Simulation of 2D and 1D Field-Effect Transistors

Semiconductor devices II - EE-567

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So Far, We Studied

1. Band Structure;

2. Defects and Capacitance of 2D Materials;

3. Contacts;

Today, simulation of quantum devices

How to simulate devices with quantum structures?

Drift-diffusion equations are not enough, we have to consider a quantum approach:

Schrodinger (Wavefunction) + Poisson (Electrostatic)
Equations

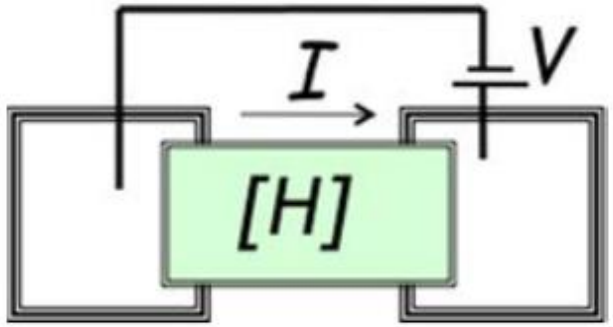
↓

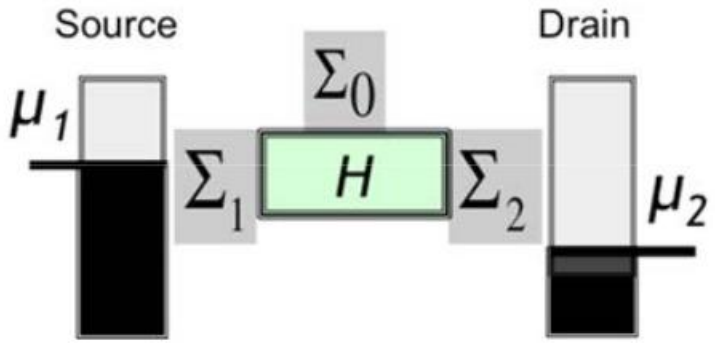
Non Equilibrium Green's Function Solver

Non-Equilibrium Green Function

- **Equilibrium** Green's Function doesn't assume approximations and a device is seen as a many body problem in which every interaction is accounted for. (Modeling is complex)

- **Non-Equilibrium** Green's Function (NEGF) considers the single particle problem (H) out of equilibrium with its interactions with the environment represented by self-energy functions (Σ). This problem can be approached more easily through computational modeling.





Non-Equilibrium Green's Function

Comparison between Equilibrium (many body) and Non-Equilibrium approaches:

Feature	Equilibrium GF	NEGF
Thermal	Equilibrium at T	General non-equilibrium
Structure	Uniform in space	Arbitrary coordinate dependence
Currents	Linear response	Arbitrary strength
Scattering	Conceptually difficult	Computationally difficult
Interaction	Many-body	Single-particle
Execution	Need a theorist on every step	Can program to an engineering tool

Extracted from Intel lecture on NEGF: https://nanohub.org/resources/18350/download/NikonovBeyondCMOS_3_NEGF.pdf

Datta, Supriyo
"Electronic transport in mesoscopic systems"
Cambridge university press (1997)

NEGF Method

Shrodinger equation with a perturbating term S → $[E - H_{op}]\psi = S$
(single-particle picture)

Green's function →

System's response — Green's function

$$D_{op}R = S \longrightarrow G = D_{op}^{-1} = [EI - H_{op}]^{-1}$$

Differental operator — Source of perturbation

Contacts and dissipating terms → $G^R = [EI - H_C - \Sigma^R]^{-1}$

Self-energy

The self-energy can be seen as an **effective Hamiltonian** expressing the interaction of the channel with the source and drain contacts as well as with a 'virtual contact' representing dissipating components.

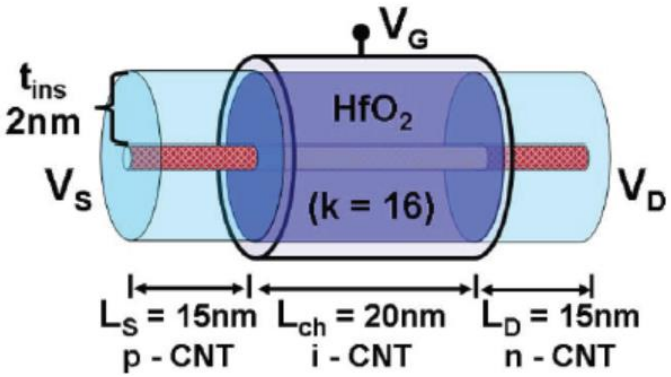
NEGF Method → Example: Carbon Nanotube

Source-drain lead terms of perturbation

$$G = [EI - H_{pz} - \Sigma_{S/D} - \Sigma_{Scat}]^{-1}$$

Channel Hamiltonian

Scattering inside the channel as a representation of **electron-phonon interactions**



The channel Hamiltonian can be discribed by a tight-binding model with a nearest-neighbor approximation → we consider the effect of each atom only on its closest neighbors.
In carbon-based electronics, ***pz* orbitals** are usually considered.

More complex materials → ***ab-initio*** treatments (e.g. DFT) are required

NEGF Method → Physical quantities

The self-energy expresses a correlation between states $(r;\ E)$ and $(r';\ E)$ ⟶ $\Sigma_{\phi}^{R} = \Sigma_{\phi}^{R}(r, r'; E)$

The Green's function represents the response of the system to S ⟶ $G^R = [EI - H_C - \Sigma^R]^{-1}$

Suffix ***R*** → **retarded** Green's function and self-energy
Suffix ***A*** → **advanced** Green's function and self-energy

By definition, G^A (Σ^A) is the **hermitian conjugate** of G^R (Σ^R).
How can they be related to physical quantities?

