Molecular transistor circuits: From device model to circuit simulation

Molecular Transistor Circuits: From Device Model to Circuit Simulation

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***Abstract*—Molecular devices have been proposed as an alternative solution for the design and fabrication of complex logic functions. In this paper a hybrid model of the molecular transistor (MT) is used to simulate different logic circuits. The model is based on the density function theory (DFT) combined with the Non Equilibrium Greens Function (NEGF) to find the transmission spectrum (TS) at equilibrium. The self-consistent method is used to calculate the I-V characteristics at non-equilibrium condition, considering the more realistic case of broadening of energy levels under the assumption of strong molecule electrode coupling.**
We have used a four terminal device with source, drain and two gate electrodes: one (backgate) used to increase the I_{ON}/I_{OFF} ratio and the other as normal control gate. The very same device is contextualized in the case of a structure feasible with currently available technology and several technological parameters are used to explore the solution space. This ensemble has been described and simulated using VHDL-AMS and allowed the design of a library of logic cells e.g NAND, NOR, Inverter and Half Adder suitable for architecture design. Results are given on both the modeling level and the circuits functional performance. Our findings represent an important breakthrough in the state of the art 1) for the methodology and design flow used and 2) for the detailed understanding on the device analyzed and optimized with the point of view of the circuit designer.

I. Introduction

As the CMOS technology is approaching its physical and technological limitations, researchers are exploring alternative technologies for future electronic circuits. Molecular devices [1], [2] can play an important role in emerging nanoelectronics due to their small size and providing features like conductance switching, rectification etc. The characteristics of these molecular devices are dominated by quantum physics, which represent a change of paradigm with respect to the conventional studies normally adopted for CMOS devices. It is then essential to understand the molecular devices behavior and their interaction in order to correctly design circuits based on them. Nonetheless, it is mandatory to develop models and methods for enabling the design with optimal trade-off between the accuracy necessary to describe quantum physics phenomena and the limited complexity necessary for designing and simulating circuits of realistic complexity.

Various methods are used to investigate the behavior of electron transport in molecular systems. The common methods are Density Function Theory (DFT) [3] and Non Equilibrium Greens Function (NEGF) [4]. Derosa et al. [5] used the combination of DFT and NEGF. They rigorously treated the open boundary condition under the influence of applied bias voltage, which is the main advantage of their approach. This is now widely used to qualitatively reproduce the $I-V$ characteristics of experimental molecular systems. However, this method is computationally demanding. Different approximation methods have been discussed to reduce the computation overhead [6], [7].

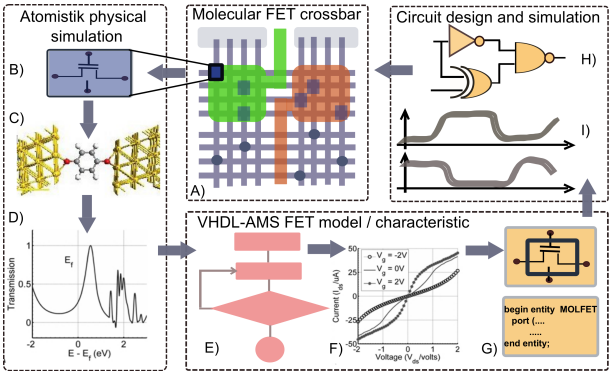

Figure 1: From device modeling to circuit simulation: A) Nanowire based crossbar architecture, B) Molecular Transistor (MT) element, C) MT Physical structure, D) MT transmission spectrum, E) Model and engine in VHDL-AMS, F) Voltage/Current (IV) characteristic, G) Modular HDL, H) Hierarchical circuits, I) Simulation output.

