Single Electron Transistor Scheme Based on Multiple Quantum Dot Islands: Carbon Nanotube and Fullerene

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Abstract

Single electron transistor (SET) is a nano dimension device that is offered by technology to solve the problem of aggressive scaling in traditional transistors. Its operation speed depends on carrier mobility of its quantum dot. In this research, fullerene (C_{60}) and carbon nanotube (CNT) are utilized as materials of quantum dots in SET. Two SETs with different multiple quantum dots as C_{60}-CNT-C_{60} and CNT-C_{60}-CNT are modeled and analyzed. The comparison study shows that total length of quantum dots as fullerene diameter and CNT length have indirect effect on its current. Moreover increasing temperature decreases its current while rising of the gate voltage increases its current. In other words, quantum dot length, temperature and gate voltage are parameters which can control SET operation. Furthermore two SETs are simulated and their stability diagrams are analyzed. The simulation results show that C_{60}-CNT-C_{60} SET has lower coulomb blockade and also it has more reliability and faster operation than CNT-C_{60}-CNT SET.

Key words: Carbon Nanotube, Fullerene, Quantum Dot, Single Electron Transistor.

1-Introduction

According to the Moore's law, the number of transistors in a chip is doubled every 2-3 years but MOSFET scaling results in performance degradations generally called short channel effects (SCEs). Novel transistors are designed to improve limitations imposed by SCEs in traditional bulk MOSFETs. Common examples which are used by the industry includes FinFETs, tunnel FETs, and nanowires FETs [1,2,3]. However, all these technologies still suffer from leakage current and power consumption. On the other hand, we know electrons cross from the transistor channel, so decreasing the number of electrons and transfer one electron from transistor channel at a very short time can improve its performance and increase its operation speed. Furthermore advanced electronic technology needs chips capable of doing more information processing in a shorter time compared with traditional chips and scaling according to Moore's law is no more adequate to achieve nano-dimension devices based on transfer of many carriers at the same time. The device which can improve these limitations in nanoscale is single electron transistor (SET). SET with its particular characteristics such as low energy consumption, nano size dimension and high operating speed can be a candidate to continue aggressive scaling [4]. SET works based on the transfer of single electrons in its channel in a very short time, so its operation speed is much higher than traditional MOSFETs and their derivatives. SET contains source and drain electrodes, gate electrode and an island between them. Its gate electrode can control electron tunneling. SET operates by moving an electron via tunneling between source and drain electrodes [5]. It has higher speed operation and lower energy consumption than Field Effect Transistors (FETs) [6, 7]. FETs work by crossing some electrons in their channels but SET operates by transfer of single electrons between electrodes and island through a tunnel Junction [8,9,10]. Any tunnel junction consists of one capacitance and a resistance in series [11]. When an electron crosses from a tunnel junction to island, the capacitor charges and tunneling of second electron is stopped [12]. This electron is transferred to the other electrode and this phenomenon is called single electron tunneling [13].

Another phenomenon is Coulomb Blockade (CB) that affects on SET operation which has been discussed by C. Gorter in 1951 [14, 15]. It occurs when the resistance of a tunnel junction becomes more than quantum resistance [16]. It prevents electron transfer to or out of SET island, so operation speed of SET depends on carrier mobility in the island [17]. On the other hand, the island has high carrier mobility in quantum size. Therefore quantum dot (QD) can be used in transistor nanostructure [18, 19]. Moreover increasing the number of QDs can reduce some operation limitations of SET such as cryogenic temperature and leakage current [20]. Increasing cryogenic temperature to room temperature is a good improvement in SET operation because CB occurs when the charging energy is less than the thermal energy (The essential energy to tunnel an electron to the QD) [21, 22]. The coulomb blockade interval makes a diamond-shaped region which is called coulomb diamond. It is function of V_g and V_{ds} while the number of electrons on the QD are fixed in any region. The curve for V_g versus V_{ds} is called charge stability diagram [23]. Furthermore, material of QD has direct effect on SET operation. There are different QDs but carbon based materials such as fullerenes and carbon nanotube (CNT) have higher carrier mobilities than other materials [12,24]. Hence, fullerene SET presents lower leakage current and CB region compared with silicon QD-SET [22]. CNT is a one dimensional material while Fullerene is classified under category of zero dimensional materials [25, 16]. Fullerenes have different natural forms as C_{38} and C_{42}. In addition, some molecules have several symmetric shapes that make direct influence on SET operation [26]. This effect is investigated for three molecules C_{38}, C_{42} and C_{60} as shown in Fig.1 and then their charge stability diagrams are reported in Fig.2 (a-f) [27]. The comparison study in Fig.2 indicates that C_{38} and C_{42} have different stability diagrams because they exhibit different types of symmetry. This problem decreases reliability of SET, so buckminster fullerene (C_{60}) is selected as SET island. Its molecule not only has one type of symmetry but also is cheaper to produce compared with other fullerene molecules while it is very stable in nano range dimensions [28].

SETs can be used in quantum computing, single electron memory and supersensitive electrometry. In this research, the advantages of two proposed SET structured are explored utilizing fullerene and CNT. Because of SET unique characteristics, it can be an alternative for the next generation of devices in electronic circuits. Moreover we investigate the impact of fullerene diameter, CNT length, temperature and the gate voltage on the SET performance. Finally a comparison study is performed between two proposed structures to reveal which one can be a suitable candidate for replacement of traditional transistors in future technology.

2-Theoritical Model

Single electron transistor works based on electron tunneling from source electrode to drain electrode. This electron transfer can be analyzed by the quantum mechanical effects describing that when electron wave crosses from different regions of the device, it has a particular wave function in each region. Therefore SET islands, drain and source are different target regions as shown in Fig. 3 where Schrodinger's equations can be written for them. The SET model is based on three islands that each island is assumed to behave like a potential well. Equations which explain wave function at regions of a fullerene island are:

$$\Psi_I = A_1 e^{k_1 x} + B_1\, e^{-k_1 x} \quad (1)$$

$$\Psi_{II} = A_2 e^{ik_2 x} + B_2\, e^{-ik_2 x} \quad (2)$$

$$\Psi_{III} = A_3 e^{ik_3 x} \quad (3)$$

where $k_1 = k_3 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$ and $k_2 = \frac{\sqrt{2mE}}{\hbar}$.

These equations can be solved using appropriate boundary conditions which can be written from continuity of the wave function and its derivative at $x = 0$ and L_1. These parts of the modeling are fully covered at the appendix A.

Therefore transmission coefficient of region with a fullerene island is calculated as:

$$T_1 = \frac{1}{1 + K_F sinh^2(k_2 L_1)} \quad (4)$$

$$K_F = \frac{(h^2 + ta'm)E - \hbar^2 E_{g_F}}{2\sqrt{ta'\hbar mE(E - E_{g_F})}} \quad (5)$$

where "L_1" is fullerene diameter, $k_2 = \frac{\sqrt{2mE}}{\hbar}$, "$E$" is the electron energy, "$m = 9.109 \times 10^{-31} kg$" is the electron effective mass in fullerene, "$\hbar = 6.582119514 \times 10^{-16} \mathrm{eV.s}$" is the reduced Planck's constant, "$a' = 3a_{c-c}$" , $a_{c-c_F} = 1.46A^0$ is the distance between neighbouring carbon atoms in fullerene molecule, "$E_{g_F} = 0.1828$" is the fullerene bandgap (C_{60} energy gap is defined as the difference between the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO)) and "*t*=2.5eV" is the hopping energy.

The Shorodinger equations are written for second part of SET with carbon nanotube island as:

$$\Psi_{III} = A_3 e^{k_1 x} + B_3\, e^{-k_1 x} \quad (6)$$

$$\Psi_{IV} = A_4 e^{ik_4 x} + B_4\, e^{-ik_4 x} \quad (7)$$

$$\Psi_V = A_5 e^{ik_1 x} \quad (8)$$

where $k_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$ and $k_4 = \frac{\sqrt{2mE}}{\hbar}$.

