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Design and modeling of molecular logic circuits based on transistor structures

S. Safapour[1] · **R. Sabbaghi-Nadooshan**[1] · **A. A. Shokri**[2,3]

Abstract Molecular electronics technology removes limitations on miniaturization of semiconductor-based devices. With shrinking device sizes, we can expect smaller but more efficient devices. This branch of research also speeds up the devices, which enables us to have faster processors in the future. In order to have progress in this branch of research, we need to have modeling based on realities. Due to the availability of semiconductor-based devices, they can be used to further the goals of modeling in this field. Here, a specific procedure for the design and modeling of the molecular logic circuit based on the transistor structures is provided. That is, we use the circuit modelling for a gated oligo-phenylene vinylene (OPV) molecule as a NMOS molecular transistor's swithch and a methyl molecule as a resistor. We also benefited from the capabilities of the LTspice simulator software. Connecting these components, we could successfully conduct the circuit simulation of the combinational logic circuits, such as decoder, encoder, multiplexer, and comparator logical molecules, and prove the validity of the model.

Keywords OPV Molecule · LTspice software · Molecular decoder · Molecular encoder · Molecular multi-multiplexer · Molecular comparator

✉ A. A. Shokri
aashokri@nano.ipm.ac.ir

[1] Electrical Engineering Department, Islamic Azad University, Central Tehran Branch, Tehran, Iran

[2] Department of Physics, Payame Noor University (PNU), P.O. Box 19395-3697, Tehran, Iran

[3] Computational Physical Sciences Research Laboratory, Department of Nano-Science, Institute for Studies in Theoretical Physics and Mathematics (IPM), P.O. Box 19395-5531, Tehran, Iran

1 Introduction

The concept of molecular electronics, also called moletronics, was first reported in 1974 when Aviram and Ratner proposed the idea of a molecular current-rectifying diode based on an asymmetric molecular tunneling junction [1]. Afterward, the study of electronic transport phenomena through these kinds of mesoscopic systems has attracted a great deal of interest in the both fields, i.e., for basic science at the nanoscale and for possible applications in Nanoelectronics. This is due to discovery of the nanofabrication techniques in materials science [2–4]. Molecular electronics, as used in this paper, is defined as the field of science that investigates the electronic and thermal transport properties of circuits in which individual molecules or an assembly of them is used as basic building blocks.

Molecular electronics has many advantages, and the size reduction is one of them. It can be said that the size reduction, because of small molecules (between 1 and 10 nm), results in higher packaging density of devices. In this case, it brings about the following advantages such as cost, efficiency, and power dissipation. As another advantage of molecular electronics branch, the increase in the device speed can be noted. Although most molecules are poor conductors, good molecular wires can reduce the transistors' transfer time [5]. Another advantage with the molecular electronics branch is its ability to establish new capabilities. Specific molecular features such as different stable geometric structures or isomers can lead to new electronic operations that are not able to have a function in the conventional solid state. However, there are also disadvantages for molecules such as the lack of stability at high temperatures. In this regard, the advantages, however, outweigh the disadvantages in molecular electronics.

In the recent years, the scientists have found that, in comparison with technology based on silicon, molecules as active

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electronic components for applications provide region for nanosized structures. The understanding of electron transport through a single molecule sandwiched between two external electrodes is a fundamental step in the development of molecular electronics devices [6]. Therefore, the electron transport through the molecular systems has been widely studied both experimentally and theoretically in the recent years [7–9]. In Refs. [10,10–13], the design of molecular logic gates has been based on diode. In 2015, Mahmoud et al have used a single tripod molecule for creating transistor molecules and molecules of NAND gate [14]. Walczak et al have created various molecular gates in the form of four-terminal devices [15]. Zahir et al have presented simulation of molecular transistor structures using the OPV molecular circuit model [16]. In Ref. [17], molecular rectifiers have been modeled based on semiconductor devices. In another work, molecular transistor structures have been simulated based on the Fermi-level shift of the transistor molecule [18].

In a previous paper [19], we have studied a nanoscale logic NOR gate by applying magnetic flux inputs in a Z-shaped graphene nanoribbon composed of an armchair ribbon device sandwiched between two semi-infinite metallic zigzag ribbon leads. We have shown that the current and conductance are highly sensitive to both the magnetic fluxes subject to the device and the size of the system. In another work [20], we have investigated the XOR and OR gate responses, theoretically in a benzene molecule threaded by a magnetic flux and two gate voltages. Also, in another work [21], the logical AND and NOR gate responses of a 1,4-2-phenyl-dithiolate molecule threaded by a magnetic flux have been explored by the Green's function method.

