Analysis of Organic Molecular Single-Electron Transistor Using $C_4H_6B_2$ with Different Metal Electrodes

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Abstract An organic molecule-based single-electron transistor (SET) is analysed by ab initio method using Density Functional Theory (DFT). Initially, benzene molecule is taken; two carbon atoms from benzene are replaced by boron atoms, and the structure of the molecule is optimized. The optimized structure $C_4H_6B_2$ is kept above the gate dielectric in the island for weak coupling. The charge energies of device are calculated in both isolated and SET environment. We have done analysis by using different electrodes with gold (work function = 5.28 eV), osmium (work function = 5.93 eV) and caesium (work function = 2.14 eV) in SET environment. By charge stability diagrams, the conductance dependence of SET on gate voltage and bias potential are verified.

Keywords Single-electron transistor (SET) · $C_4H_6B_2$ · Ab initio · Density functional theory (DFT) · Non-equilibrium greens function (NEGF) · Coulomb blockage

1 Introduction

The number of transistors integrated on chip doubles approximately in every two years. Scaling cannot last for ever because below gate length of 10 nm many parasitics and second-order effects create problem. For continuation of Moore's law, different methods came to existence like spintronics and tunnel junctions. When transistors enter the nanometer regime, they suffer from many second-order effects and leakage current issues. Limitations of transistor scalings such as drain leakage have reached peak level, and hence different approaches depending on

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electron spin transfer, tunnel junction, and confinement of channel material are used.

Enormous attention is given by industries and academic researchers on active electronic unit in single molecules. Single molecules have several unique properties which can be used in electronic unit. Fabricating such small scale devices will be advantageous because of self-assembly and their diversity and functionality.

For smaller and faster switches, single-electron transistors (SETs) have become an alternative. SET allows more number of transistors to be integrated on chip. In present years, the main focus is on using organic molecules as island in SET [1–5].

2 Single-Electron Transistor

SET involves adding a gate control to a coulomb blockade structure as shown in Fig. 1. SET exploits quantum effect of tunnelling to control and measure the movement of single electron. In SET, charge passes through the island in quantized manner. For electron to tunnel from source to island the energy must be equal to $e^2/2c$ (coulomb energy) as shown in Fig. 2, where C is self-capacitance of island.

$$C = e^2 \Delta E, \tag{1}$$

where ΔE is the separation between the energy levels of island.

If the energy is below coulomb energy, electron does not hop and current does not flow.

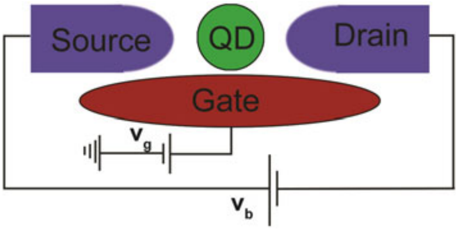
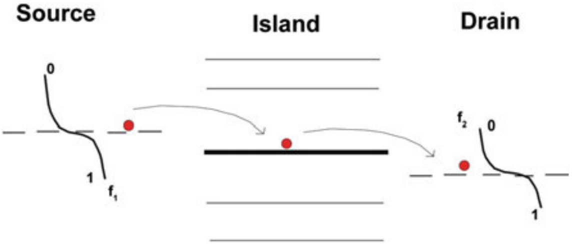


Fig. 1 Single-electron transistor

Fig. 2 Electron tunnelling



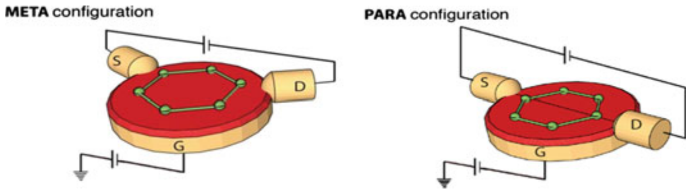


Fig. 3 Meta configuration and para configuration

When the bias voltage between drain and source is increased, the electron is passed through island when energy reaches coulomb energy.

In Meta configuration contact atoms are next nearest neighbours, and in Para configuration the atoms on opposite ends of molecule are coupled to leads, as shown in Fig. 3 [6–10].