These set of equations should also be solved and the boundary conditions can be written at points $x = 0$ and L_2. These parts of model are also fully covered at the appendix A.

Therefore transition coefficient of region with a CNT island is calculated as

$$T_2 = \frac{1}{1+K_{CNT} sinh^2(k_4 L_2)} \quad (9)$$

$$K_{CNT} = \frac{(\hbar^2 + ta'm)E - \hbar^2 E_{g_{CNT}}}{2\sqrt{ta'\hbar m E(E - E_{g_{CNT}})}} \quad (10)$$

where "L_2" is the CNT length, $k_4 = \frac{\sqrt{2mE}}{\hbar}$, $a_{c-c_{CNT}} = 1.42A^0$ is the distance between neighbouring carbon atoms, "$E_{g_{CNT}} = \frac{0.8\text{eV}}{d(nm)}$" is the CNT band gap where $d = 2R$ is the CNT diameter and "t=2.7eV" is the hopping energy of CNT.
The first proposed SET comprises three islands as two fullerene molecules and one CNT. Therefore the product of three calculated transmission coefficients as obtained in Eqs. (4) and (9) results in the total transmission coefficient as:

$$T_{Total_1} = T_1 \times T_2 \times T_1 \quad (11)$$

$$T_{Total_1} = \frac{1}{K_F{}^4 k_2{}^4 L_1{}^4 + 1 + 2K_F^2 k_2^2 L_1^2 + K_{CNT}^4 K_F^2 k_2^4 k_4^2 L_1 L_2 + K_{CNT}^4 k_4^2 L_2^2 + 2K_F^2 K_{CNT}^2 k_2^2 k_4^2 L_1^2 L_2^2} \quad (12)$$

where"L_1" is diameter of fullerene and "L_2" is CNT length. The parameters were defined previously.

SET current with three multiple islands as two fullerene molecules and one CNT can be calculated based on the Landauer formalism as:

$$I = \int_0^{\eta} T(E).F(E)dE \quad (13)$$

where "T(E)" is the total transmission coefficient of SET (T_{total_1}) and F(E) is Fermi probability function defined as $F(E) = [\frac{1}{\exp\left(\frac{E-E_F}{k_B T}\right)+1}]$, where "E" is electron energy, "E_F" is Fermi energy, "T" is temperature and "k_B" presents the Boltzmann's constant.

Based on proposed model, the current versus voltage characteristic of the SET with three islands as two fullerene molecules and one CNT in the parabolic-band region can be expressed as:

$$I = \int_0^{\eta} \frac{1}{\frac{K_F{}^4 (Ak_B T(x+d_F))^2 L_1{}^4 + 1 + 2K_F^2 \left(Ak_B T(x+d_F)\right) L_1^2 + K_{CNT}^4 K_F^2 (Ak_B T(x+d_F))^2 \left(Ak_B T(x+d_{CNT})\right) L_1 L_2}{\frac{1}{+K_{CNT}^4 \left(Ak_B T(x+d_{CNT})\right) L_2^2 + 2K_F^2 K_{CNT}^2 \left(Ak_B T(x+d_F)\right)\left(Ak_B T(x+d_{CNT})\right) L_1^2 L_2^2}}} \frac{dE}{e^{x-\eta}+1} \quad (14)$$

where"L_1" is diameter of fullerene and "L_2" is length of CNT , $x = \frac{E-E_g}{k_B T}$, $\eta = \frac{E_F - E_g}{k_B T}$, $E_g = \frac{E_{g_F} + E_{g_{CNT}}}{2}$, $d_F = \frac{E_{g_F}}{k_B T}$, $d_{CNT} = \frac{E_{g_{CNT}}}{k_B T}$, $A = \sqrt{\frac{2m}{\hbar^2}}$ and other parameters were defined previously.

The second proposed SET comprises three islands as two CNTs and one fullerene molecule. The product of three transmission coefficients as calculated in Equations (4) and (9) will be total transmission coefficient which is now given by:

$$T_{Total_2} = T_2 \times T_1 \times T_2 \quad (15)$$

$$T_{Total_2} = \frac{1}{{K_{CNT}}^4 {k_4}^4 {L_2}^4 + 1 + 2K_{CNT}^2 k_4^2 L_2^2 + K_F^4 K_{CNT}^2 k_4^4 k_2^2 L_2 L_1 + K_F^4 k_2^2 L_1^2 + 2K_{CNT}^2 K_F^2 k_4^2 k_2^2 L_2^2 L_1^2} \quad (16)$$

where all of the parameters in Eq. (16) were previously defined. Therefore the SET current with three multiple islands as one fullerene molecule and two CNTs can be calculated based on the Landauer formalism as:

$$I = \int_0^{\eta} \frac{1}{{K_{CNT}}^4 (Ak_BT(x+d_{CNT}))^2 {L_2}^4 + 1 + 2K_{CNT}^2 (Ak_BT(x+d_{CNT})) L_2^2 + K_F^4 K_{CNT}^2 (Ak_BT(x+d_{CNT}))^2 (Ak_BT(x+d_F)) L_1 L_2} \frac{1}{+K_F^4 (Ak_BT(x+d_F)) L_1^2 + 2K_F^2 K_{CNT}^2 (Ak_BT(x+d_{CNT}))(Ak_BT(x+d_F)) L_1^2 L_2^2} \frac{dE}{e^{x-\eta}+1} \quad (17)$$

where all parameters were defined previously.

3- Results and discussion

The proposed models depend on some parameters such as temperature, island length and gate voltage. The impact of CNT length on the current in the first proposed SET is investigated and plotted in Fig. 4. The gate voltage is 1mV, temperature is 300^0 K and the fullerene diameter is 1nm. The variations in Fig. 4 indicates that CNT length has an indirect effect on the SET current because increasing CNT length increases distance between source and drain therefore leakage current increases in SET .This SET contains two fullerene molecules where the effect of their diameters on the current is shown in Fig. 5. The gate voltage is 1mV, temperature is 300^0 K and CNT length is 1nm. Fig. 5 shows that decreasing of fullerene diameter decreases leakage current, so it increase SET current. Another effective factor in the proposed model is the temperature. The impact of temperature on the SET I-V characteristics is illustrated in Fig. 6. Here the gate voltage is chosen as 1mv, CNT length and fullerene diameter are both 1nm. It can be seen that the temperature has indirect effect on the proposed model. The increasing temperature increases electron tunneling to QD but electron accumulation occurs in QD, so electron transfer decreases and current decreases in higher temperature. Moreover effect of the gate voltage on SET current is investigated and sketched in Fig. 7. The temperature is 300^0 K, CNT length and fullerene diameter are both 1nm. The curves in Fig. 7 show that increasing of the applied gate voltage increases SET current.

The next proposed SET for our study is comprised of three islands: two CNTs in the channel sides and one fullerene molecule in the middle as shown in Fig. 8.

The current versus voltage characteristic of the second proposed SET with one fullerene molecule in the channel and two carbon nanotubes on its sides depends on some factors. The island length affects on SET current. Impact of the CNT length on SET current is investigated as shown in Fig. 9. The gate voltage is 1mV, temperature is 300^0 K and fullerene diameter is 1nm. It confirms that the CNT length has indirect effect on the SET current. The impact of fullerene molecule diameter on the SET current is plotted in Fig. 10. Here, the gate voltage is assumed to be 1mV, temperature is 300^0 K and CNT length is 1nm. It confirms that increasing fullerene diameter decreases SET current as expected. Both Fig .9 and Fig .10 show the bigger QD has the more leakage current, so lower SET current occurs in this case. Moreover the current is affected by changing the temperature as illustrated in Fig. 11. Again, the gate voltage is 1mv, CNT length and fullerene diameter are both 1nm. It reveals the fact that increasing of the temperature decreases SET current that shows electron accumulation in QDs and decreasing current. Another important factor is the gate voltage as plotted in Fig. 12. The temperature is 300^0 K, CNT length is 1nm and fullerene diameter is 1nm. The current versus voltage characteristics of different gate voltages in Fig. 12 show this factor has direct influence on the SET current.