In a recent work [22], we have used the circuit modeling of gated oligo-phenylene vinylene (OPV) molecule as a NMOS molecular transistor's switch as well as a resistor as the representative of a methyl molecule. We also benefited from the capabilities of the LTspice simulator software [23]. Connecting these components, in the present work, we investigate the circuit simulation of the basic molecular logic gates and decoder, encoder, multiplexer, and comparator logic circuits and prove the validity of the model. Due to the existence of semiconductor elements such as transistors and resistance, circuit-simulation method presented in this paper is more realistic and practical than the other simulation methods in previous articles. The application of these results can form a base for the design of molecular electronics devices.

The paper is organized as follows: In Sect. 2, the system composed of a gated OPV molecule with oxygen-linker groups is defined, and the proposed model for calculating the outputs of the logic circuit is discussed. Then, we discuss the numerical results of the circuit simulation of the decoder, encoder, multiplexer, and comparator logical molecules on the output in Sect. 3. Furthermore, the validity of the model will be confirmed in this section. The last section of the paper is devoted to the discussion and conclusion of our findings.

2 Theoretical framework

The understanding of electron transport through a single molecule sandwiched between two external electrodes is a fundamental step in the development of molecular electronics devices [6,24]. In other words, the electron transport through the molecular systems has been widely studied both experimentally and theoretically in recent years [7–9,25]. Conjugated molecules are more suitable than saturated ones for improving fabrications in molecular devices. This is because of the small energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and also the facile tuning of electronic and optical properties.

The charge distribution in inter atomic covalent bonds is determined based on the electronegativity of constituent atoms. Therefore, in the molecule of NC2, regarding the higher electronegativity of nitrogen than the two adjacent atoms, the charge distribution on nitrogen is seen to be more. Electrostatically, all the things which absorb the negative charges have the positive potential. Therefore, the potential barrier can be discussed for the behavior of these atoms, and it can be seen like the potential behavior of an nMOSFET transistor. The behavior of the adjacent atoms can be modeled as an nMOSFET transistor the gate of which is connected to the drain. For example, in the molecule of NC2, two nMOSFET transistors can be used which are in front of each other and have different threshold voltages. The gate of these transistors is connected to the drain because of the controlling effect of the adjacent atoms. The reason behind selecting nMOSFET transistor for modeling interatomic behavior and how to determine their threshold voltages will be explained further [17].

The threshold voltage of the transistors is inversely related to the drain current. In other words, the increasing of the threshold voltage of the transistors decreases their drain current. Therefore, this property is used for the modeling of potential barrier behavior of molecule atoms. For example, in case of potential barrier of NC2, the potential barrier height of the right carbon with nitrogen is less than the potential barrier height of the left carbon and nitrogen. Therefore, the threshold voltage of upper transistor, modeling the behavior of the right carbon with nitrogen, is considered less than the lower transistor, modeling the behavior of the left carbon with nitrogen, so that the drain current of the upper transistor is more than the drain current of the lower transistor. Molecules behave like atoms, and so they can be modeled similarly. For a simple phenyl ring with ethylene chain attached to it, the electrical charges pass between two adjacent carbon atoms,