Let's define the *electron Green's functions* → $G^n(r, r'; E) = 2\pi \cdot \psi(r)\psi(r')^*$

And the so-called *spectral function* is the NEGF equivalent of the density of states → $A = G^n + G^p$

NEGF Method → Scattering states

G^R represents the *e* wavefunction related to a impulsive source S → $\psi(r) = \int G^R(r, r_1) \cdot S(r_1) \cdot dr_1$

We define Σ^{in} as the self-energy of scattering *into* a state → $\Sigma^{in}(r_1, r_1') \sim S(r_1)S^*(r_1')$

Thus, by taking the complex conjugate: $G^n(r, r'; E) = 2\pi \cdot \psi(r)\psi(r')^*$ ⟶ $G^n = G^R \Sigma^{in} G^A$

We define Σ^{out} as the self-energy of scattering *out of* a state.
Intuitively, by following the same steps, we obtain the relationship for holes ⟶ $G^p = G^R \Sigma^{out} G^A$

As we defined the spectral function *A*, we can consider the total scattering between states as the sum between in and out self-energies →

Broadening function

$\Gamma = \Sigma^{in} + \Sigma^{out}$

NEGF Method → Reservoirs

In order to deal with a real device structure, we can consider *i* terminals (contact leads) that act as **reservoirs of states in equilibrium**.

Then, it is possible to assign electrochemical potentials to each contact and consider its effects on the channel states through Γ, also called the **broadening function**.

In such a case, the electron and hole states, as well as the the *in* and *out* scattering components, can be described by Fermi-Dirac statistics:

$$G^n(E) = f(E) \cdot A(E) \;\; ; \;\; G^p(E) = (1 - f(E)) \cdot A(E)$$

$$\Sigma_i^{in}(E) = f(E) \cdot \Gamma_i(E) \;\; ; \;\; \Sigma_i^{out}(E) = (1 - f(E)) \cdot \Gamma_i(E)$$

NEGF Method → Current

Continuity equation: $$i\hbar\nabla J = q[(H_c\psi)^*\psi - \psi^*(H_c\psi)] = -q\left\{[(H_c(r) - H_c(r')]\psi(r)\cdot\psi(r')^*\right\}_{r=r'}$$

We define $\nabla J = I_{op}(r, r', E)$ as the **current operator** ⟶ $$I_{op}(E) = \frac{iq}{h}[H_c G^n - G^n H_c]$$

The broadening function can be expressed as → $$\Gamma = i(\Sigma^R - \Sigma^A) = \Sigma^{in} + \Sigma^{out}$$

and is the **main contribution to the current**, since it expresses the presence of movement of carriers out of the channel.

NEGF Method → Current

The current is obtained by considering the current operator components such that r = r':

$$\int \nabla J(r;E)dr = \int I_{op}(r,r;E)dr = Tr[I_{op}]$$

← Trace of I_{op} matrix

By performing algebraic operations on what we obtained and adding some more knowledge on what contributes to the current, we can derive the following:

Landauer-Buttiker formalism in NEGF

$$I(E) = \frac{q}{h} \cdot Tr[\Gamma_1 G^R \Gamma_2 G^A] \cdot (f_1 - f_2) \longrightarrow I = g_s g_v \frac{q}{h} \cdot \int_{-\infty}^{+\infty} \overbrace{Tr[\Gamma_1 G^R \Gamma_2 G^A]}^{T(E)} \cdot (f_1 - f_2) \cdot dE$$

NEGF Method → Current

$$I = g_s g_v \frac{q}{h} \cdot \int_{-\infty}^{+\infty} \overbrace{Tr[\Gamma_1 G^R \Gamma_2 G^A]}^{T(E)} \cdot (f_1 - f_2) \cdot dE$$

This expression is reminescent of the Landauer-Buttiker formalism for quantum transport, which is used for example in 1D Tunneling Field-Effect Transistors (TFETs) as: $I_t = g_v \frac{q}{\pi\hbar} \cdot \int_0^{qV} T_{WKB} \cdot [f_v(E) - f_c(E)] \cdot dE$

So why using NEGF?

The main point of NEGF is to have the possibility of including self-energy functions representing different types of physical phenomena in the channel, such as phononic scattering. Moreover, it is indipendent on the specific system, allowing to study situations where an analytical expression is not available.

→ Quantum transport can be studied for any system with a known Hamiltonian and self-energies

Self-consistent device simulation

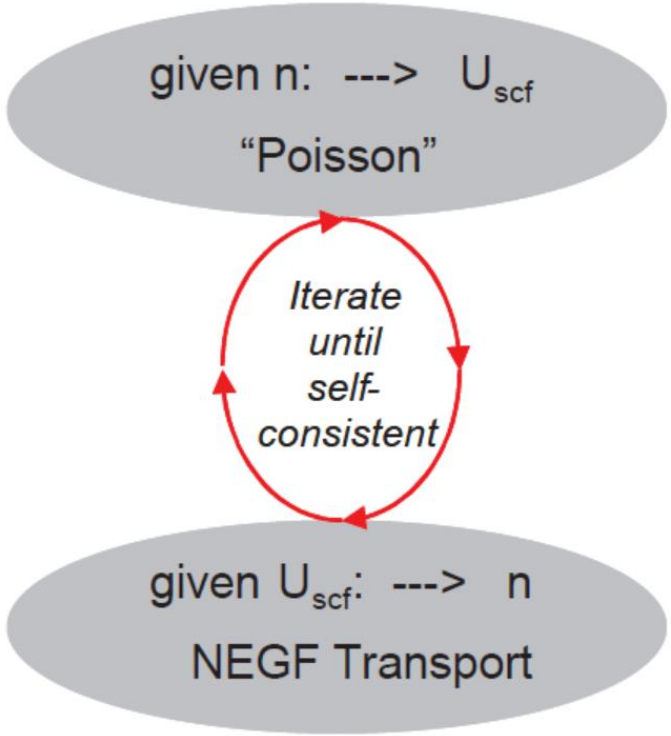
Poisson's equation:

$$\nabla^2 U(r,z) = -\frac{\rho(r,z)}{\epsilon}$$

Charge density distributions from NEGF:

$$n(z_j) = \sum_{m,s} \frac{1}{\Delta z} \cdot \int_{-\infty}^{+\infty} \frac{G^n_{i,j}(E,m)}{2\pi} \cdot dE$$

$$p(z_j) = \sum_{m,s} \frac{1}{\Delta z} \cdot \int_{-\infty}^{+\infty} \frac{G^p_{i,j}(E,m)}{2\pi} \cdot dE$$