In this paper we aimed at finding optimal solutions to the mentioned problems. We started from a computationally efficient hybrid model i.e the combination of DFT and NEGF to find the transmission spectrum at equilibrium. We applied the self consistent method to calculate the $I-V$ characteristics at non-equilibrium condition. We included then the device model in a high level simulator and designed a library of different logic circuits based on this model referring to a possible architectural implementation. We simulated them including then the quantum physics phenomena in the functional logic results. The state of the art [8]–[10] reports several logic circuit implementations based on the molecular device models. Most of these circuits are build on 2-D array of wires. However, in all these circuit implementations the device model used only considers weak coupling / discrete energy levels. In this paper we considered a more realistic case of broadening of energy levels under the assumption of strong molecule-electrode coupling. Another important point to be considered and often neglected in literature is the leakage current, that occurs at zero gate voltage and low bias voltage in case of strong molecule-electrode coupling. We used a four terminal molecular field effect transistor (MOLFET) with back gate electrode to handle the problem of leakage current. We tested different molecules and selected the one with the highest I_{ON}/I_{OFF} ratio with the application of an optimized back gate voltage. The transistor model is described and simulated using VHDL-AMS, and is then used to build basic logic circuits in

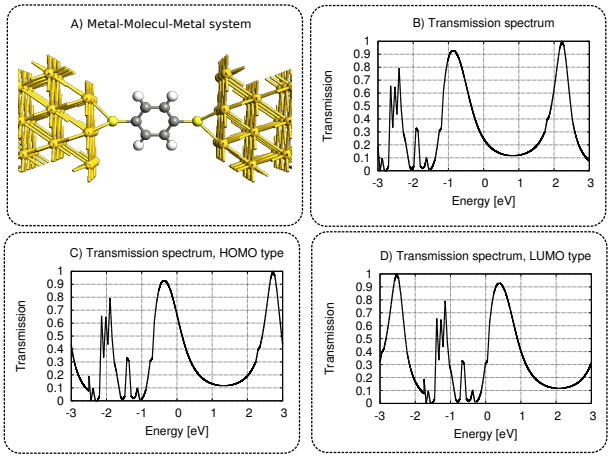

Figure 2: A) Schematic diagram of benzene molecule with thiol group sandwiched between two electrodes, B) transmission spectrum at $V_{gb} = 0$, C) transmission spectrum at $V_{gb} < 0$ and D) transmission spectrum at $V_{gb} > 0$.

a crossbar like architecture. In this work we used the crossbar architecture presented in [10] with the proposed modification of the back gate voltage regions for the MOLFET arrays.

Fig. 1 shows the methodology proposed for creating the architecture (A). We started with the structural metal-molecule-metal arrangement (B-C) from which the transmission spectrum of the device at equilibrium (D) is calculated and then with the iterative algorithm at non equilibrium (E), the shifted transmission spectrum and the $I-V$ characteristics are obtained (F). This transistor modeling is translated to the VHDL-AMS description (G) and then the logic circuits are organized (H) using the transistor model and simulated (I).

To summarize, our work contributes then to the advancement of the state of the art through several achievements: i) we introduce an accurate model and demonstrate its validity, ii) we introduce the use of a back gate electrode and demonstrate its effectiveness in order to enable the use of this type of device for logic purposes, iii) thanks to the way the model is conceived it requires reduced computational effort, so we could include it in a circuit level simulator and we could associate it to parameters related to technological related issues, iv) we designed a set of benchmark circuits based on this device and were able to simulate their correct functionality, their current/voltage levels and their dependency on technological choices.

The rest of the paper is organized as follows. The device model is described in sec. II. VHDL-AMS description of the transistor model is given in sec. III. The details of the architecture and results are in sec. IV and section V concludes the paper.

II. Device Model and Characterization

A. Hybrid model: Fig. 2 (A) shows the configuration of molecular transistor, in which the conductive channel is replaced by sandwiching a molecule between two electrodes and a capacitive gate. We studied this structure at equilibrium by using Atomistix ToolKit (ATK) [11], [12], where we placed an optimized molecule between two gold electrodes. For DFT exchange correlation, we used local density approximation (LDA) with unpolarized spin. Transmission function and details of energy level of the molecular system are calculated using Kyrlov [13] self-energy calculation.