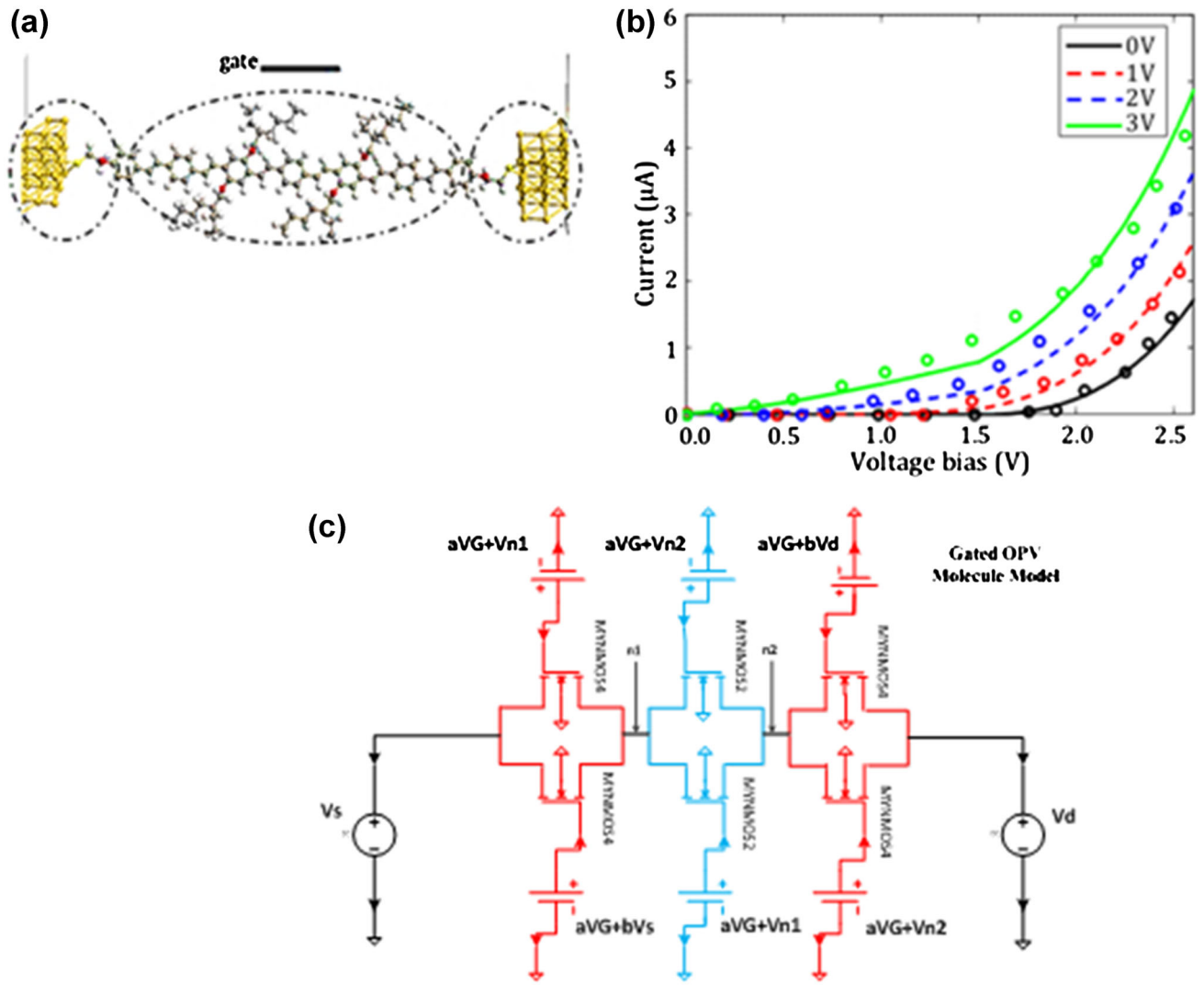


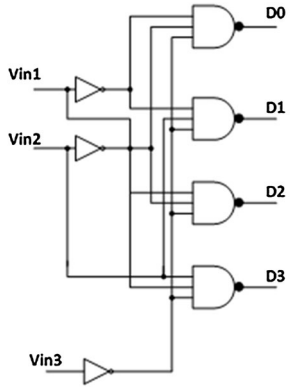
Fig. 1 **a** Gated OPV molecule with oxygen linkers on both sides. **b** Characteristic curve obtained from gated OPV molecule circuit model (integrated lines) together with the characteristic curve obtained from atomic simulation of molecule (*small circles*). **c** Gated OPV molecule circuit model [17]

due to sigma bonds. Therefore, such a molecule can be modeled with a transistor with low threshold of $V_{\text{th}} = 0.1$ V. An atom like oxygen which is shown with a high electronegativity is modeled with an amount of high threshold $V_{\text{th}} = 0.2$ V [17].