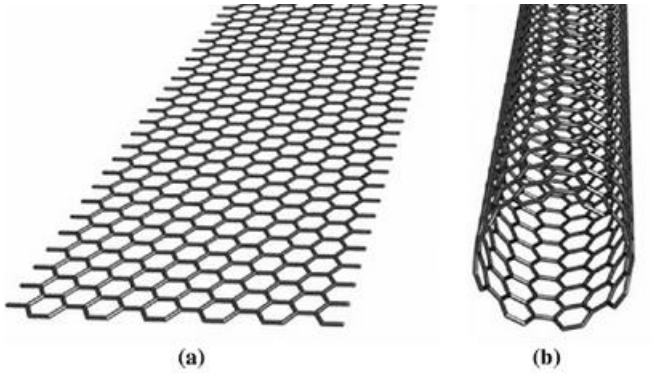


Self-consistent calculation of the **current** in the device

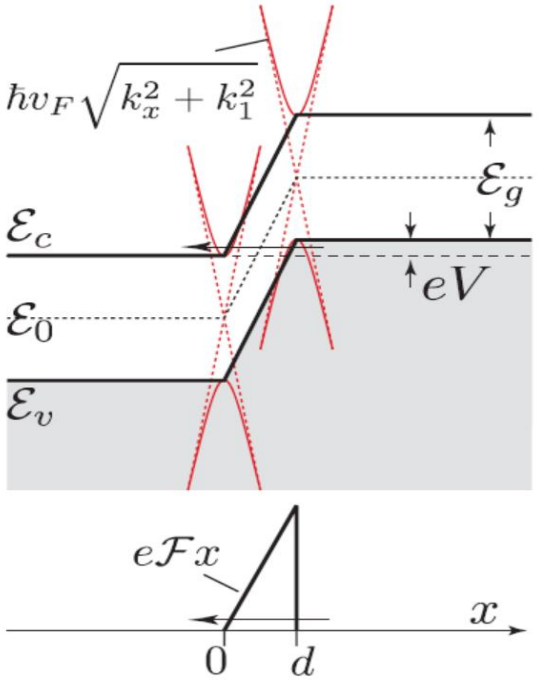
Application:
1D Tunnel Field-Effect Transistors

TFETs based on Carbon Nanotubes (CNT) or Graphene Nano Ribbons (GNR):

- Radial or lateral quantization → opening of a bandgap



GNR CNT



$$E \approx \pm\hbar v_F \cdot \sqrt{k_x^2 + k_n^2} \longrightarrow T_{WKB}^{(CNT,GNR)} \approx exp\left(-\frac{\pi E_g^2}{4\hbar v_F q\mathcal{E}}\right)$$

Analytical approach → Landauer – Buttiker formalism for the ON current:

$$I_t = g_v \frac{q}{\pi\hbar} \cdot \int_0^{qV} T_{WKB} \cdot [f_v(E) - f_c(E)] \cdot dE$$

- Valid in structure with **monodimensional** transport
- $T_{WKB} = T(E)$ optimization → high ON currents

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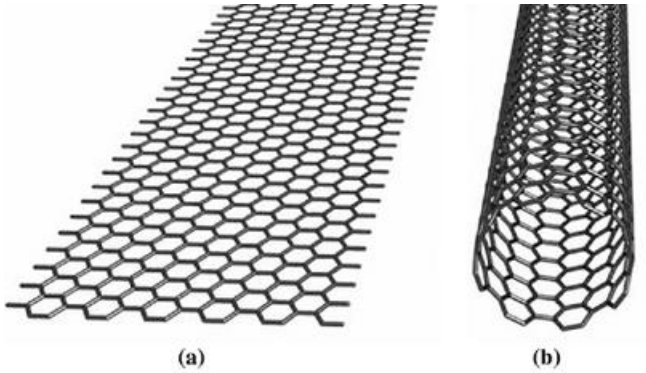
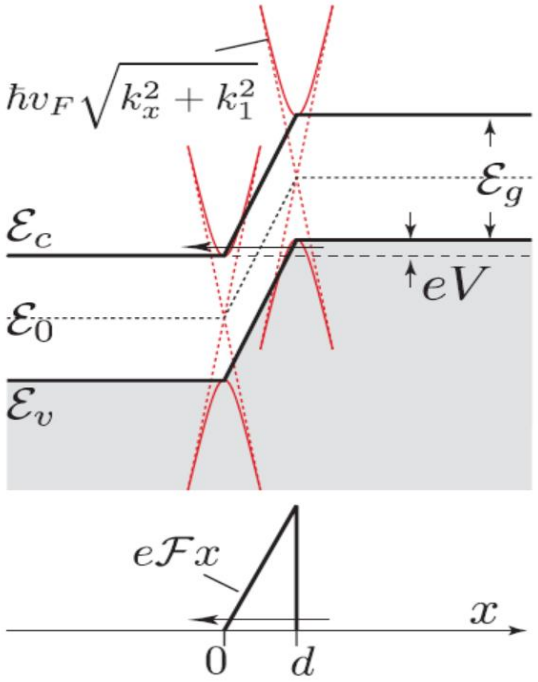


GNR CNT



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What about the OFF current?

Phonon-assisted tunneling is determinant → **NEGF** is required

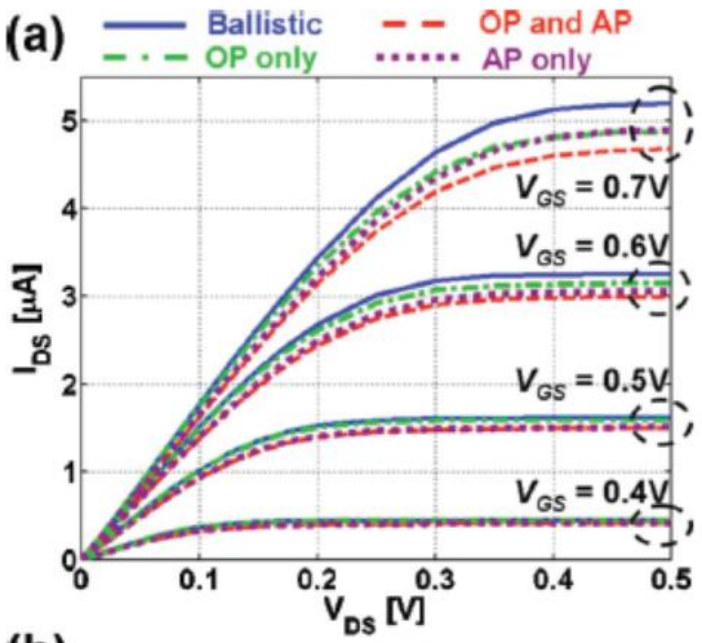
Application:
1D Tunnel Field-Effect Transistors