When a molecule is bound to metallic electrodes, a charge exchange occurs between molecule and electrodes, causing a shift of the molecular energy states. Thus at equilibrium, the energy levels of molecule and contacts get aligned with respect to one Fermi energy level E_f. Energy levels above E_f are known as Lowest Unoccupied Molecular Orbitals (LUMOs) and levels below E_f are known as Highest Occupied Molecular Orbitals (HOMOs). When a molecule is strongly coupled with electrodes, energy levels broaden and interact with each other. In order to take this into account, NEGF-DFT formalism is used to find the transmission spectrum, as shown in Fig. 2 (B), where each peak corresponds to a molecular energy level. These peaks and the extracted transmission spectrum of the system are then used to estimate the new transmission spectrum at non-equilibrium conditions. When the applied voltage involves important peaks in the spectrum, the charging effect should be taken into account to estimate the shift of molecular energy levels (U_{SCF}). In our model, the shift of molecular orbitals is obtained by the self-consistent loop [6], [7]. In particular, $U_{SCF} = U_0(N - N_0)$, where U_0 is the charging energy (its value is taken as $1eV$). N_0 is the number of electrons at equilibrium hosted by the molecular orbitals. N is the electron population out of equilibrium and it is calculated by means of self-consistent field loop. New energies of states of molecular orbitals E_{new} are obtained by adding the self-consistent field energy U_{SCF} and the contribution of the gate potential to molecular orbital shift eV_{geff}. Particularly, in our model when the electrostatic potential is applied to the gate electrode, only a part of this electrostatic potential would effect the molecular energies. If molecular energy levels are not in resonance with E_f, the applied gate voltage shifts linearly the energy level with respect to E_F by $E = E_0 - e|\alpha|V_g - U_{SCF}$, where α is the gate efficiency factor which defines the amount of energy that would effect the molecular energy levels.

Once the position of the transmission spectrum is estimated for each pair of voltages (V_g,V_{ds}) the current I through the system can be calculated using the Landauer formula

$$I(V) = 2q/\hbar * \int T(E,V)(f_L(\mu_L) - f_R(\mu_R))dE \qquad (1)$$

where f_L, f_R, μ_L and μ_R correspond to left Fermi-Dirac function, right Fermi-Dirac function, left chemical potential and right chemical potential, respectively. The integral is calculated over the bias window, defined as the difference between the positions of μ_L and μ_R.

In section III we describe its implementation using the VHDL-AMS engine. As the details are strictly related to quantum physics, and though it is an important contribution of this work, we do not detail this implementation in the present description and we focus more on the method and its impact on the device understanding and on the results at circuit level. For the same reasons, we thoroughly validated the method with several molecules and conditions. Here we show Benzene molecule link with different anchoring groups (cyanide, Oxygen and Sulfur) validation case in Fig. 3. In this case, the results of ATK show an extremely good agreement with the results obtained by the proposed method with in the applied range of voltages.

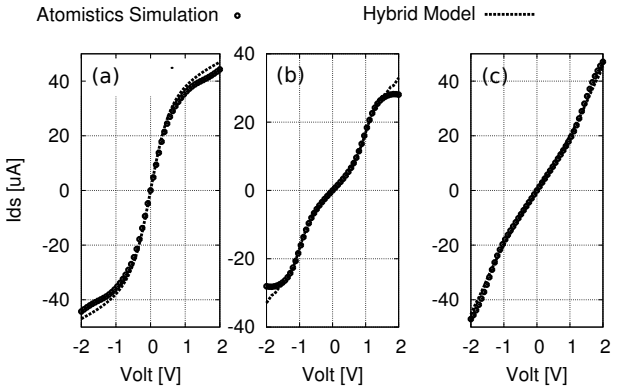

Figure 3: Comparison between the results obtained through the proposed model and the ATK simulation. I/V curves are reported for Benzene with (a) cyanide (b) oxygen and (c) Sulfer link group molecules.

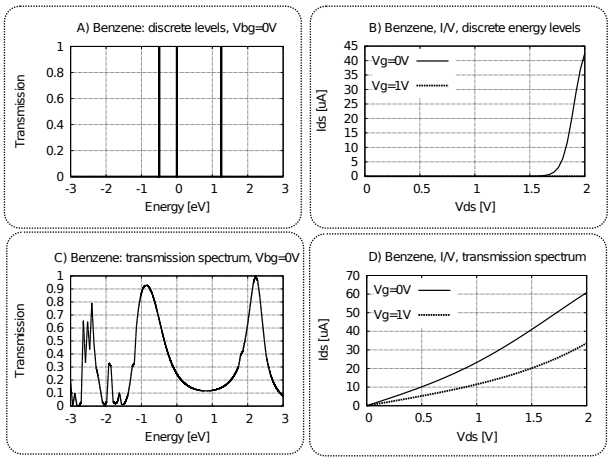

Figure 4: A) and B) discrete level and I-V characteristics of benzene molecule with thiol group. C) and D) Transmission spectrum and I-V characteristics of benzene molecule with thiol group. Back gate voltage V_{bg} is zero.