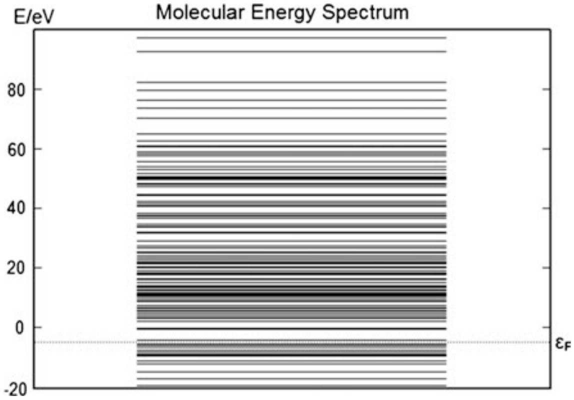
3 Theoretical Approaches

There are different experimental techniques and many theoretical approaches to describe transport in molecular devices. Combination of Density Functional Theory (DFT) with non-equilibrium greens function (NEGF) method is a standard way to study transport in nano-scale. The molecular energy spectrum consists of molecular energy levels as shown in Fig. 4, where Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO).

Basically Fermi-level can be seen as the energy level that lies between occupied and unoccupied states. It can be anywhere in HOMO-LUMO gap.

We define the ionization energy (E^I) as the energy required for removal of single electron from the molecule. It is equal to $-E_{HOMO}$.

Fig. 4 Molecular energy spectrum of $C_4H_6B_2$ with para configuration



The affinity energy (E^{A}) is defined to be the energy gained by adding a single electron to the molecule and it is equal to $-E_{\mathrm{LUMO}}$.

In weak coupling regime, the transport is described by sequential tunnelling.

For movement of electron from source to island, island must have lower energy compared to source.

$$E^{\mathrm{source}}(M) + E^{\mathrm{Island}}(N) \geq E^{\mathrm{source}}(M-1) + E^{\mathrm{Island}}(N+1). \tag{2}$$

For movement of electron from island to drain, the drain must have lower energy compared to island.

$$E^{\mathrm{drain}}(K) + E^{\mathrm{Island}}(N+1) \geq E^{\mathrm{drain}}(K+1) + E^{\mathrm{Island}}(N). \tag{3}$$

Charging energy of island is

$$\Delta E^{\mathrm{Island}}(N) = E^{\mathrm{Island}}(N+1) - E^{\mathrm{Island}}(N). \tag{4}$$

Form the Eqs. (2, 3 and 4), the following variables are given as follows:

N	is the number of initial electrons on island;
M	is the number of initial electrons on source electrode;
K	is the number of initial electrons on drain electrode
$E^{\mathrm{Island}}(N)$	It gives energy of island as function of number of electrons on island;
$E^{\mathrm{source}}(N)$	It gives energy of source as function of number of electrons on source; and
$E^{\mathrm{drain}}(N)$	It gives energy of drain as function of number of electrons on drain.

4 Computational Procedure

By using electrostatic gate, the charging energy of the molecule is modified. Tuning the gate voltage, the energy levels can be moved inside and outside of bias window. Dependency of SET conductance on gate voltage and bias potential is emphasized by charge stability diagram. We also analysed total energy as function of gate voltage in SET environment.

We analysed the total energy by changing the electrodes (work function of gold is 5.28 eV, osmium is 5.93 eV and caesium is 2.14 eV) and plotted the graphs. Total energies and charging energies of molecule for various charge states (2, 1, 0, −1, −2) are calculated using ATK 12.8 Tool kit. These are based on non-equilibrium greens function and density functional theory (DFT).

$C_4H_6B_2$ molecule is used as an island in SET placed between metallic drain and source electrodes above dielectric slab with Para configuration. The dielectric slab of dielectric constant $10\varepsilon_0$ and 3.8 Å thickness lies on metallic back gate. In order to keep the perpendicular component of electric field zero at boundaries, we used Newman boundary condition. Energy zero is kept at absolute zero [11–17].

5 Results and Discussion

Initially, benzene molecule is taken and the charging energies and total energy are calculated. Figure 5 shows the charge stability diagram of benzene. Then the benzene molecule is taken and two carbon atoms are replaced by boron, and structure is optimized and placed in SET environment and even top view of set environment is seen in Fig. 6. Charging energy of $C_4H_6B_2$ in Para configuration is