The impact of island material on the SET operation can be illustrated using its charge stability diagram. Two proposed SETs with different islands $C_{60} - CNT - C_{60}$ and $CNT - C_{60} - CNT$ are designed with Atomistic Toolkit software [27], so their charge stability diagrams are simulated and plotted in Fig. 13. The important parameters which are extracted from stability diagrams of two structures as shown in Fig. 13 are summarized in table1. It clearly shows the range of gate and drain voltage for each diamond and the associated area. The sum of coulomb diamond areas for C_{60}-CNT-C_{60} SET is 1.329 while this summation for CNT-C_{60}- CNT SET equals 7.538.

Table1: Important parameters extracted from Fig. 13.

Diamond	$V_{ds_{min}}, V_{ds_{max}}$	ΔV_{ds}	Vg_{min}, Vg_{max}	ΔVg	Area
C_{60}-CNT-C_{60} Diamond 1	-0.297,0.319	0.616	-1.164,-0.869	2.033	0.626
C_{60}-CNT-C_{60}	-0.312,0.319	0.631	-0.862,-0.529	1.391	0.438

Diamond 2					
C_{60}-CNT-C_{60} Diamond 3	-0.529,-0.204	0.733	-0.521,-0.204	0.725	0.265
CNT-C_{60}- CNT Diamond 1	-0.372,0.364	0.736	-3.159,-2.781	5.940	2.185
CNT-C_{60}- CNT Diamond 2	-0.595,0.572	1.167	-2.773,-2.192	4.965	2.897
CNT-C_{60}- CNT Diamond 3	-0.669,0.651	1.320	-2.182,-1.540	3.722	2.456

The comparison study of coulomb diamond patterns in Fig. 13 indicates that not only SET with two fullerene molecules and one CNT has smaller coulomb diamonds but also has lower coulomb blockade range and zero conductance region than other proposed SET. It reveals the fact that the most important factor in SET operation is the island length and since SET with $C_{60} - CNT - C_{60}$ islands has smaller islands, it presents lower coulomb blockade range and faster and better operation compared with $CNT - C_{60} - CNT$ SET.

4-Conclusion

Single electron transistor (SET) based on quantum dot can improve problems of integrated circuit scaling. Quantum dots such as fullerene and carbon nanotube can be utilized to increase operation speed of SET. In this research, two SETs with fullerene (C_{60}) and CNT islands as $\mathrm{C_{60} - CNT - C_{60}}$ SET and $\mathrm{CNT - C_{60} - CNT}$ SET were analyzed and also some effective factors on SET operation were investigated. The comparison study indicates that decreasing fullerene diameter, CNT length and temperature increase SET current but applied gate voltage has a direct effect on the current. Moreover proposed SETs were simulated and simulation results were compared together. Comparison study showed that $\mathrm{C_{60} - CNT - C_{60}}$ SET has lower coulomb blockade range and also higher operation speed than $\mathrm{CNT - C_{60} -}$ CNT SET. It confirms effective role of island length and its material in SET operation and

SET reliability. Therefore selecting suitable material for the island and the associated length can control the current value. Furthermore current can be tuned by temperature and applied gate voltage.

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Appendix A

The Schrodinger equations are solved for the first part:

$$\frac{\hbar^2}{2m}\frac{d^2\psi_I(x)}{dx^2}+(E-V)\psi_I(x)=0 \qquad x\leq 0 \qquad \text{Region I} \tag{A1}$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2}+E\psi_{II}(x)=0 \qquad 0<x<L_1 \text{Region II} \tag{A2}$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_{III}(x)}{dx^2}+(E-V)\psi_{III}(x)=0 \qquad x\geq L_1 \qquad \text{Region III} \tag{A3}$$

The boundary conditions can be written from continuity of the wave function and its derivative at $x=0$ and L_1 as:

$$A_1+B_1 = A_2+B_2 \tag{A4}$$

$$k_1A_1-k_1B_1 = ik_2A_2-ik_2B_2 \tag{A5}$$

$$A_2e^{ik_2L_1}+B_2\,e^{-ik_2L_1} = A_3e^{k_1L_1} \tag{A6}$$

$$ik_2A_2e^{ik_2L_1}-ik_2\,B_2\,e^{-ik_2L_1} = k_1A_3e^{k_1L_1} \tag{A7}$$

The Schrodinger equations are solved for second part as:

$$\frac{\hbar^2}{2m}\frac{d^2\psi_{III}(x)}{dx^2}+(E-V)\psi_{III}(x)=0 \qquad x\leq 0 \qquad \text{Region III} \tag{A8}$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_{IV}(x)}{dx^2}+E\psi_{IV}(x)=0 \qquad 0<x<L_2 \text{Region IV} \tag{A9}$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_{V}(x)}{dx^2}+(E-V)\psi_{V}(x)=0 \qquad x\geq L_2 \qquad \text{Region V} \tag{A10}$$

These boundary conditions can be written at $x=0$ and L_2 as:

$$A_3 + B_3 = A_4 + B_4 \quad \text{(A11)}$$

$$k_1 A_3 - k_1 B_3 = ik_2 A_4 - ik_2 B_4 \quad \text{(A12)}$$

$$A_4 e^{ik_4 L_2} + B_4 e^{-ik_4 L_2} = A_5 e^{k_4 L_2} \quad \text{(A13)}$$

$$ik_4 A_4 e^{ik_4 L_2} - ik_4 B_4 e^{-ik_4 L_2} = k_1 A_5 e^{k_4 L_2} \quad \text{(A14)}$$

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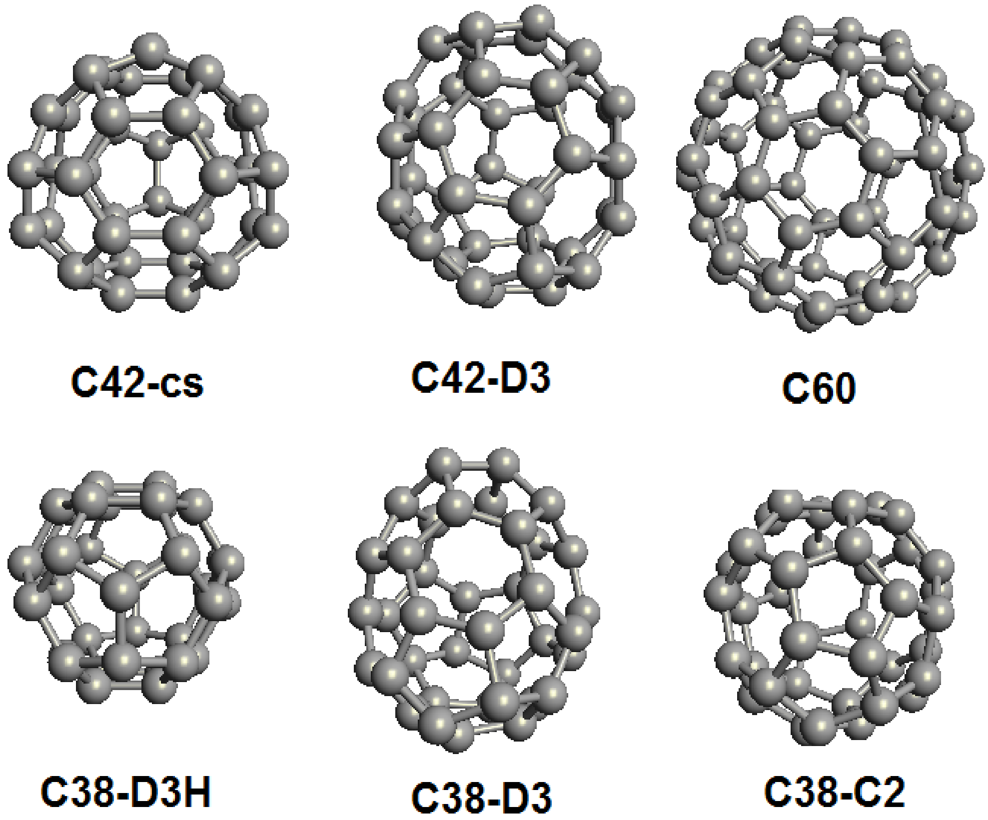
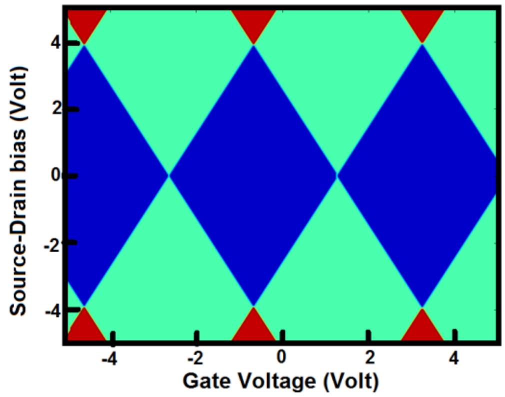
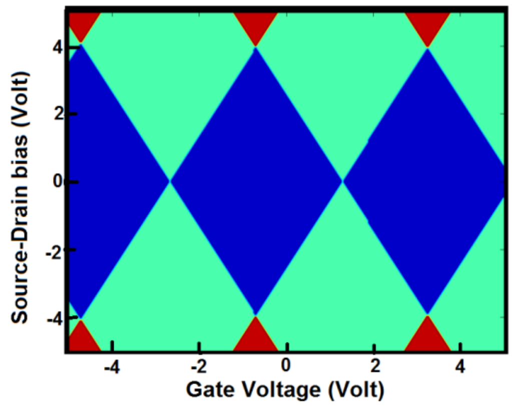


