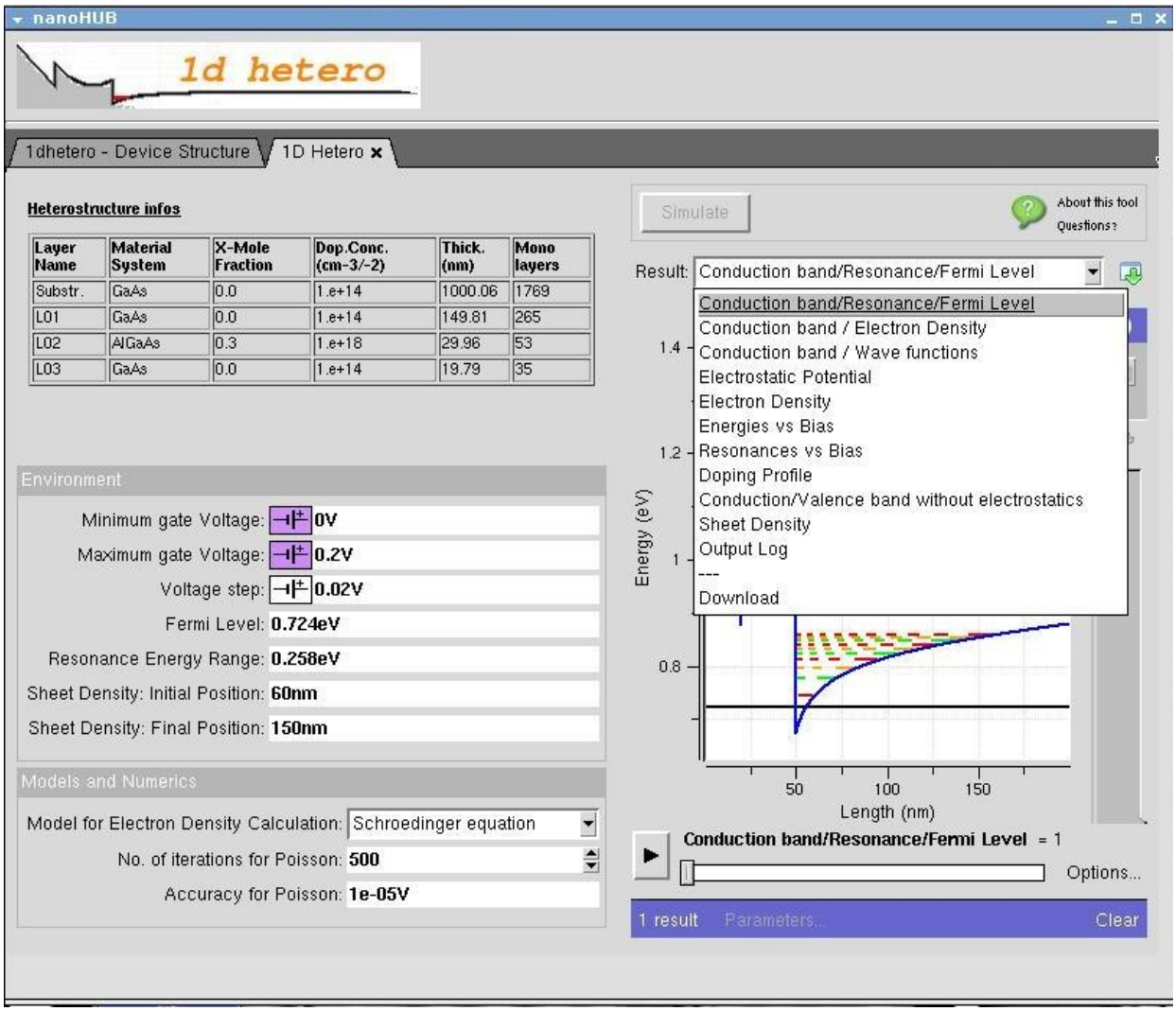


Once the user click on the “Simulate” button, the simulation starts. Some message shows up on the screen during the calculations so that the user can understand what's going on.

The values reported in the table are the bias, which represents the currently applied gate voltage (in Volts), the time of computation for that particular bias (in seconds), the numerical accuracy, which is the accuracy reached on the potential profile during the Schroedinger-Poisson iteration, and the convergence results, which reports if the iteration converged or not.

The first picture the user faces after the simulation calculations is the above one. This picture represents the conduction band along the Fermi level and the resonances.