Figure 1 shows a molecule of gated OPV with oxygen-linker groups which are linked on both sides with methyl linker to the source and drain metal electrodes. The molecule has seven rings of benzene. The circuit model shown in Fig. 1 introduces the electrostatic coupling of gate to the molecule by parameter a. Assuming that the thickness of the oxide layer that separates the gate from the molecule is 100 nm, the parameter of a defines poor coupling and is considered equal to 0.08. Assuming that there are 3 nm methyl connectors on both sides of the molecule, parameter b is considered equal to 0.46. These parameters create the closest match between the voltage–current curves of the circuit model and the voltage–current curves rising from the atomic simulation of the molecule. Fig. 1 depicts that the voltage–current curves obtained through atomic simulation of the molecule and circuit model are in good agreement [17].

2.1 The OPV transistors

The transmission characteristics of the metal–molecule–metal (m–M–m) are limited to molecular energy levels close to the Fermi level and inside the bias window [18]. If the HOMO level is close to E_{F}, the positive gate voltage shifts the transmission spectrum to a point a little farther than E_{F}. A decrease in the current can be observed, which is consistent with PMOS operation. On the other hand, if the LUMO level is close to E_{F}, the positive gate voltage shifts the transmission spectrum toward EF, and the current increases, which is



Vin1	Vin2	Vin3	D0	D1	D2	D3
X	X	1	1	1	1	1
0	0	0	0	1	1	1
0	1	0	1	0	1	1
1	0	0	1	1	0	1
1	1	0	1	1	1	0

Fig. 2 Schematic model of a 2 × 4 decoder (*above*) and its truth Table (*below*)

consistent with NMOS operation [18]. It can be said that, for the OPV molecule, the increasing gate voltage increases the source–drain current in the molecule, allowing it to be used as an nMOSFET molecular transistor.

This OPV molecule circuit model is known as a NMOS molecular transistor. Resistance is used as an indicator of the methyl molecule that plays the role of insulator. The molecular transistor model and resistance are considered packages that can be connected using the features of LTspice. Figure 1 shows the gated OPV molecular current–voltage curve. In the model, the conduction threshold voltages of different currents passing through the molecule are used for different gate voltages. The gate voltages 0 and 2 V are considered for logic levels 0 and 1, respectively. The voltage on two sides of the molecule is 1.2 V, so that the current through the molecule can be cut and connected at 0 and 2 V. Other gate voltages can be tried with the other source–drain voltages; however, the 1 V gate voltage as logic level 1 reduces power consumption in the model. The molecule for which gate voltages 0 and 2 V are applied can be used as a transistor switch, and different logic circuits can be modeled with resistance, an indicator of the methyl molecule.

It should be noted that the used transistors in the gated OPV molecular circuit model (molecular transistor) are level 1 with parameters KP = 5E-7, $\gamma = 0.586$, $\lambda = 0$, $V_{To} = V_{th}$($V_{To} = 0.1$ V for MYNMOS2 and $V_{To} = 0.2$ V for MYNMOS4) [17]. Also, the other parameters of the transistors, W and L, can be changed based on more matching the curves obtained from molecular circuit model with the curve obtained from atomic simulation. Note that $a = 0.08$ and $b = 0.46$ were determined based on electrode–molecule coupling [17].