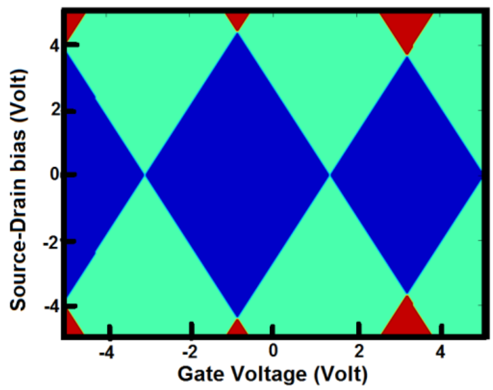
Fig.1. C_{38} and C_{42} molecules with different types of symmetry and C_{60} molecule [23].



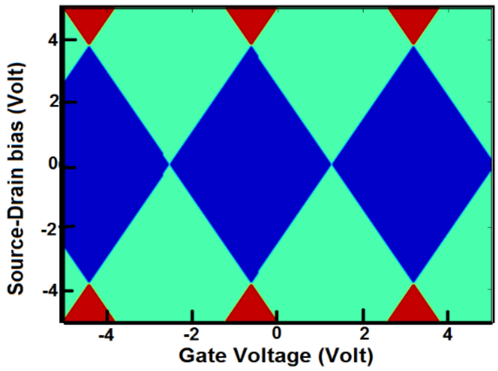
a) C_{38} molecule -D_3H



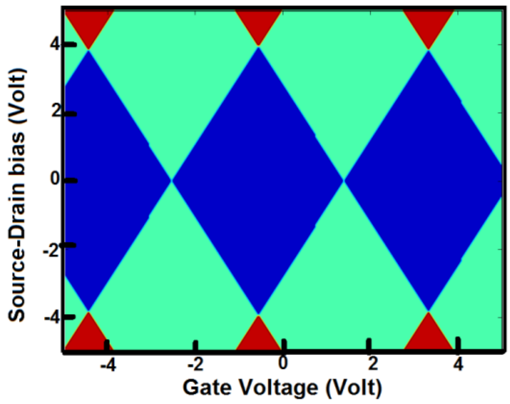
b)C_{38} molecule -C_2



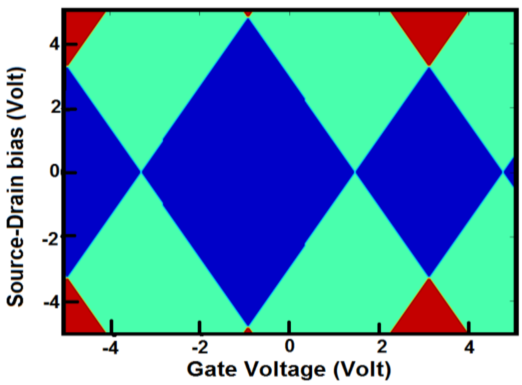
c) C_{38} molecule –D_3



d) C_{42} molecule -CS



e) C_{42} molecule –D_3



f) C_{60} molecule

Fig. 2. Stability diagrams of C_{38} and C_{42} with different types of symmetry and C_{60}.

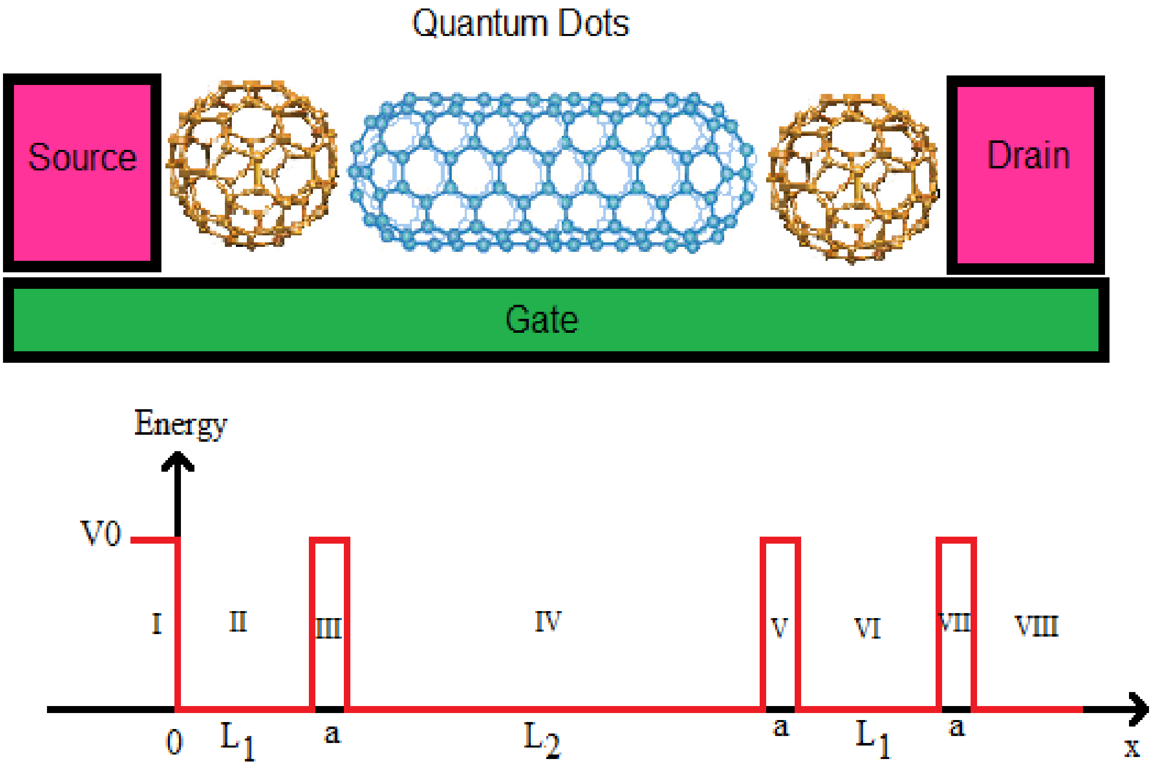


Fig. 3.Top: SET with three islands (two fullerene molecules in the sides and one carbon nanotube in the middle: $C_{60} - CNT - C_{60}$), Bottom: SET energy versus position in the channel region.