Koswatta, Siyuranga O., Mark S. Lundstrom, and Dmitri E. Nikonov.
"Performance comparison between pin tunneling transistors and conventional MOSFETs."
IEEE Transactions on Electron Devices (2009)

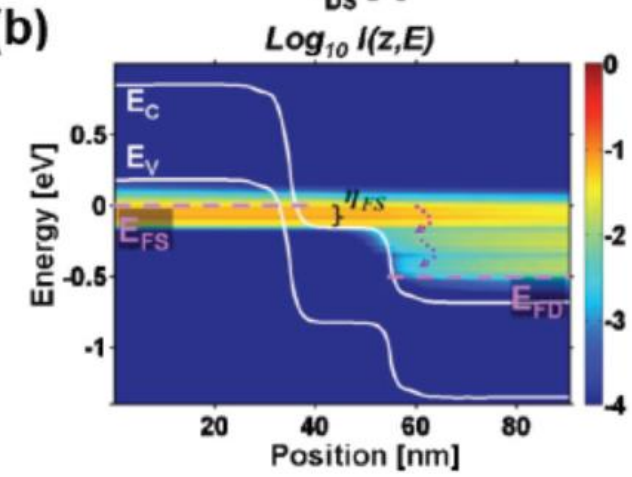
TFETs based on Carbon Nanotubes (CNT) p-i-n TFET:

- The ON current is dominated by band-to-band tunneling (BTBT)
- The Landauer-Buttiker formalism for ballistic transport is a good approximation for the ON current
- The full treatment of phonon-electron interactions in a self-consistent Poisson-NEGF approach reveals relatively small degradation of the ON current due to phonon scattering only for larger biases

  → backscattering due to AP (negligible)
  → emission of OP (dependent on bias)



CNT



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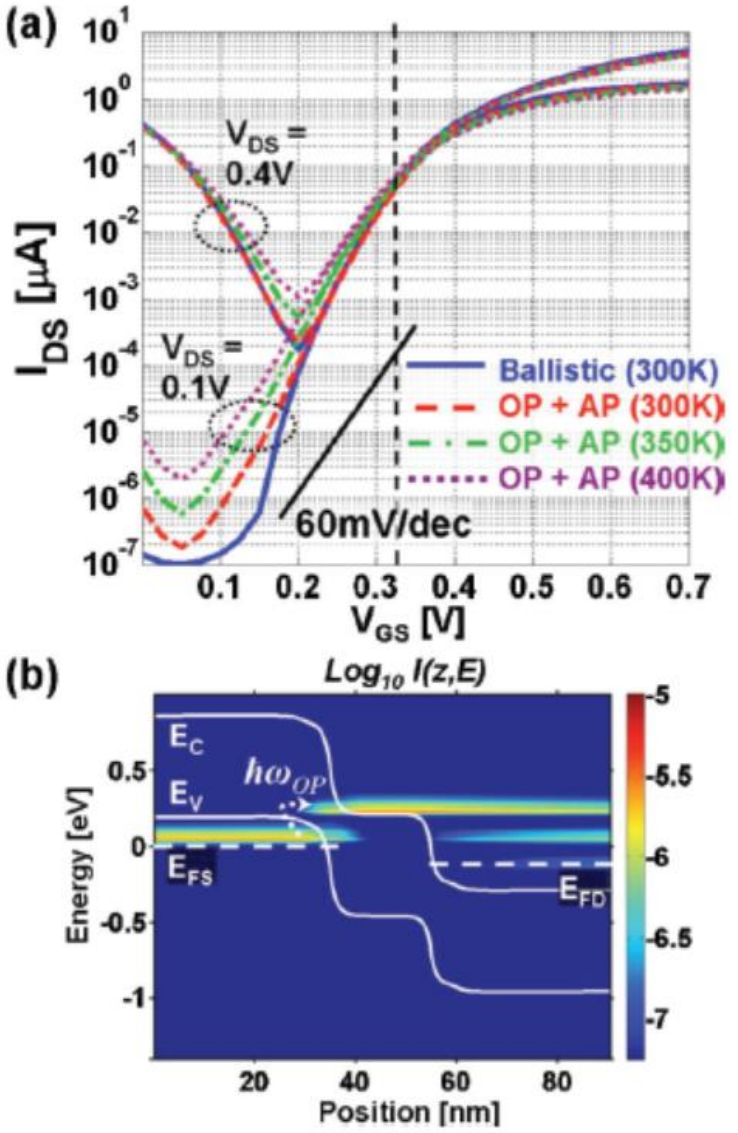
TFETs based on Carbon Nanotubes (CNT) p-i-n TFET:

- The OFF current is dominated by phonon-assisted tunneling of electrons
- High-energy OPs are determinant

  → phononic modes degradate SS

- Ambipolar TFET behavior due to tunneling holes. The ambipolar branch appears at higher V_{GS} for lower V_{DS} due to Drain-Induced Barrier Lowering (DIBL)



CNT

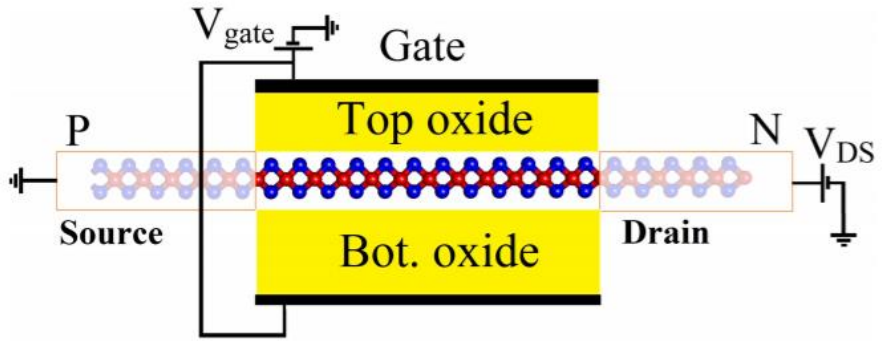
Application:
2D Tunnel Field-Effect Transistors