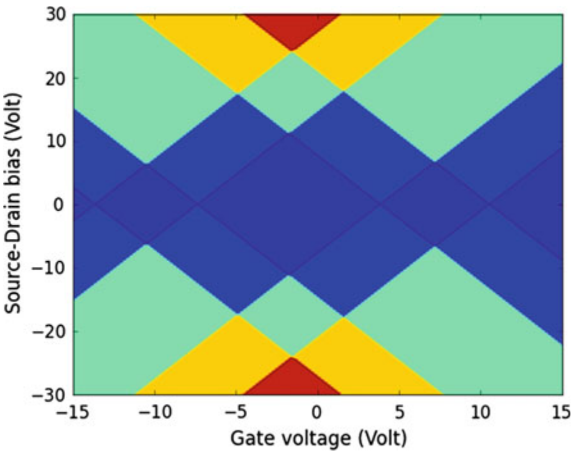


Fig. 5 Charge stability diagram of benzene, the colours represent: (0) *blue*, (1) *light blue*, (2) *green*, (3) *orange* and (4) *red* (Color figure online)

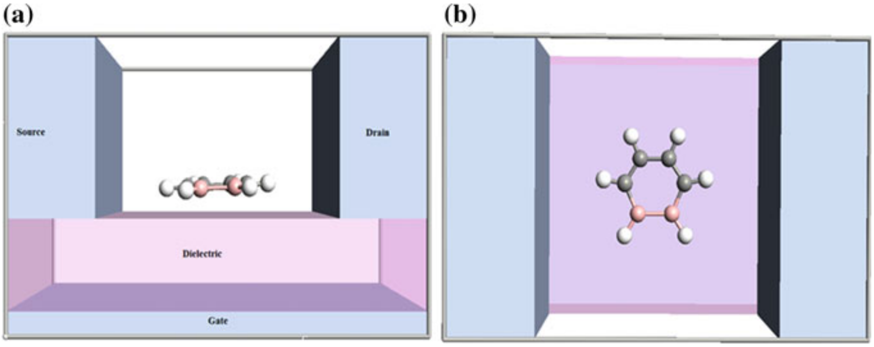


Fig. 6 **a** $C_4H_6B_2$ molecule in SET Environment. **b** Top view of $C_4H_6B_2$ molecule in SET

computed by the total energies of island for different charge states of molecule (−2, −1, 0, 1, 2) in both SET and isolated phases.

The Total Energy of Benzene molecule we obtained is −1040 eV.

The Total Energy of $C_4H_6B_2$ molecule is −880.41 eV.

As the Total Energy of $C_4H_6B_2$ is negative and more compared to Benzene, the coupling of $C_4H_6B_2$ molecule with the source and drain will be weak. Due to weak coupling of $C_4H_6B_2$ molecule with the source and drain, when the electron hops from source to island the electron gets more time to localize. So electron loses all information about its original state in the source electrode and it operates in incoherent transport regime.

Highest Occupied Molecular Orbital (HOMO), $E_{\mathrm{HOMO}} = -5.94$ eV.

Lowest Unoccupied Molecular Orbital (LUMO) $E_{\mathrm{LUMO}} = -0.747$ eV.

Table 1 defines the charging energies of $C_4H_6B_2$ molecule in both isolated and SET environments with different charge states. We obtain $E^{\mathrm{I}} - E^{\mathrm{A}} = -10.49$ eV in the isolated phase and $E^{\mathrm{I}} - E^{\mathrm{A}} = -10.74$ eV in SET environment.

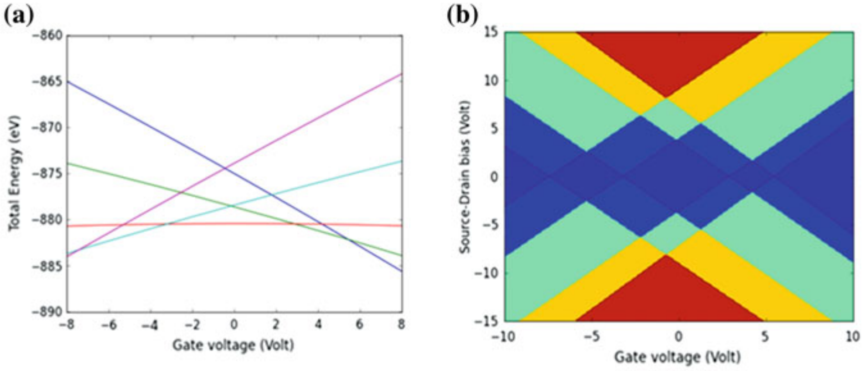
The affinity energy (E^{A}) and the ionization energy (E^{I}) of $C_4H_6B_2$ are 1.001 eV and −9.05 eV in isolated phase and E_A and E_I of $C_4H_6B_2$ is obtained as 3.46 eV and −9.05 eV in SET environment, respectively. In isolated condition, charging energy of $C_4H_6B_2$ at zero state has highest charging energy of 1.001 eV and at −2 charge state it has lowest charging energy of −24.1 eV. In SET environment, at −1 state it has highest charging energy, where at negative potential the positive charges are stabilized and at −2 charge state it has highest charging energy of −17.14 eV. In SET environment, positive charges are stabilized.