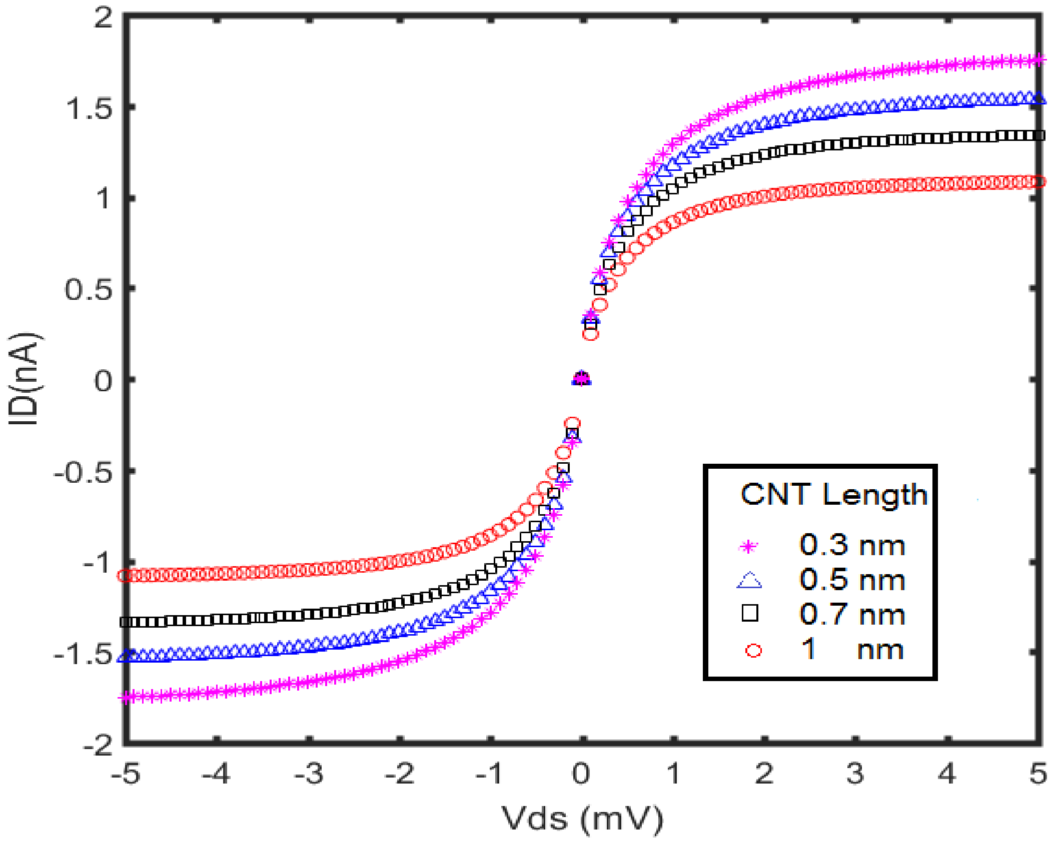


Fig. 4. I-V characteristics of the proposed SET ($C_{60} - CNT - C_{60}$ islands) for different CNT lengths.

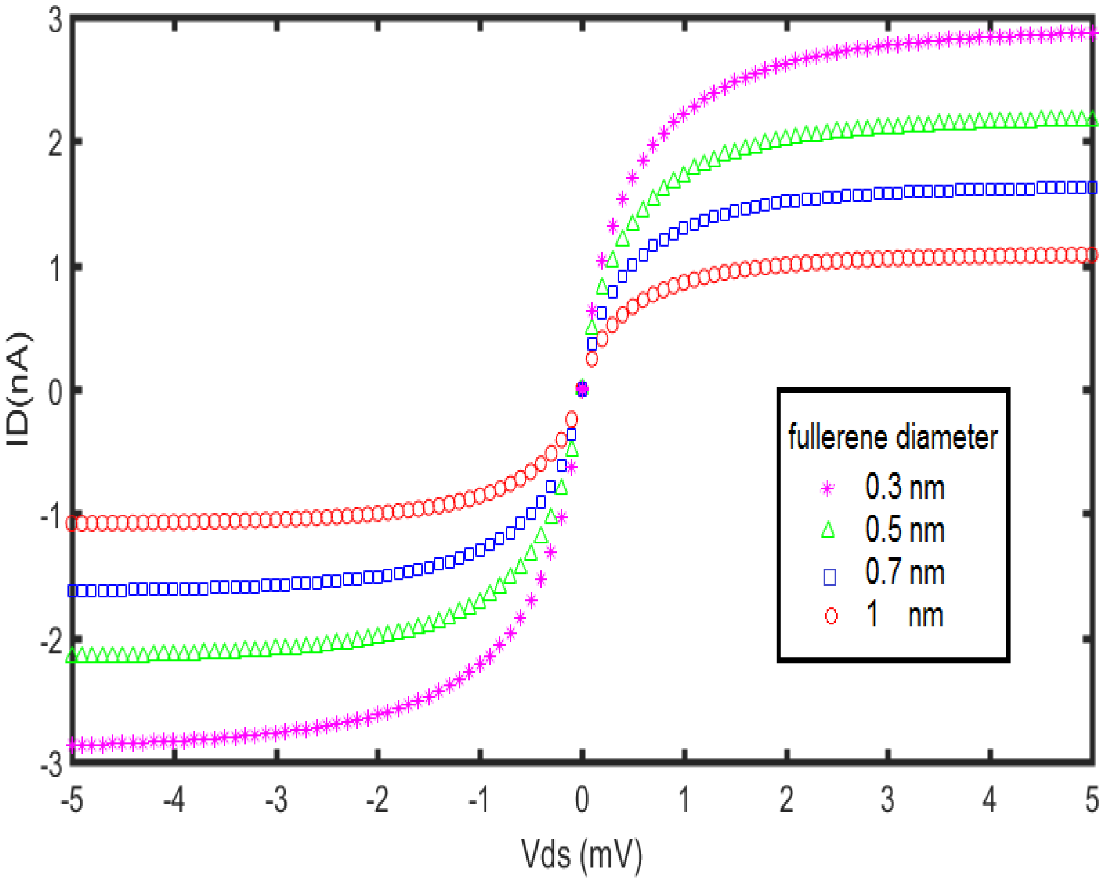


Fig. 5. I-V characteristics of the proposed SET ($C_{60} - CNT - C_{60}$ islands) for different fullerene diameters.