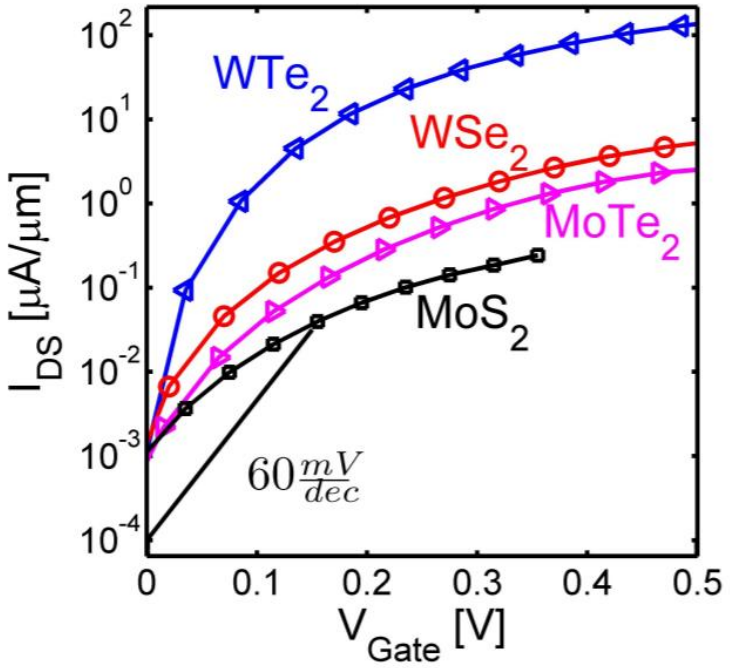
Ilatikhameneh, Hesameddin, et al.
"Tunnel field-effect transistors in 2-D transition metal dichalcogenide materials."
IEEE Journal on Exploratory Solid-State Computational Devices and Circuits (2015)

Simulations on TFETs based on 2D materials:

- Full consideration of band structure
  → NEGF for a complete quantum treatment
- Different 2D materials investigated
- ON currents can be compared based on semiclassical knowledge of the tunneling probability T_{WKB}
  → low effective mass and low gaps are preferable

Material	I_{ON}	Eg	m_r^*	λ	Λ	η
WTe_2	127	0.75	0.17	0.45	2.45	3.15
WSe_2	4.6	1.56	0.21	0.41	2.5	5.2
$MoTe_2$	2.3	1.08	0.32	0.5	2.7	5.8
MoS_2	0.3	1.68	0.29	0.38	2.5	6.3





Application:
Vertical Heterostructure TFETs

Szabo, Aron, Steven J. Koester, and Mathieu Luisier.
"Ab-initio simulation of van der waals MoTe 2–SnS 2 heterotunneling fets for low-power electronics."
IEEE Electron Device Letters (2015)

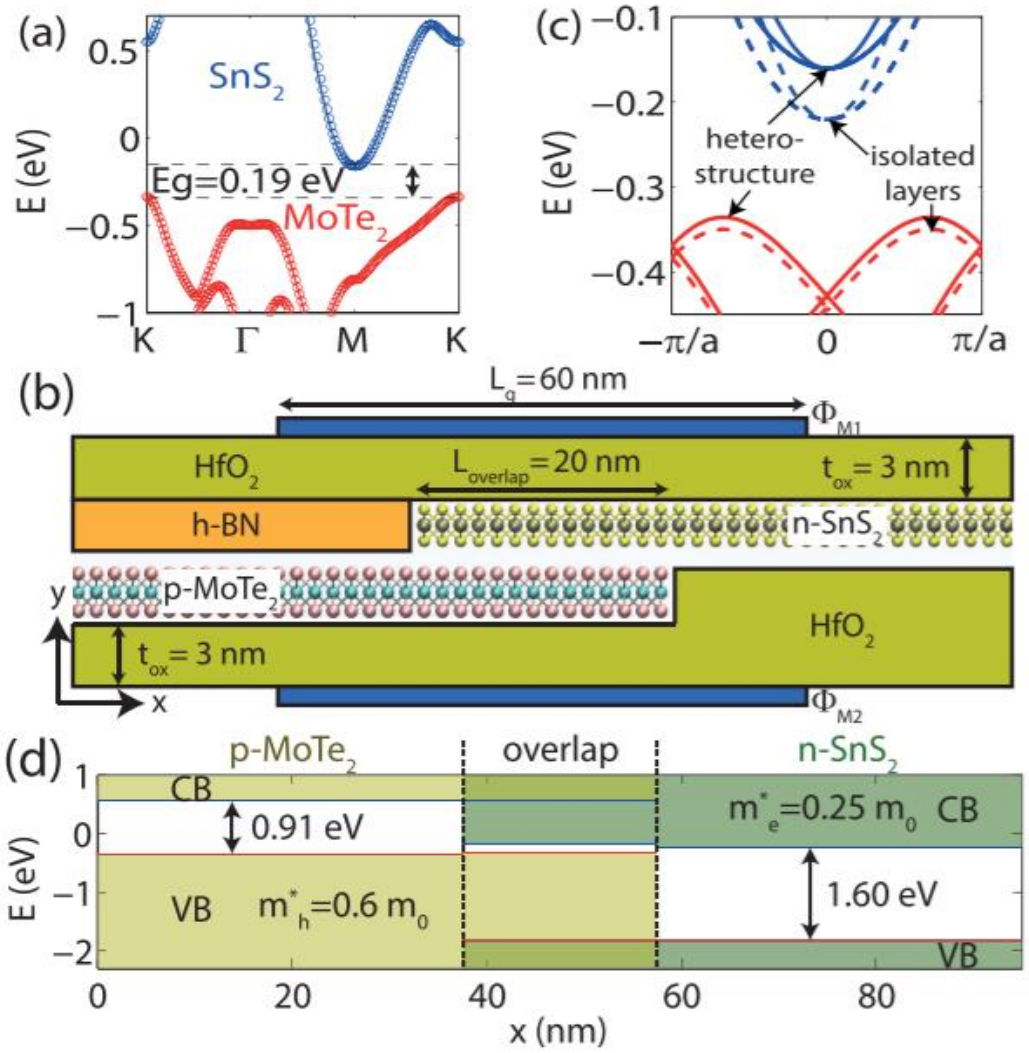
Simulation of heterostructure devices:

- DFT calculations for band structure of single layer and heterobilayer regions

  → staggered gap, good for tunneling FETs

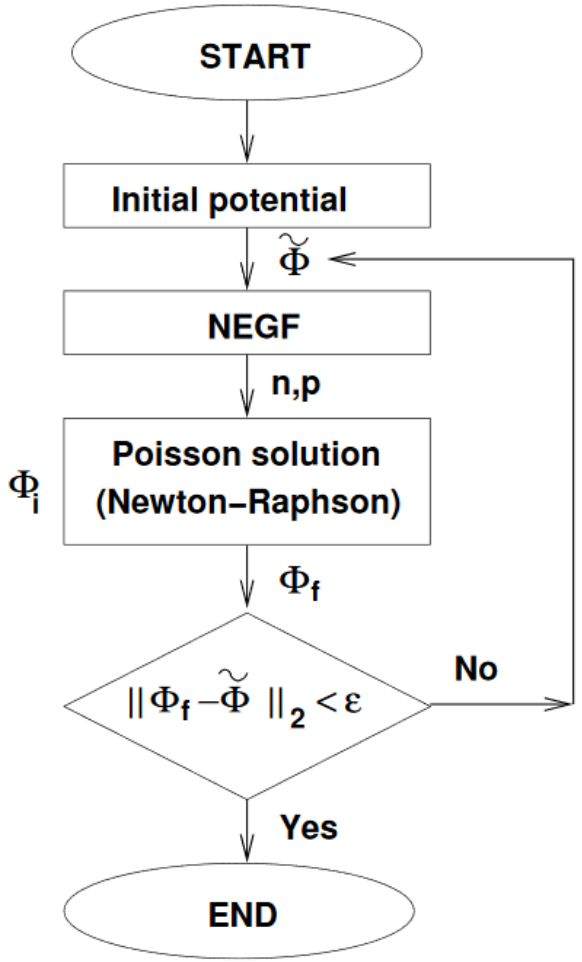
- Quantum transport approach for band-to-band tunneling between TMDs

- Advantage: small tunneling length, equal to distance between layers → high ON current



NanoTCAD ViDES

Method:



Simulator for Nanoelectronics developed at the University of Pisa by Prof. Iannaccone, Prof. Fiori & others:

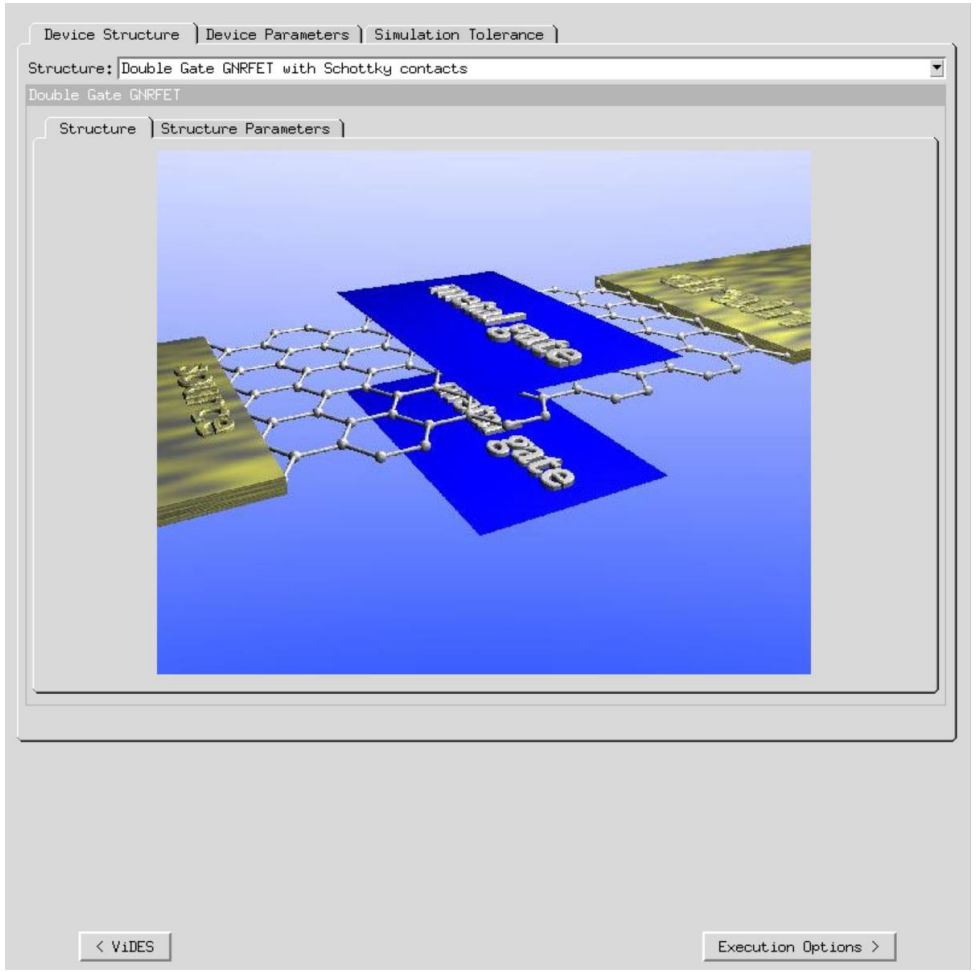
- Nanowires
- Carbon Nanotubes
- Graphene
- Transition Metal Dichalcogenides