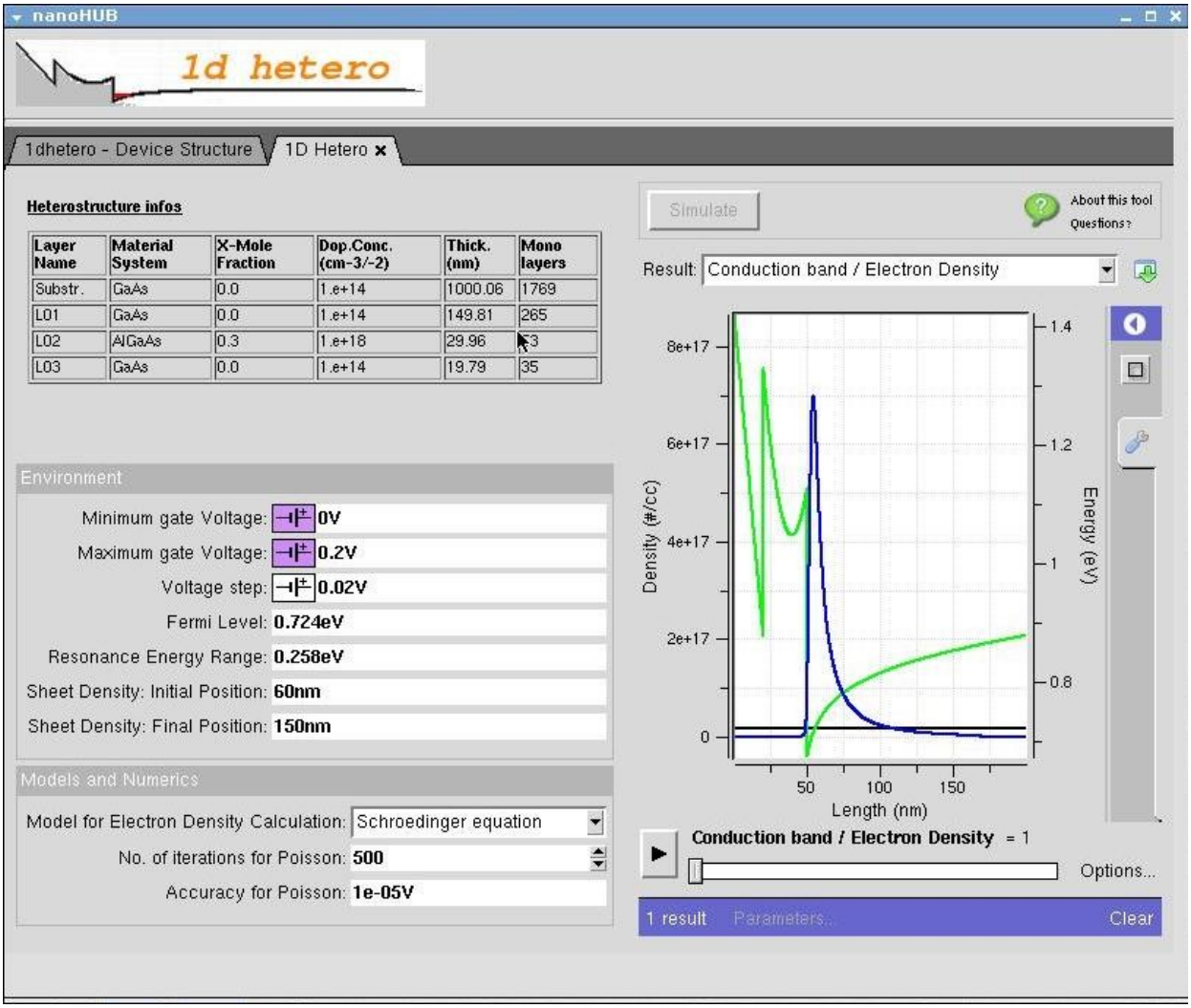
1DHetero displays the energy resonances as horizontal lines at the resonance energy E superimposed on the band profile plot. Each line represent the normalized electron wavefunction probability wherever it exceeds 50% of its local maximum value.



If the user click on the “Result” menu bar, a menu appears by means of which it is possible to visualize several different graphs. Many of those graphs give very good insights of the dynamic involved in the simulated device.

For example, the user can visualize the Electron density along with the conduction band, the wave functions, the electrostatic potential and so on.

In the following we report two pictures showing what can be practically visualized. All the pictures refer to the HFET simulated and described in the first part of the tutorial.



In this picture, the electron density is reported in function of spatial position. The green plot represents the conduction band.

As one can see a peak is reported in the proximity of the AlGaAs layer. It is possible to see how the peak slightly penetrate the AlGaAs layer, which is what one expects from such a quantum calculation.

In this graphs, the calculated eigenenergies are reported in function of the applied potential.

It is possible to see how the energies go down as the applied bias increases. This is what the experimentalists obtain during measurements so the calculated result is physically reasonable.