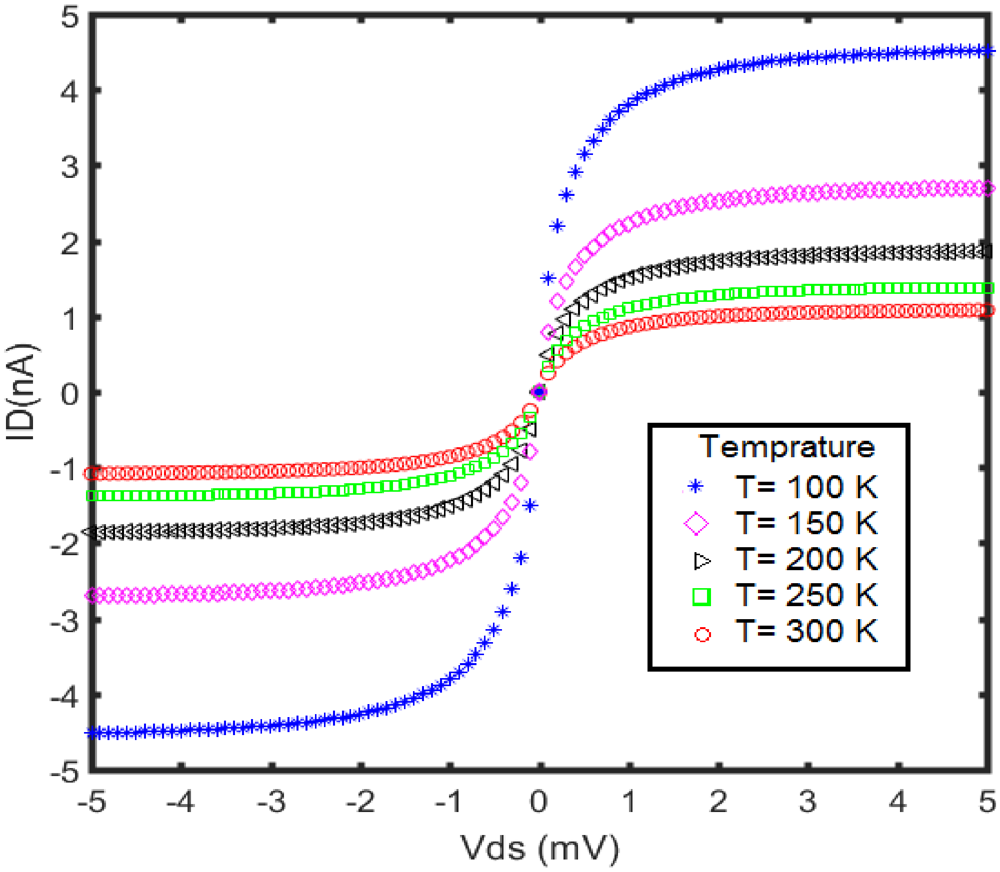


Fig. 6. I-V characteristics of the proposed SET ($C_{60} - CNT - C_{60}$ islands) at different temperatures.

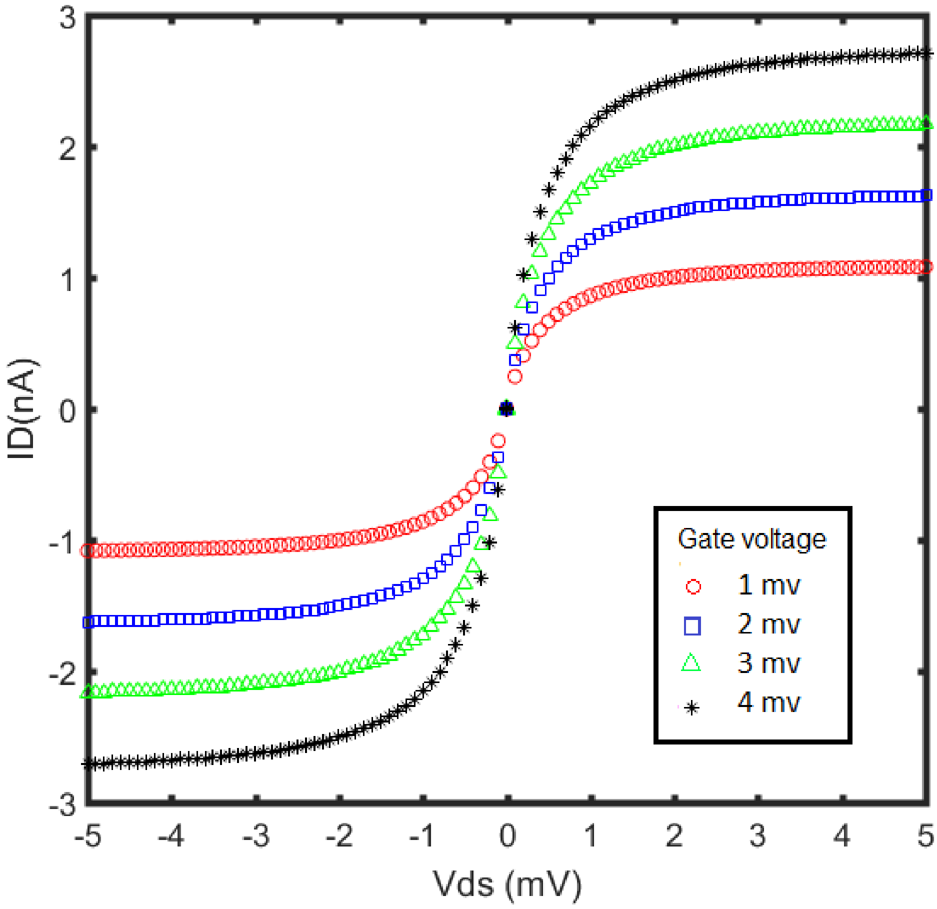


Fig. 7. I-V characteristics of the proposed SET ($C_{60} - CNT - C_{60}$ islands) for different gate voltages.

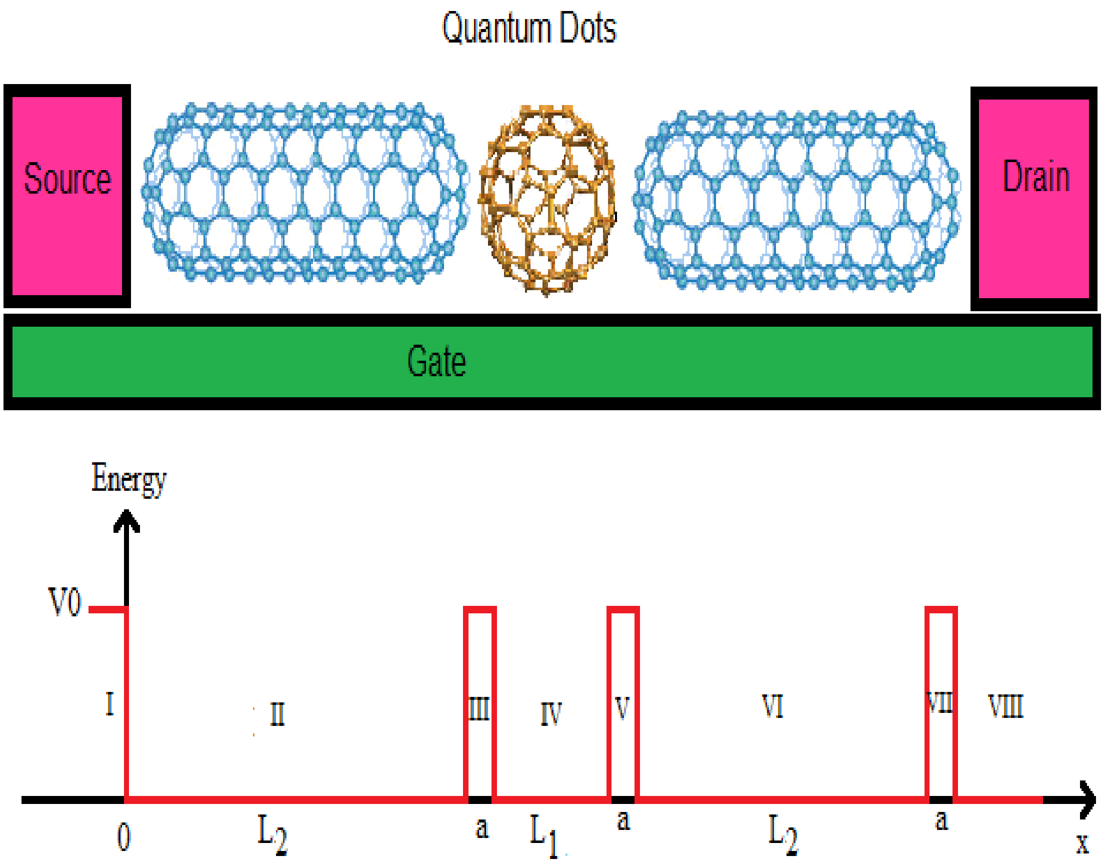


Fig.8. Top: SET with three islands (two CNTs in the sides and one fullerene molecule in the middle: $CNT - C_{60} - CNT$), Bottom: SET energy versus position in the channel region.