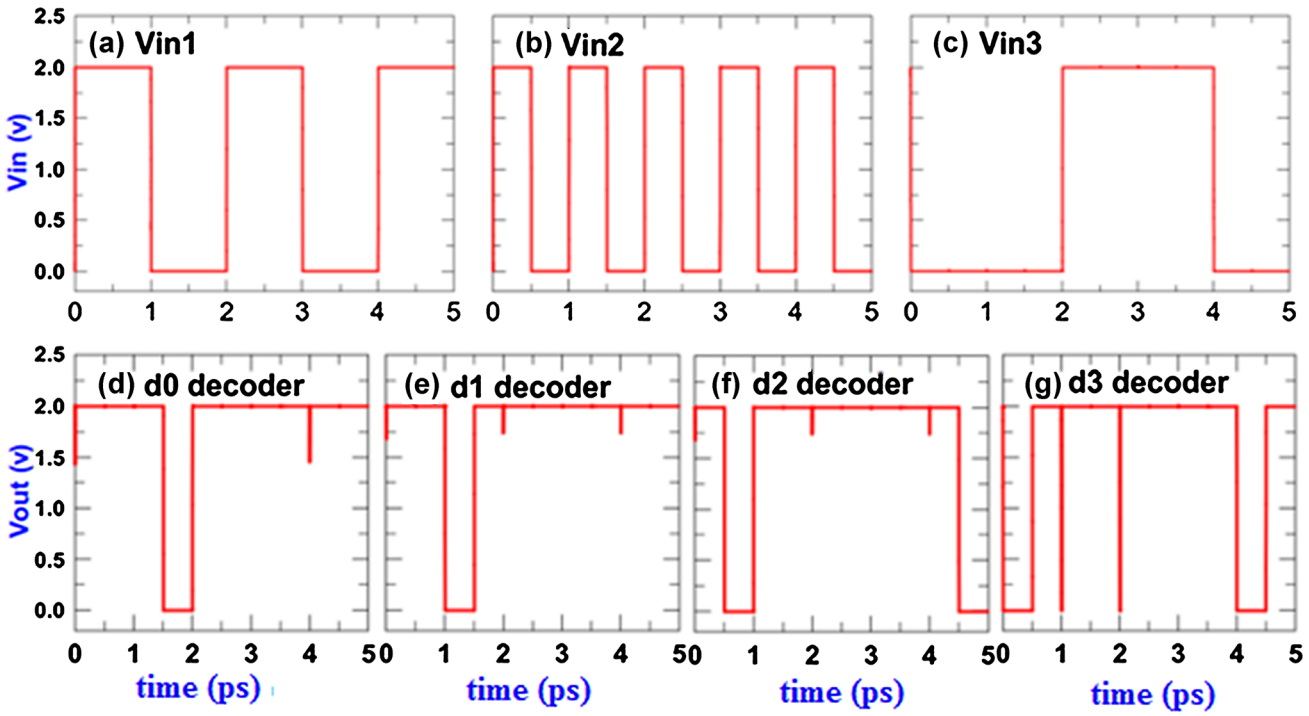
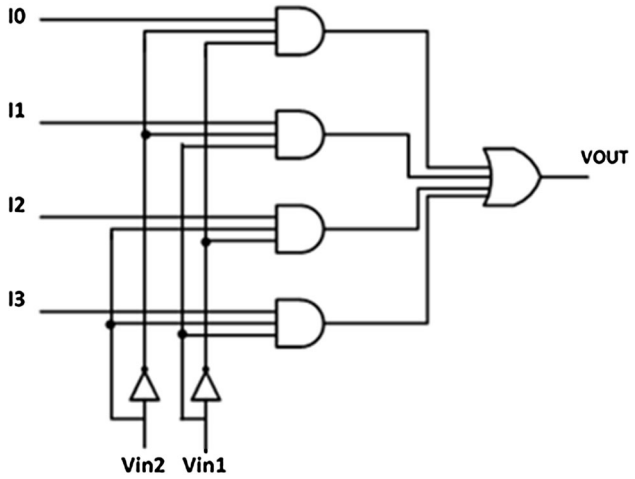


Fig. 3 Outputs of decoder molecule model. **a** Input Vin1. **b** Input Vin2. **c** Input Vin3. **d** Output (D0). **e** Output (D1). **f** Output (D2). **g** Output (D3)



Vin2	Vin1	Vout
0	0	I_0
0	1	I_1
1	0	I_2
1	1	I_3

Fig. 4 Schematic model of a four-to-one multiplexer circuit (*above*) and its truth Table (*below*)

In our simulation method, two features of LTspice software are utilized [22,23]: (a) current-dependent current source and (b) Arbitrary behavioral current sources. In first case, the circuit element applies a current between nodes. The current applied is equal to the value of the gain times the current through the voltage source. In second feature, there are current sources and the currents passing through them are the maximum or minimum of the currents passing through molecular transistors. In the next section, we investigate the molecules of decoder, encoder, multiplexer, and comparator, which are simulated by using this method.

3 Numerical results and discussion

The molecule geometry properties in the nanowire have been used to design logic gates by different methods. These logic gates consume electric input voltage, which operate as clock of logic circuits as shown in the related figures to output voltages. Based on the above consideration, we have proposed the circuit models of basic gates molecules in the previous work [22]. Accordingly, here, we simulate the molecules models connecting to the decoder, encoder, multiplexer and comparator.