B. The impact of broadening on the transmission spectrum: Although a stand alone molecule is described by discrete energy levels, when it is coupled to electrodes, the molecular energy levels broaden and overlap each other, as shown by the shape of the transmission spectrum. In Fig. 4, the I-V characteristics are compared simply considering the discrete levels and the broadening in the transmission spectrum. For discrete level case, there is a step change from OFF current ($V_g = 0V$) to ON current ($V_g = 1V$) as shown in fig. 4(B) and can be easily controlled by gate. In this case, the ratio I_{on}/I_{off} is high. On the contrary, if the broadening is strong as in the transmission spectrum in figure Fig. 4(C), the current can flow through the device even at very low applied voltages and thus I_{on}/I_{off} ratio is very low, as shown in Fig. 4(D). A wrong estimation of the ratio I_{on}/I_{off} could compromise the proper functioning of the logic circuit. This behavior further confirms that for more realistic and accurate circuit simulation the transmission spectrum based on broadening has to be taken into account, as in our model.

C. Transmission Spectra and Related parameters: The transport property of metal-molecule-metal is usually dominated by the molecular energy levels that are close to the Fermi energy level and are also inside the bias window. If HOMO level is close to E_f (as shown in Fig. 2 (C)) and the positive gate voltage shifts the transmission spectrum away from E_f, a decrease of the current is observed. In this condition HOMO behaves like valence band in silicon device and this is analogous to PMOS operation. Thus, we will call this condition *P-type* hereinafter. On the contrary, if LUMO level is close to E_f (as shown in Fig. 2 (D)) the positive gate voltages pushes the transmission spectrum towards E_f, the current increases as well. This condition is analogous to NMOS type conduction and we will refer to it as *N-type* condition.

From a technological and circuit level point of view, it is also important to consider that the transmission spectrum of the molecular electronic system is greatly dependent on the type of molecule used as a channel and on the type of the *anchoring group* for metal-molecule coupling. Fig. 5 shows the molecules used in this work as conductive channel: A) Benzene linked through fluorine, B) Benzene linked through cyanide, C) Benzene linked through oxygen, D) Oligo Phenylene Vinylene linked through thiol.

D. The back gate: In this work, we proposed the use of a second gate electrode called *back gate* on which a fixed voltage is applied to configure the device. The reasons behind this are twofold: first, the molecular orbital and the related transmission spectrum can be shifted to change the system from n-conduction type (N-type) to p-conduction type (herein P-type) and vice versa. Second, the transmission spectrum shift is tuned in such a way that the number of molecular orbitals inside the bias window changes and the ratio of I_{on}/I_{off} increases. Fig. 6 shows the transmission spectrum and I-V characteristics of Benzene molecule with thiol group at different back gate voltages. When $V_{bg} < 0$ is applied, the gap between Fermi energy level E_f (shown by vertical dotted lines) and HOMO increases. In this case the I_{on}/I_{off} ratio increases. However, when $V_{bg} > 0$, LUMO-E_f gap decreases, and thus the conduction of the molecular transistor is changed to N-type.

E. Effect of linkers and back gate voltage: In Fig. 7 the I-V characteristics of the benzene molecule with different linkers

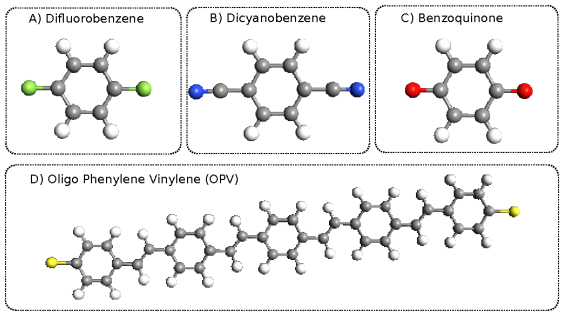

Figure 5: Different Molecules used to construct conductive channel in molecular FET. A) Benzene linked through fluorine (leftmost and rightmost atoms), B) Benzene linked through cyanide, C) Benzene linked through oxygen, D) Oligo Phenylene Vinylene in a chain of 5 molecules linked through thiol.