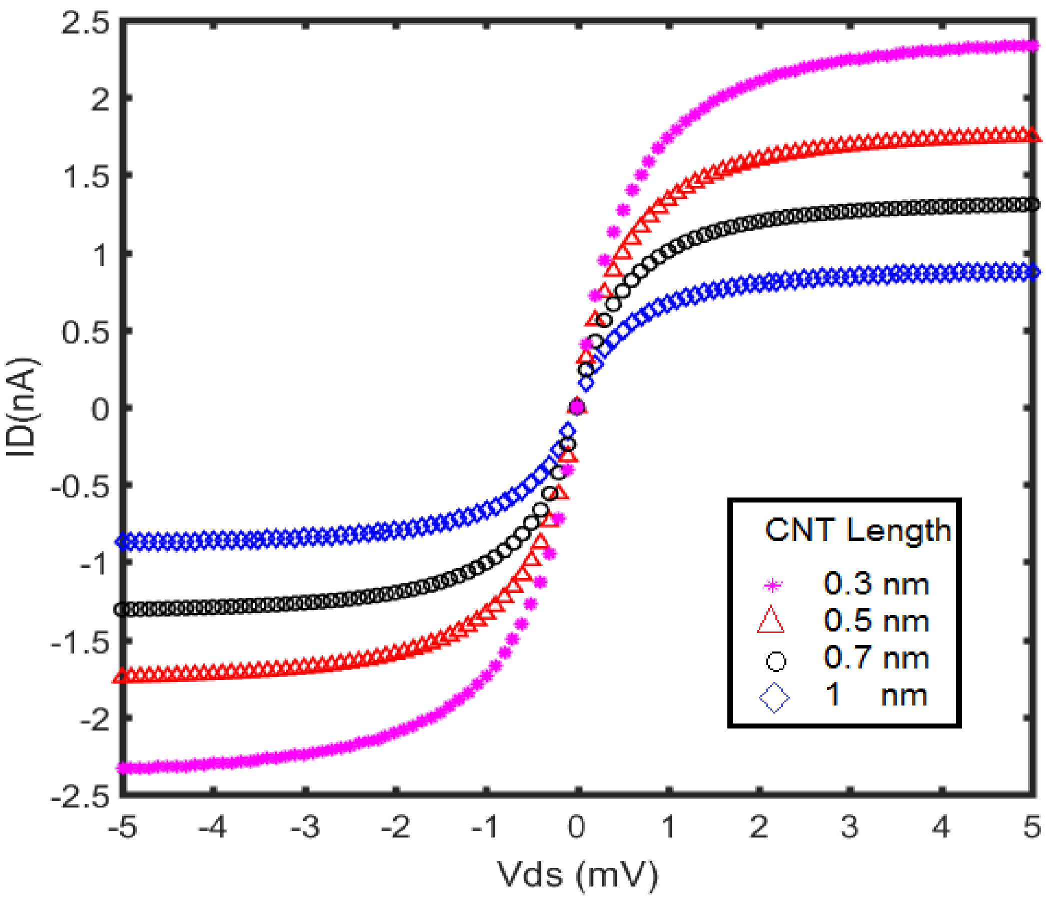


Fig. 9. I-V characteristics of the proposed SET ($CNT - C_{60} - CNT$ islands) for different CNT lengths.

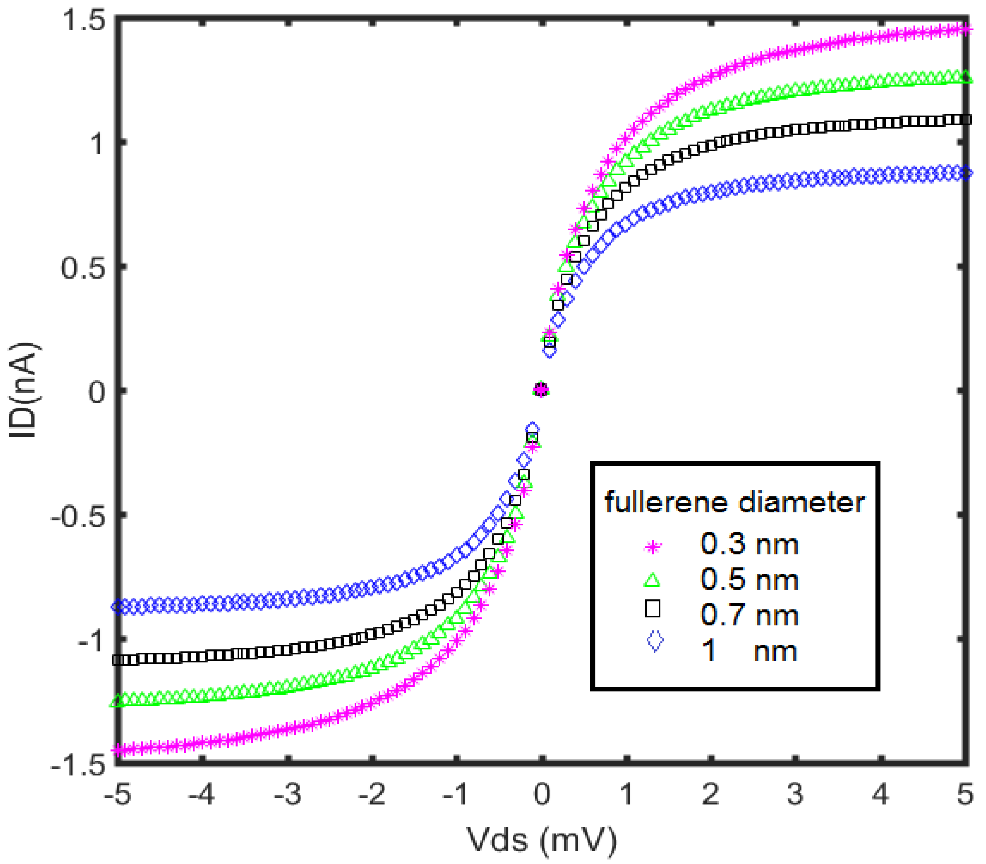


Fig. 10. I-V characteristics of the proposed SET ($CNT - C_{60} - CNT$ islands) for different fullerene diameters.

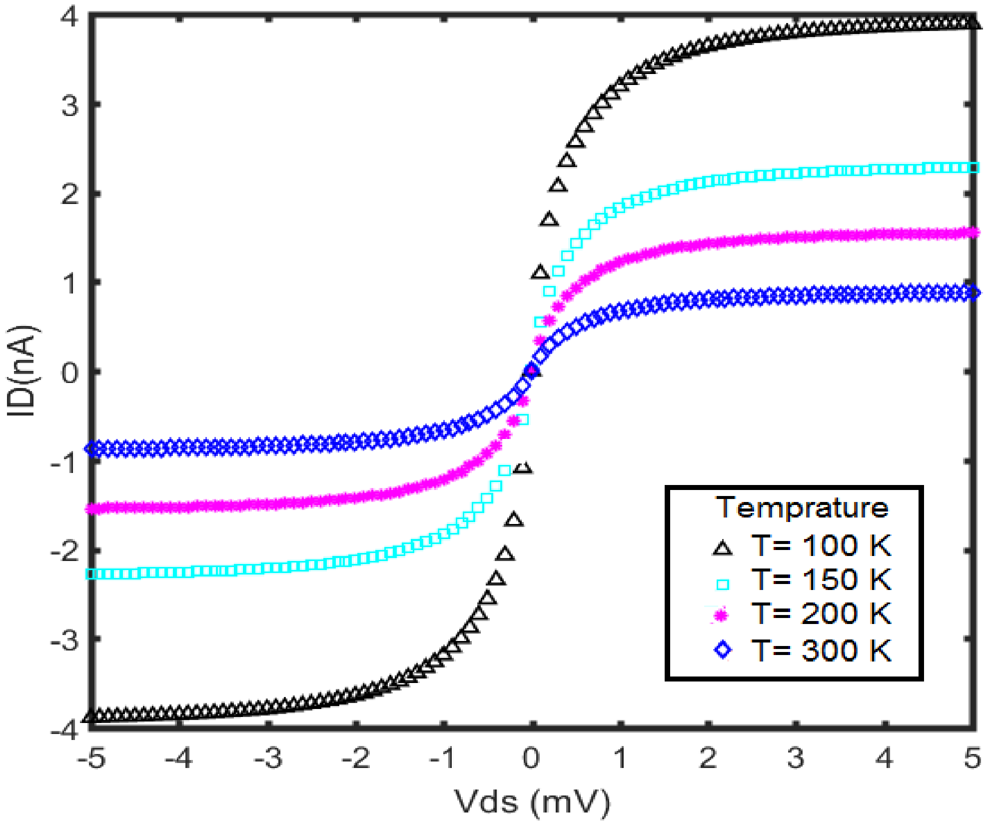


Fig. 11. I-V characteristics of the proposed SET ($CNT - C_{60} - CNT$ islands) at different tempratures.