3.1 Circuit model of a decoder molecule

Figure 2 shows a decoder circuit with its truth Table. As can be seen in this figure, the decoder consists of four NAND molecule models and three NOT molecule models connected via the features of LTspice software. The logic state is volatile

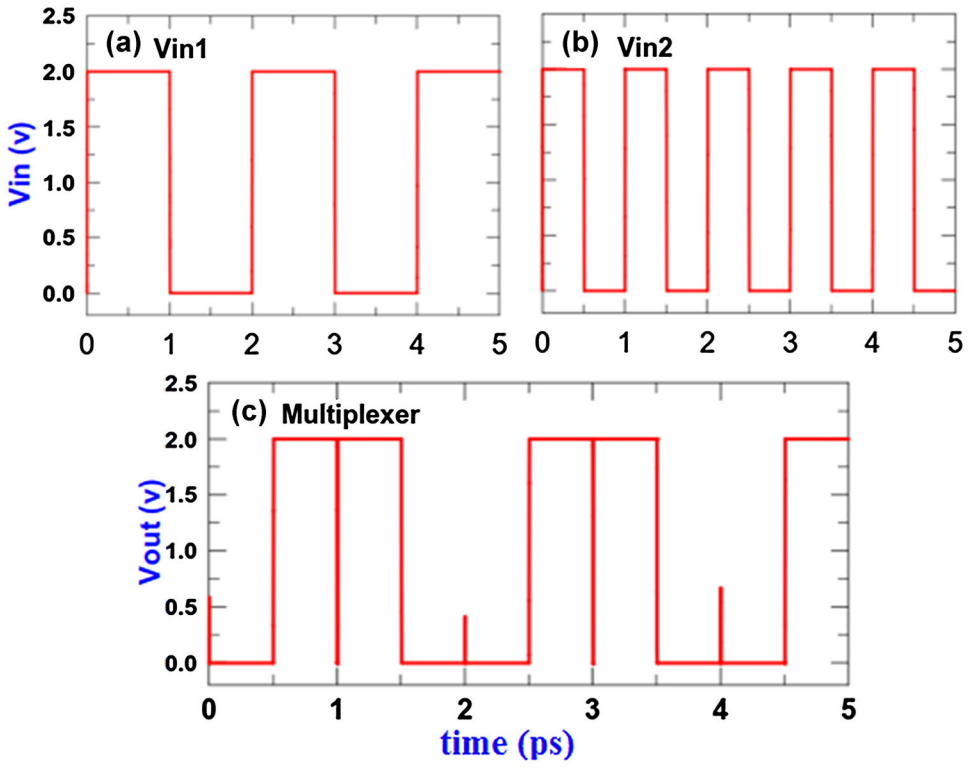
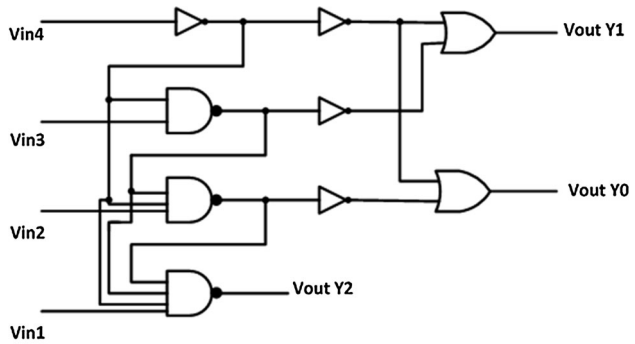


Fig. 5 Results of 4–1 multiplexer. **a** Input Vin1. **b** Input Vin2. **c** Output multiplexer



Vin4	Vin3	Vin2	Vin1	Vout Y1	Vout Y0	Vout Y2
X	0	0	0	0	0	1
0	0	1	X	0	1	1
0	1	X	X	1	0	1
1	X	X	X	1	1	1
0	0	0	0	X	X	0

Fig. 6 Schematic model of 4–2 encoder circuit (*above*) with its truth Table (*below*)

allowing zero standby power to keep the computing results. The outputs of the decoder molecule model for inputs Vin1, Vin2, and Vin3 are shown in Fig. 3. As example in Fig. 3, when Vin1 and Vin2 are low, output (D0) is low, and other outputs are high as the truth table. In order to determine the speeds of such circuits, we can easily calculate two output frequencies and switching time parameters in the model. For example, according to decoder output D0, one can consider that the switching time is 3 fs. Also, the output frequency D0 according to Fig. 1 is 250.287 GHz. It should be noted that the range of time has been on the order of picoseconds as shown in the figures.