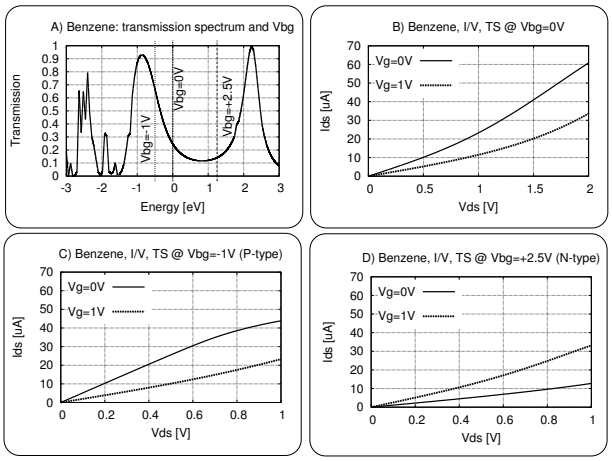

Figure 6: A) Position of E_f represented by vertical line at three different back gate volt. V_{bg} , B) $I-V$ characteristics of benzene molecule, $V_{bg} = 0V$. C) $I-V$ characteristics of benzene, $V_{bg} = -1V$. D) I_V characteristics of benzene, $V_{bg} = 2.5V$.

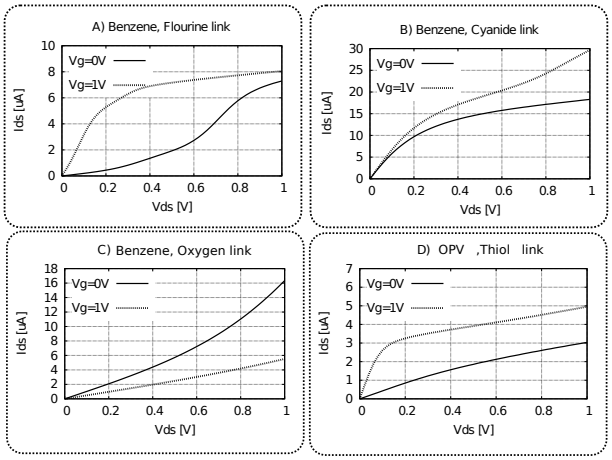

Figure 7: $I-V$ characteristics of different molecules showing different I_{on}/I_{off} ratio. Back gate Voltage is considered zero for all cases.

are reported. The figure shows that the I_{on}/I_{off} ratio depends on the linker and in all the cases it is very low. Among all, the most performing from a circuit point of view is the oxygen linker, since the I_{on}/I_{off} ratio at $V_{ds} = 1V$ is the highest. We further analyzed two different length of OPV molecule i.e. OPV with 5 rings (OPV5) and OPV with seven rings (OPV7) to improve the I_{on}/I_{off} ratio. The transmission function and corresponding $I-V$ characteristics of the molecules are shown in Fig. 8, where back gate voltages are used to tune the Fermi level for two reasons: to optimize the I_{on}/I_{off} ratio and to change the conduction from N-type to P-type. In this paper, OPV7 molecule is used for circuit simulations based on the following properties: 1) OPV7 has more benzene rings and thus realization of OPV7 based molecular devices are possible, 2) no sub-peaks between LUMO and HOMO are present in the transmission spectrum of the molecule and 3) high I_{on}/I_{off} ratio, with appropriate back gate voltage, makes it suitable for