Simulator for exercises

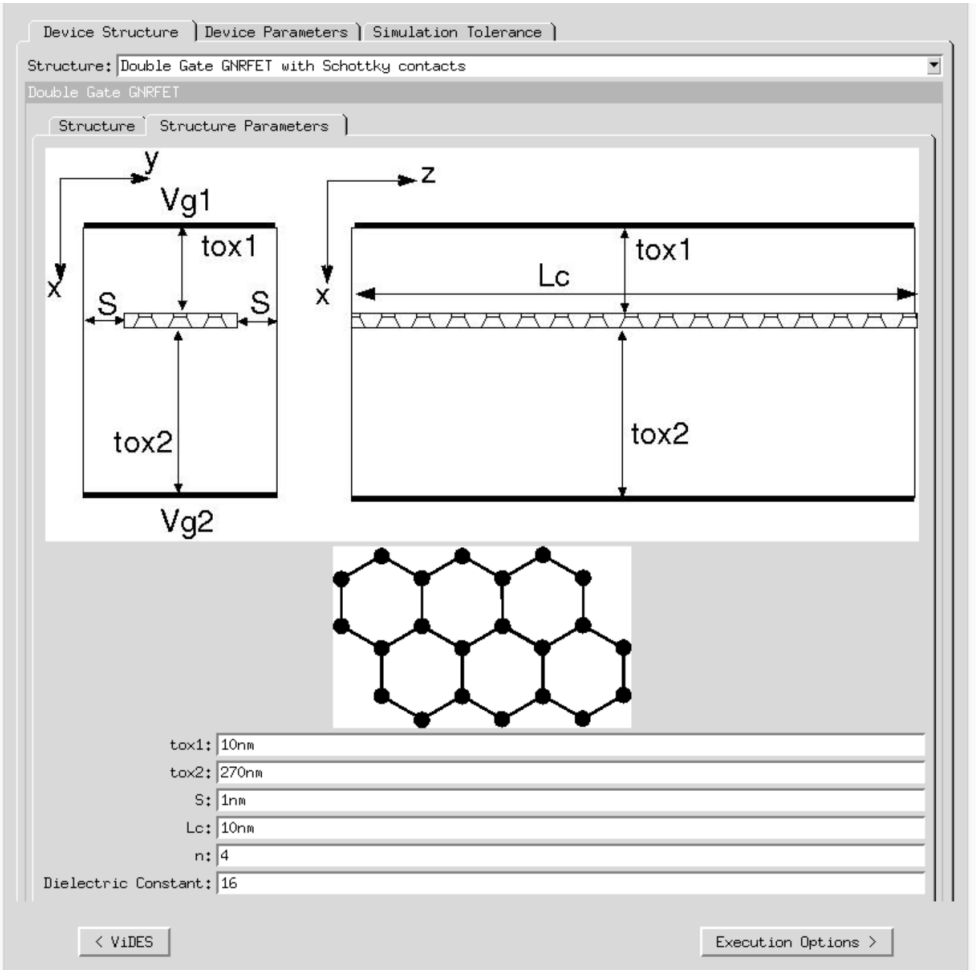
https://nanohub.org/resources/vides/

NanoTCAD ViDES – How to setup a simulation

Select device structure:

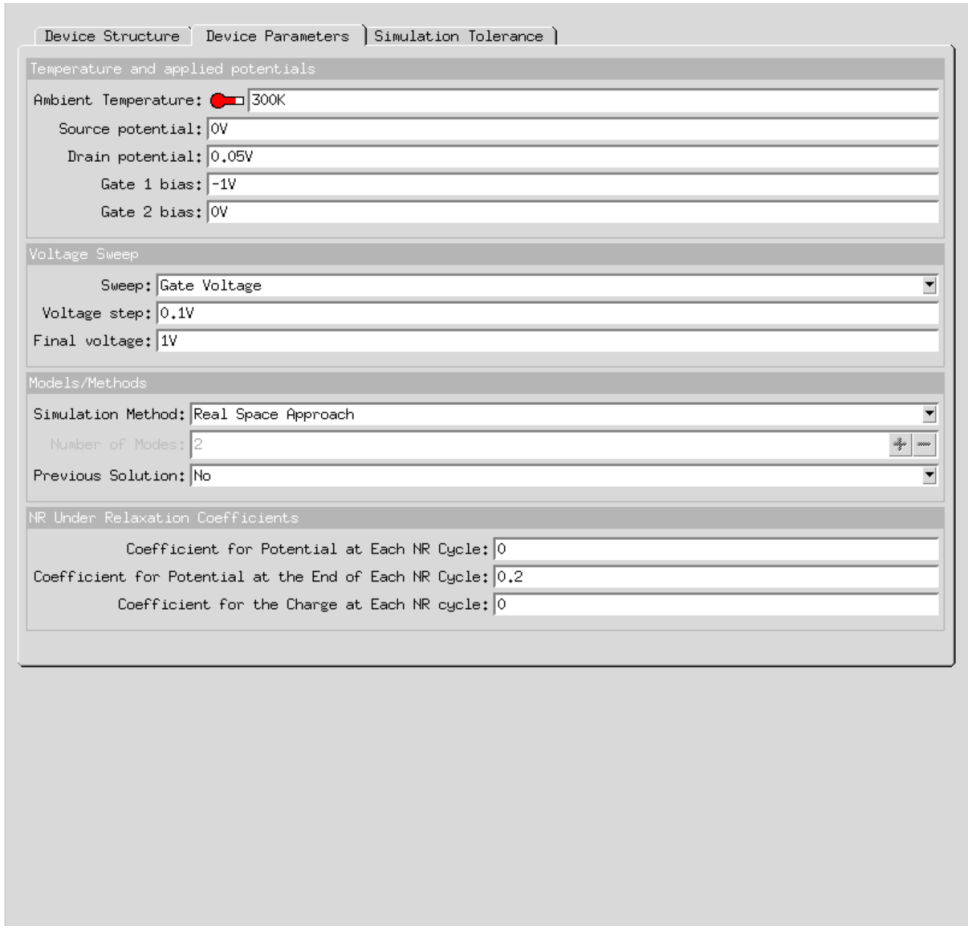


Define device structure parameters:

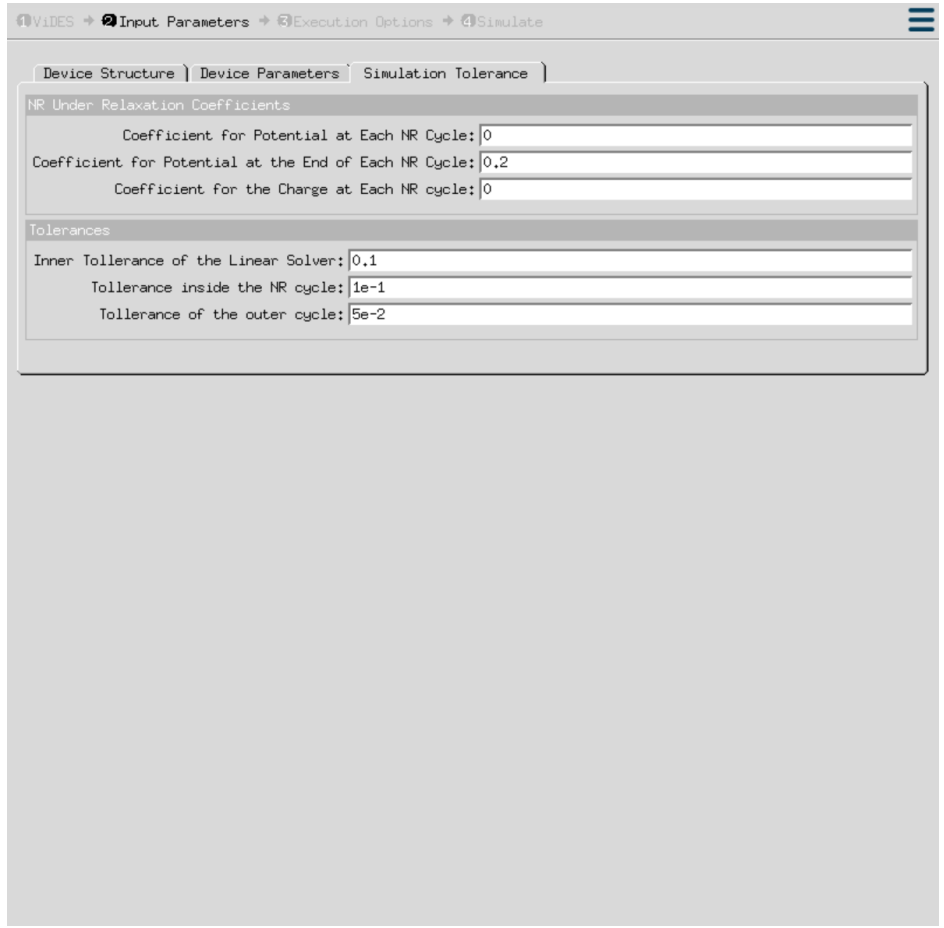


NanoTCAD ViDES – How to setup a simulation

Define Electrical Parameters:



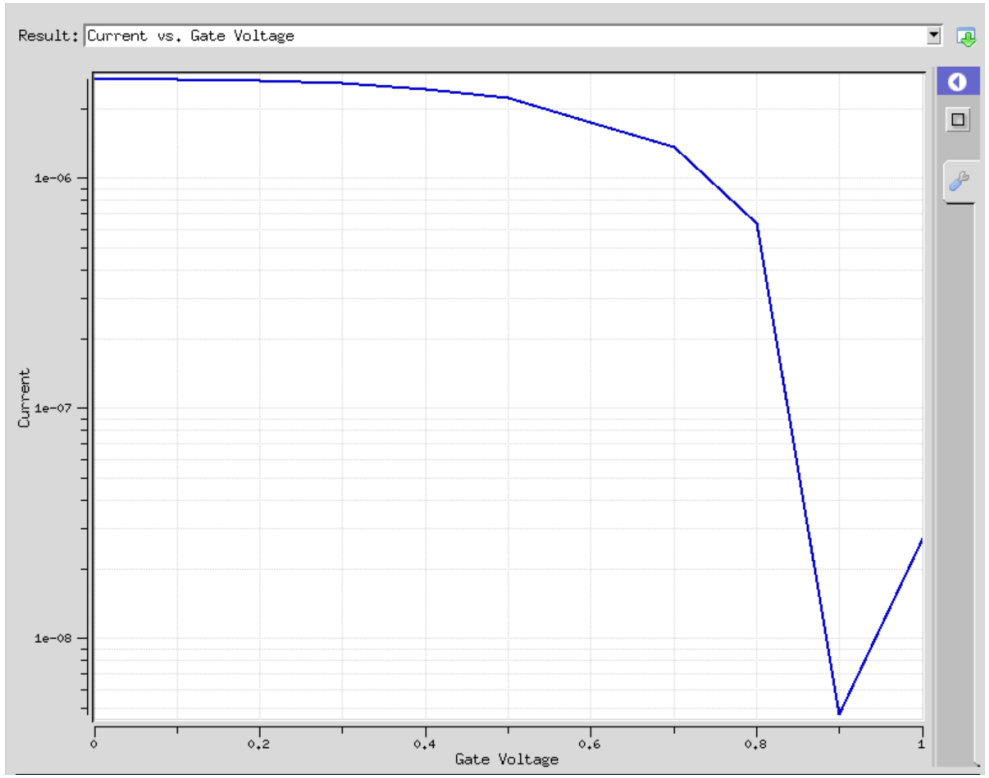
Define Simulation Parameters (don't need to change):



NanoTCAD ViDES – How to setup a simulation

Select Simulation and have fun:

Sample of Result:



Exercise

Type of Device:

1. Double Gate GNRFET with doped contacts
2. Parameters: - tox = 10nm
   - L = 10nm, 20nm, 100nm.
   - L_C (length contact) = 10nm, 20nm, 100nm.
3. Electrical Simulation:
   - I_{DS} versus V_{DS} (linear and in Saturation)
   - I_{DS} versus V_{DS} (Calculate the oxide breakdown voltage for this device and use it as the maximum gate voltage).
4. If you are curious, see the effect of temperature on device performance.

Observation:

Simulations are quite time consuming.