3.2 The model of 4–1 multiplexer molecule

As already pointed out, a hybrid tunnel junction like a NMOS molecule transistor can be designed as built-up logic gates. Hence, we have shown a multiplexer circuit with its truth Table in Fig. 4. It is seen that the multiplexer consists of four AND molecule models, two NOT molecule models, and one OR molecule model connected with properties of LTspice software (The first feature, the second feature). The outputs of the multiplexer molecule model for inputs Vin1 and Vin2 are shown in Fig. 5. Note that we have considered $I_0 = 0$ V, $I_1 = 2$ V, $I_2 = 2$ V and $I_3 = 0$ V in this simulation. For instance, in Fig. 5, when Vin1=0 and Vin2=0, the output $I_0 = 0$V is selected.

3.3 The model of 4–2 encoder molecule

Figure 6 represents an encoder circuit along with its truth table. As can be seen in this figure, the encoder consists of three NAND molecule models, four NOT molecule models, and two OR molecule models connected with properties

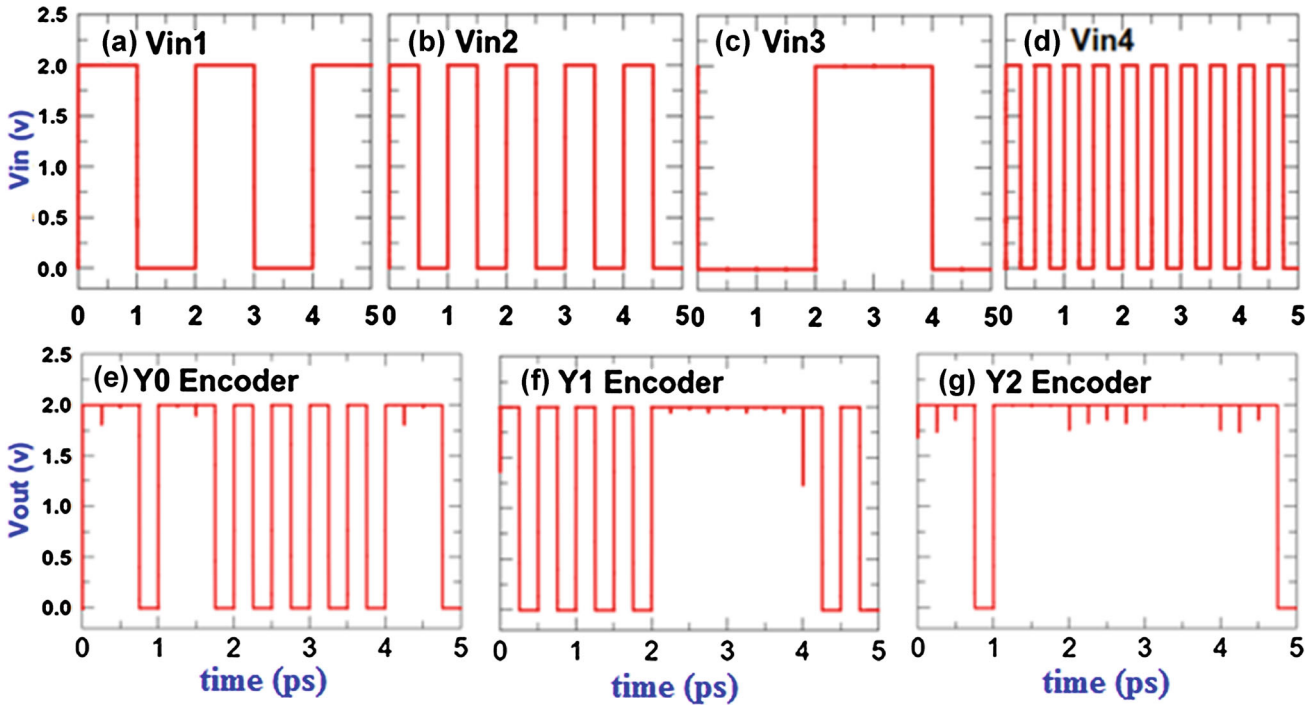
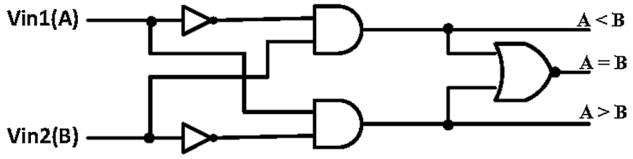