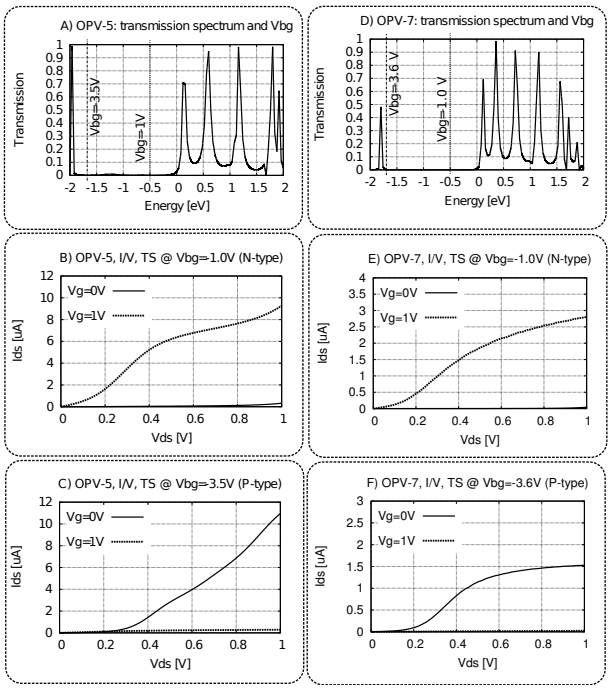

Figure 8: Transmission spectrum and $I-V$ characteristics of OPV5 (A,B,C) and OPV7 (D,E,F) molecules. Both P-type (C,F) and N-type (B,E) obtained using different back gate voltages (V_{bg}) are shown in relation to their transmission spectra.

low power complementary logic circuits.

III. VHDL-AMS Description of Transistor Model

The transistor model as described in the previous section was implemented in VHDL-AMS. The circuit level implementation of the proposed model thus includes: i) the incorporation of the transmission spectrum of a molecular FET at equilibrium into the VHDL-AMS description, ii) the iterative calculation of the self consistent field energy and of the new molecular energy levels due to charging effect, iii) the calculation of the shifted transmission spectrum based on the self consistent field and finally, iv) the calculation of the current from this shifted transmission spectrum.

As described in the previous section, the transmission spectrum at equilibrium is calculated through ATK toolkit. We took 100 values of the transmission spectrum in the range of -2eV to 2eV with the interval dE of 0.04eV. These values in the form of array of constant numbers, along with the fundamental constants used in the transistor model, are defined in packages in VHDL-AMS. The rest of the steps are implemented in a function that is also defined in a package in VHDL-AMS. Figure 9 shows the VHDL-AMS description of the transistor model. In the following section we show the results of its application to logic gates.

IV. Circuits

We designed a small library of logic gates based on the transistor model proposed in section II and described and simulated them using VHDL-AMS. We used the Advance MS

```
ENTITY MOLFET IS
Generic (----);
Port(-----);
End Entity MOLFET;
ARCHITECTURE behav OF MOLFET IS
--Declaration of Quantities
begin
-- DL_SCF (discrete molecular level- self consistent
field) function call.
I == DL_SCF(EF,E0,U0,G1,G2,A,V,VG1,VG1_back);
END ARCHITECTURE behav;

--- Function DL_SCF is defined in a package
FUNCTION DL_SCF (EF,E0,U0,G1,G2,A,Vds,Vg,Vg_back:REAL)
RETURN REAL IS VARIABLE Ids:REAL;
----Variable Declarations----------
---- Here all the variables used in the code are
declared
BEGIN
-- self consistent calculations--
G  := G1+G2; UL1 := -A*Vg; UL2 := -A*Vg_back; UL :=
UL1+UL2;
E1 := E0+UL;  F0 := 1.0/( 1.0 + exp((E0-EF)/KT));
N0 := 2.0 * F0;                  -- number of electrons
U1 := EF - ((1.0 - VDF)*Vds); U2 := EF + VDF*Vds;
while dU > 1.0e-6 loop
E1 := E0+Uscf+UL;       --- New molecular energy levels
F1 := 1.0/( 1.0 + exp((E1-U1)/KT));
F2:= 1.0/( 1.0 + exp((E1-U2)/KT));
N := 2.0*((G1*F1)+(G2*F2))/G;    -- Electron population
Uc := U0*(N-N0);                 -- SCF energy
dU := ABS(Uscf - Uc);
Uscf := Uscf + 0.1*(Uc-Uscf);
end loop;
-- shifting of transmission function--
 TQ_SHIFT = shift(TQ,N_SHIFT)  -- function for
calculating the shift in transmission function
-- calculating current--
for i in 0 to 100 loop
F11(i):= 1.0/(1.0+exp((E(i)-U1)/KT));
F22(i):= 1.0/(1.0+exp((E(i)-U2)/KT));
FT(i):= F22(i)-F11(i);
SUM1:= SUM1+ (TQ_SHIFT(i)*FT(i)); SUM := dE*SUM1;
Ids := (2.0*Q*Q/H)*SUM;
end loop;
-----------------------------------------------
RETURN Ids;
END FUNCTION DL_SCF;
```