We calculated total energy of different charge states of isolated and SET environment as function of gate potential. From Figs. 7 and 8, we can see the results of Total energy versus gate voltage.

Charging energy in SET phase is reduced due to stabilization of charge on island by electrostatic surrounding. Stabilization occurred since the $C_4H_6B_2$ molecule was

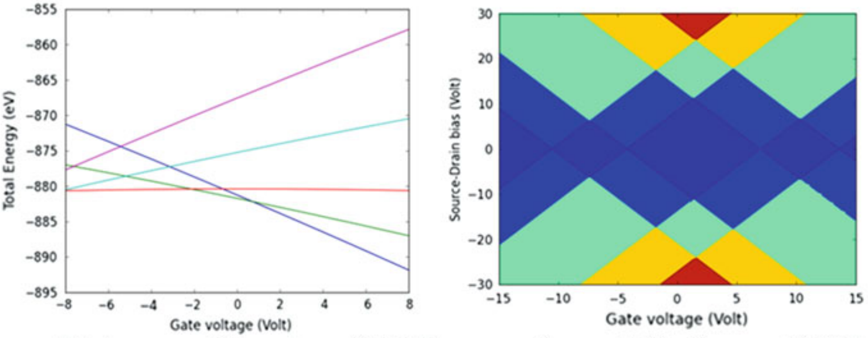
Table 1 Energies of $C_4H_6B_2$ molecule in isolated and SET environments

Environment	Energy	State	Charging energy (eV)
Energies of $C_4H_6B_2$ molecule in isolated condition	$E^{\mathrm{I}+1}$	2	−24.1
	E^{I}	1	−9.05
	E^{A}	0	1.001
	$E^{\mathrm{A}-1}$	−1	−3.35
Energies of $C_4H_6B_2$ molecule in SET environment	$E^{\mathrm{I}+1}$	2	−17.14
	E^{I}	1	−7.28
	E^{A}	0	3.46
	$E^{\mathrm{A}-1}$	−1	5.53



Total energy vs Gate voltage of $C_4H_6B_2$

Charge stability diagram of $C_4H_6B_2$



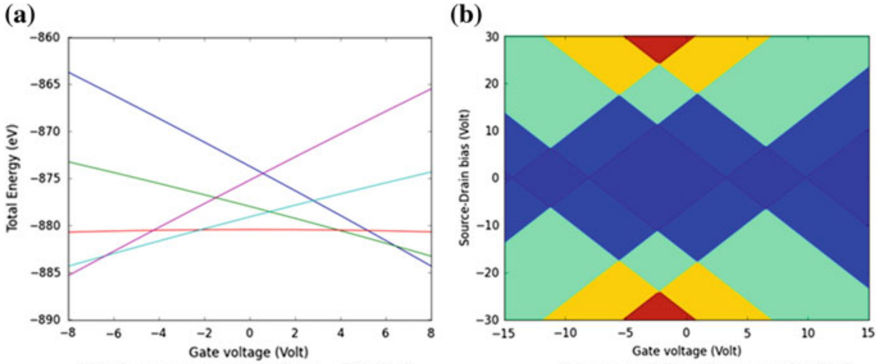
Total energy vs Gate voltage of $C_4H_6B_2$

Charge stability diagram of $C_4H_6B_2$

Fig. 7 **a** Total energy as the function of gate voltage of $C_4H_6B_2$ molecule with different electrodes [Gold (W = 5.28 eV) and caesium (w = 2.14 eV)]. *Curve* represents the charge state: *violet* [2], *turquoise* [1], *red* [0], *green* [−1] and *blue* [−2]. **b** Charge stability diagram of $C_4H_6B_2$ molecule with different electrodes. Gold (W = 5.28eV) and caesium (w = 2.14eV). The *colours* represent: (0) *blue*, (1) *light blue*, (2) *green*, (3) *orange* and (4) *red* (Colour figure online)

kept flat on dielectric. By tuning the gate voltage in SET, the charging energy of island can be modified. It moves the energy levels of SET in and out of the bias window. As it can be illustrated with charge stability diagram, number of energy levels in bias window is shown by colour [codes (0) blue, (1) light blue, (2) green, (3) orange and (4) red]. The work function of electrodes is changed and simulated total energies versus gate voltage are plotted as shown in Figs. 7 and 8.