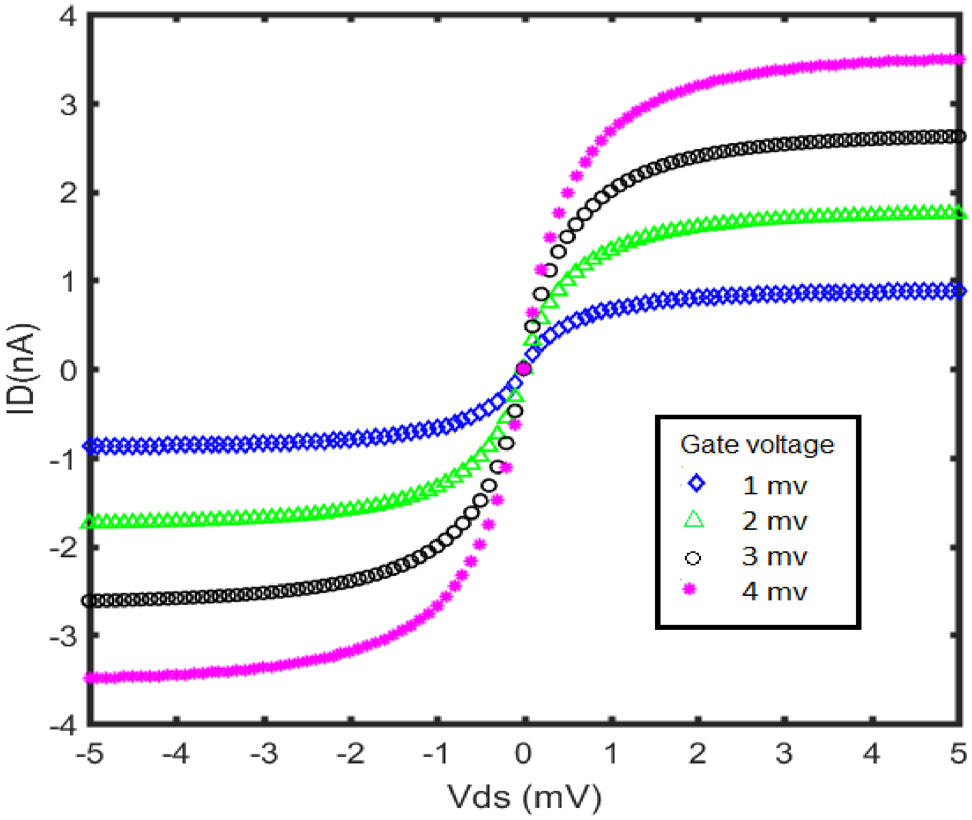


Fig. 12. I-V characteristics of the proposed SET ($CNT - C_{60} - CNT$ islands) for different gate voltages.

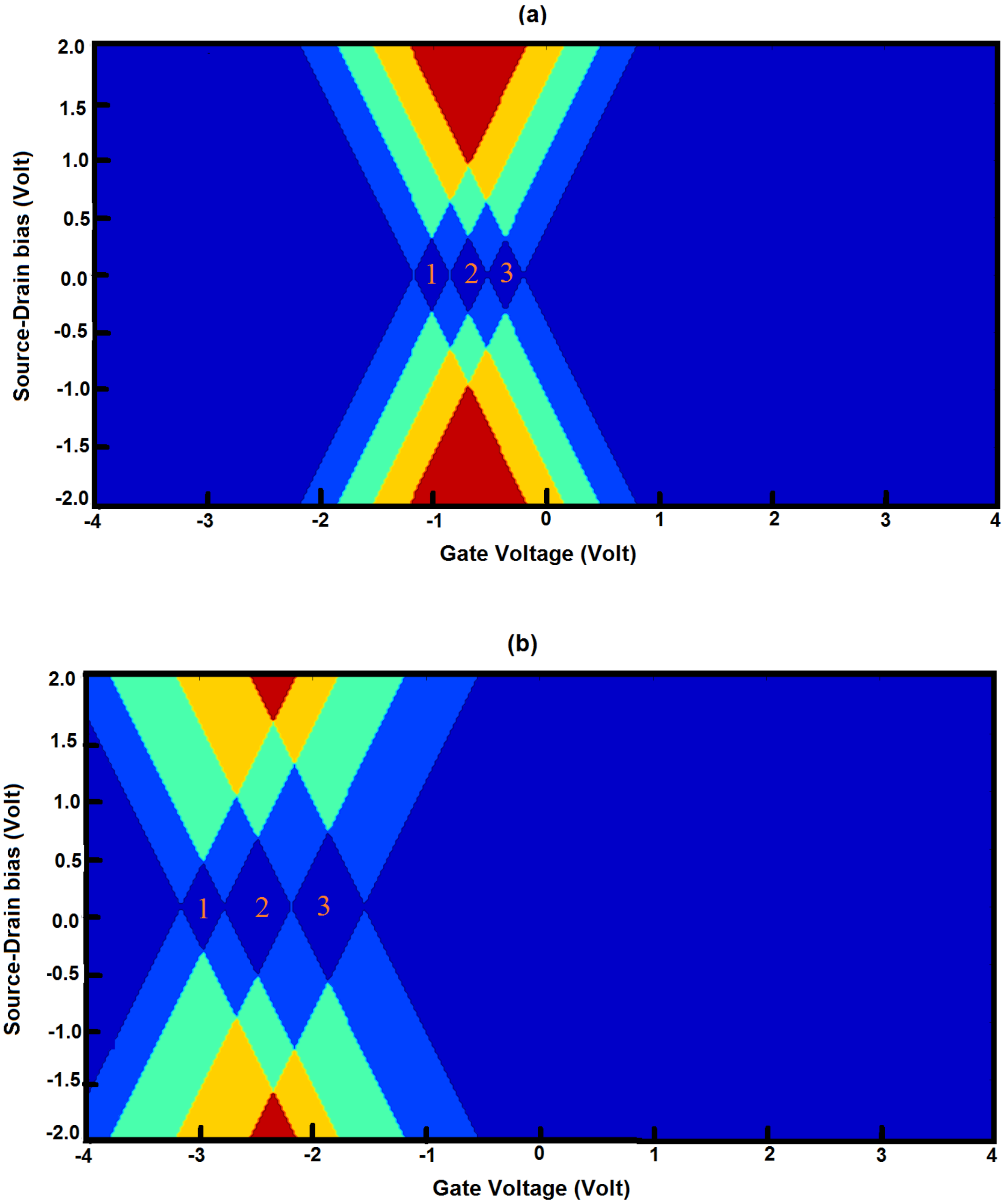


Fig. 13. The charge stability diagrams of two proposed SETs with three islands :(a) islands as $C_{60} - CNT - C_{60}$, (b) islands as $CNT - C_{60} - CNT$.