Figure 9: VHDL-ams code for Molecular FET

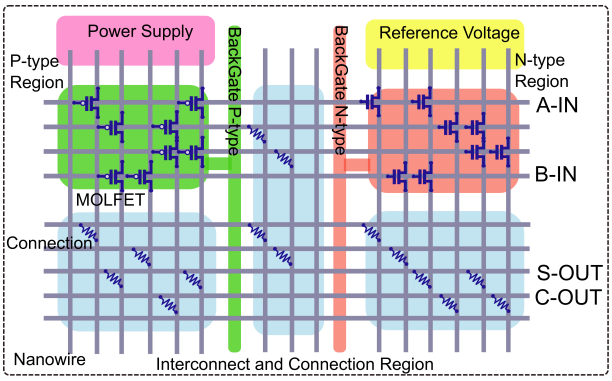

Figure 10: Crossbar architecture of Half Adder

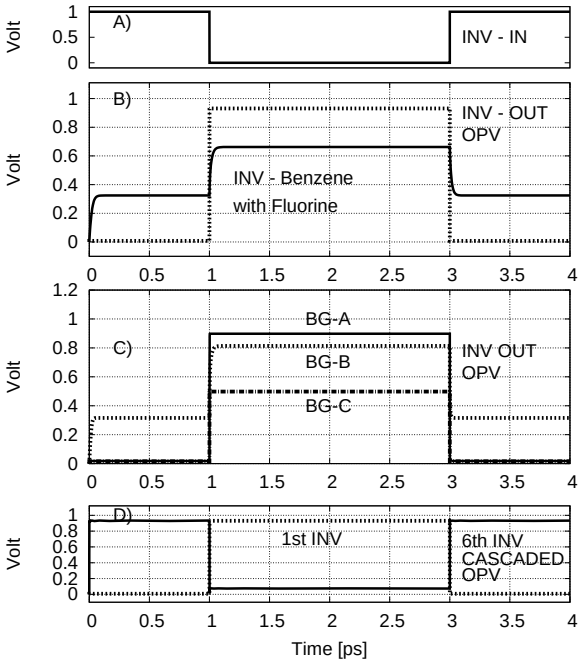

Figure 11: Output of inverter with different molecules and back gate voltages: A) inverter input. B) Inverter output for two types of molecules (OPV and benzene). C) Inverter output for OPV with three back gate voltages. BGA refers to the optimal back gate voltage: V_{bg}-P-type=-3.6V, V_{bg}-N-type=-0.9V. BGB refers to V_{bg}-P-type=-3.0V, V_{bg}-N-type=-1.5V and BGC refers to V_{bg}-P-type=-4.2V, V_{bg}-N-type=-0.3V. D) Output of six cascaded inverters.

(ADMS) simulator 2008.1 from Mentor Graphics. The logic circuits are implemented in a crossbar like architecture based on the structure proposed in [10]. There the authors built the logic circuits using arrays of nanowires and configurable FETs and switches. We started from this structure and modified it in order to include the back gate electrode that we differentiate for the N-type and P-type molecular transistor regions. We designed basic gates like inverter (INV), NAND and NOR gates and we also proposed the architecture of Adder. One for all, the crossbar architecture of the Half Adder (HA) circuit is shown in Fig. 10. The different regions of the architectures are highlighted and mentioned in the figure. P-type and N-type regions include nanowires and molecular transistors (left and right top zones). Interconnect and connection regions enable the communication between N-type and P-type devices as well as between devices and I/O. Back gate for both the N-type and P-type are electrodes that also need interconnection space. We used the resistors at the junctions for connecting the vertical and the horizontal wires. It is worth to note that our method can be applied to any other architecture that could arise as a winner from the experimental side. Currently this structure can be considered as a good starting point as several subparts have been already experimentally demonstrated for different types of technologies (carbon nanotubes, silicon nanowires and related transistors, molecular transistors considered alone, etc.).