Number of energy levels in bias window is directly related to conductance. With different electrodes (caesium, gold and osmium) separately in SET environment, the charge stability diagrams are plotted. It is seen in Figs. 7 and 8.



Total energy vs Gate voltage of $C_4H_6B_2$ Charge stability diagram of $C_4H_6B_2$

Fig. 8 **a** Total energy as the function of gate voltage of $C_4H_6B_2$ molecule in para configuration with osmium electrodes (w = 5.93 eV). *Curve* represents the charge state: *violet* [2], *turquoise* [1], *red* [0], *green* [−1] and *blue* [−2]. **b** Charge stability diagram of $C_4H_6B_2$ molecule with osmium electrodes (w = 5.93 eV). The *colours* represent: (0) *blue*, (1) *light blue*, (2) *green*, (3) *orange* and (4) *red* (Colour figure online)

6 Conclusions

In this work, we have taken benzene molecule and replaced the two carbon atoms with boron and optimized the structure. We used that molecule as island, and with different charge states we have calculated the Charging Energy, Total Energy, HOMO and LUMO. By this organic molecule, we got highest negative total energy, so it causes weak coupling of molecule with the source and drain. When the electron hops from source to island, the electron gets more time to localize and hence the electron loses all information about its original state in the source electrode and it operates in incoherent transport regime.

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References

1. 1965—Moore's Law: Predicts the Future of Integrated Circuits. Computer History Museum. Retrieved 2009-03-19 (2007)
2. Yoon, Y., Ganapathi, K., Salahuddin, S.: Nano Lett. **11**, 3768 (2011)
3. Mak, K.F., Lee, C., Hone, J., Shan, J., Henix, T.F.: Phys. Rev. Lett. **105**, 136805 (2010)
4. Abhinav, E., Chary, M., Vemana, D.: Strain-induced on germanene monolayer 6nm short channel FET from first-principle study. In: 2014 International Conference on Circuits, Communication, Control and Computing (I4C), pp. 1, 4, 21–22 Nov 2014. doi:10.1109/CIMCA.2014.7057743

5. Brandbyge, M., Mozos, J.L., Ordejon, P., Taylor, J., Stokbro, K.: Density-functional method for nonequilibrium electron transport. Phys. Rev. B **65**, 165401 (2002)
6. Josephson, B.D.: Possible new effects in superconductive tunnelling. Phys. Lett. **1**, 251 (1962). doi:10.1016/0031-9163(62)91369-0
7. Julliere, M.: Tunneling between ferromagnetic films. Phys. Lett. A **54**(3), 225–226 (1975). doi:10.1016/0375-9601(75)90174-7
8. Grabert, H., Devoret, M.H. (eds.): Single Charge Tunneling: Coulomb Blockade Phenomena in Nanostructures. Plenum Press, New York (1992)
9. Fulton, T.A., Dolan, G.J.: Observation of single-electron charging effects in small tunnel junctions. Phys. Rev. Lett. **59**, 109–112 (1987). doi:10.1103/PhysRevLett.59.109
10. Yano, K., Ishii, T., Hashimoto, T., Kobayashi, T., Murai, F., Seki, K.: Technical Digest of the 1993 International Electron Device Meeting, p. 541 (1993)
11. Atomistix Toolkit Version 12.8: Quantum wise A/S. http://quantumwise.com
12. Ghorbani-asl, M., Borini, S., Kuc, A., Heine, T.: Phys. Rev. B **23**, 235434 (2013)
13. Etymology for ab initio. etymonline.com. Retrieved 7 Feb 2010
14. Erdogan, E., Popov, I.H., Enyashin, A.N., Seifert, G.: Eur. Phys. J. B **85**, 33 (2012)
15. Tour, J.M., et al.: Recent advances in molecular scale electronics. Ann. New York Acad. Sci. **852**, 197–204 (1998)
16. Splendiani, A., Sun, L., Zhang, Y., Li, T., Kim, J., Chim, C.Y., Galli, G., Wang, F.: Nano Lett. **10**, 1271 (2010)
17. Popov, I., Seifert, G., Tománek, D.: Phys. Rev. Lett. **108**, 156802 (2012)