Fig. 7 Outputs of encoder molecule model. **a** Input Vin1. **b** Input Vin2. **c** Input Vin3. **d** Input Vin4. **e** Output Y0. **f** Output Y1. **g** Output Y2



Inputs		Outputs		
Vin2	Vin1	A > B	A = B	A < B
0	0	0	1	0
0	1	1	0	0
1	0	0	0	1
1	1	0	1	0

Fig. 8 Schematic model of a one-bit comparator circuit and its truth Table

of LTspice software (The first feature, the second feature). The outputs of encoder molecule model for inputs Vin1, Vin2, Vin3, and Vin4 are shown in Fig. 7 confirming the 4–2 encoder operations.

3.4 A one-bit comparator molecule model

Figure 8 shows a comparator circuit with truth table. As can be seen in this figure, comparator consists of two AND molecule models, two NOT molecule models, and a NOR molecule model connected with properties of LTspice software (The first feature, the second feature). The outputs of a comparator molecule model for inputs Vin1 and Vin2 are presented in Fig. 9. As we see in Fig. 9, when Vin1=1 and Vin2=0, output (A > B) is high, and two other outputs are low.

4 Conclusions

In this paper, we used the circuit modeling of gated OPV molecule as a NMOS molecular transistor's switch, as well as a resistor as the representative of a methyl molecule. We also benefited from the capabilities of the LTspice simulator software. Connecting these components, we could successfully perform the circuit simulation of combinational logic circuits, such as decoder, encoder, multiplexer, and comparator logical molecules, and prove the validity of the model. One of the capabilities of the LTspice software is the use of current sources current for which is obtained from maximizing or minimizing the passing current through transistor molecules. Another one is the use of voltage sources, which are serially located in the circuit and which calculate the current passing through the transistor molecule and methyl molecule (resistor). The circuits selected for modeling are only a small sample of logic circuits, and we can model other various logic circuits. These progresses may be useful in experimental works, which open a new way to explore logic gates.

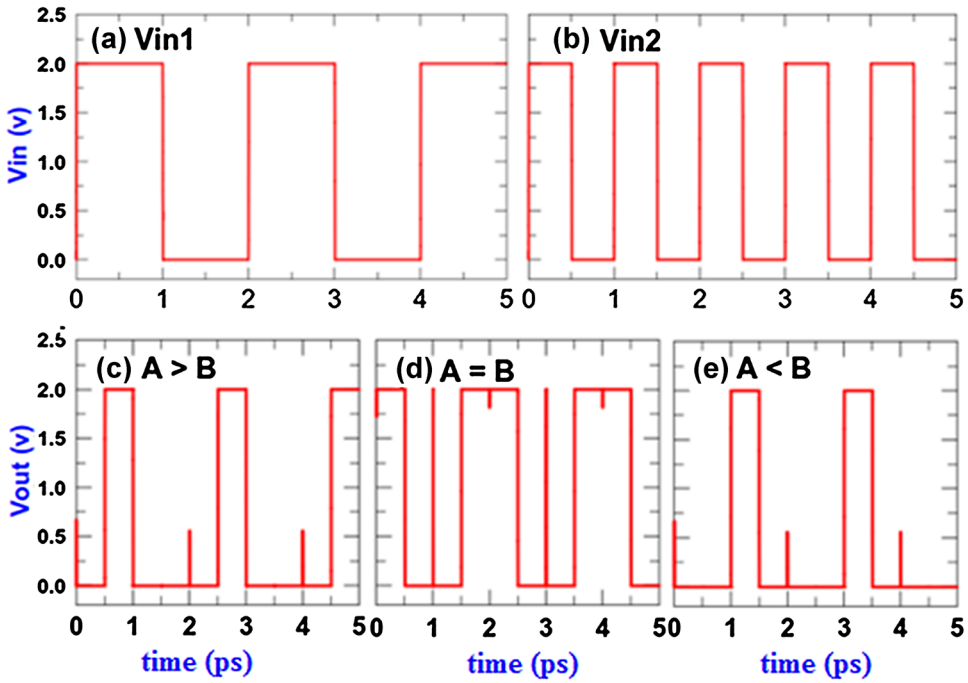


Fig. 9 Outputs of a comparator molecule model. **a** Input Vin1. **b** Input Vin2. **c** Output A > B. **d** Output A = B. **e** Output A < B

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