In the following we show the results of the simulations, that are useful not only to validate the correct functionality of the structure, but especially to see the impact of the technological choices on the circuit performance and organization. A disclaimer should be done about the transient simulations we are going to show. At the current status of the state of the art no dynamic simulations has been done for molecular devices. Some models have been proposed that take into account the dynamic variation of the voltage applied to the transistor gate and that modifies the conduction mechanism accordingly. In this work we applied the model proposed in [8], but the results on the dynamic part (e.g. gate delay) should be considered valid from a behavioral point of view, not from a quantitative

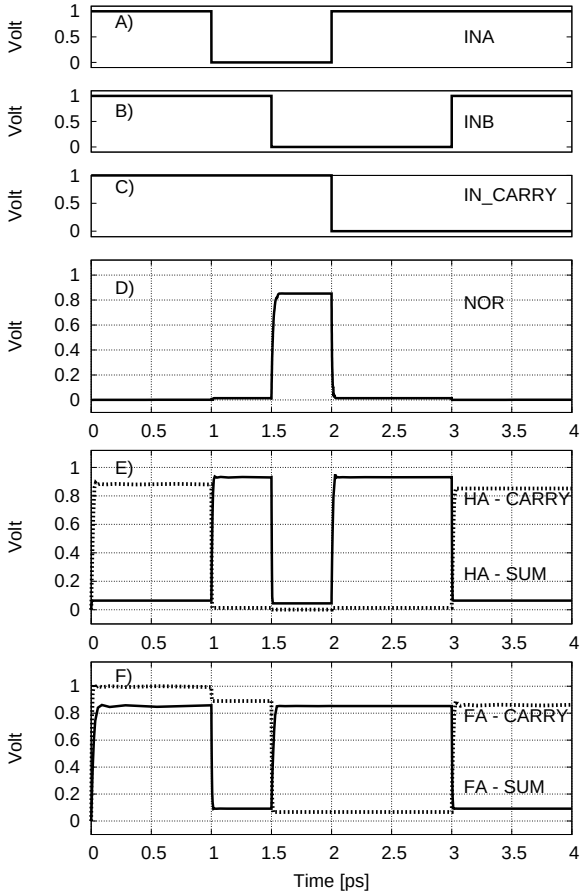

Figure 12: Output waveforms of NOR (D), HA (E) and FA (F) circuits.

point of view.

Inverter, different molecules-linkers and back gates. In almost all the cases the OPV7 molecule, for which the I_{ON}/I_{OFF} ratio is the highest on the basis of our findings, is used here as channel in the transistor model. An example of a comparison between the OPV behavior and the Benzene with fluorine linker is shown in Fig. 11 (B), where clearly the benzene results in lower voltage levels. Fig.11 (C) shows instead the INV output in the case of OPV when optimal (BGA) or suboptimal (BGB, BGC) back gate voltages are selected (values are in the figure caption). This demonstrates the importance of the introduction of back gate to control not only the P-type and N-type behavior, but also to find the optimal conduction as with the back gate voltage the I_{ON}/I_{OFF} ratio is inversely proportional to the leakage current.

NOR, HA and FA. With the application of these optimal back gate voltages found for the OPV7 molecule, we simulated some other basic logic gates and circuits: NAND, NOR, half adder (HA) and full adder (FA). We have not considered the parasitic resistances and capacitances in these simulations as they are related to specific technology used for the nanowire; their relation with the circuit/transistor performance will be the object of a separate study. The output waveforms of NOR, HA and FA circuits are shown in Fig. 12. The waveforms show that, with the application of suitable back gate voltage and OPV7 molecule, we are able to achieve high I_{ON}/I_{OFF} ratio in case of strong molecule-electrode coupling.

Cascaded gates. Finally we simulated a cascade of six inverter circuits. Results in Fig. 11(D) show that, thanks to the good I_{ON}/I_{OFF} ratio, the voltage levels are maintained and in this condition it is conceptually possible to design circuits organized with chain of basic blocks. Clearly at this point important considerations at the technological level should be done in order to take into account the parasitics elements and other parameters that could have an impact on long chains of elements.

V. Conclusion

We simulated different logic circuits in a crossbar like architecture using a new hybrid model of the molecular transistor. We used in the model the more realistic case of broadening of energy levels under the assumption of strong molecule-electrode coupling. We used a four terminal device with two gate electrodes. We handled the problem of leakage current and small I_{ON}/I_{OFF} ratio by using the back gate terminal and selecting the suitable molecule. We selected the optimum back gate voltages for the N-type and P-type MOLFETs and the molecule with the highest I_{ON}/I_{OFF} ratio. The transistor model is implemented using VHDL-AMS. We build and simulated some basic logic circuits, demonstrated their functional performance and their dependency on technological choices.

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