



Electronic and dynamics properties of a molecular wire of graphane nanoclusters

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ARTICLE INFO

Article history:

Received 17 June 2011

Received in revised form 31 August 2011

Accepted 19 September 2011

Available online 4 October 2011

Communicated by R. Wu

Keywords:

Molecular wire

Quantum dots

Graphane

ABSTRACT

In this work we study the electronics and dynamical properties of an array of graphane nanoclusters. The electronic properties are obtained from first principles calculations. The dynamical study is performed by solving the time-dependent Schrödinger equation, adopting the occupation number Hamiltonian and using parameters obtained with first principles calculations. The thermal behavior is simulated by a stochastic algorithm. Our results show that for a set of geometric parameters of the array of nanoclusters, the system exhibits bi-stability in the charge configuration, excitation energies that allow operation at room temperature, operation times below the picosecond and scalability.

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1. Introduction

The limits to miniaturization of electronic devices are reached with sizes where quantum mechanics rules over the dynamics of the system. Because of this, enormous efforts are being made in the search of new technologies to store and process information that can efficiently replace classic electronics. The proposal for quantum systems for carrying out computation represents an attempt to create a new generation of information processors [1]. The major advantage of quantum computation is that it can solve numeric problems that cannot be solved by classical computation. However, it remains the problem of the coherence of the proposed systems. Some significant advances have been made in addressing this difficulty using dislocated qubits with global control protocols [2], with small molecular systems. On the other hand, a completely different solution to the quantum computation has been attempted by using cellular automata architecture to develop classical computational processes with quantum entities. Important advances have been made with automata based on quantum dot arrays (QCA), the idea for which was proposed by C. Lent and collaborators [3]. The original idea was introduced as a system of quantum corrals with four quantum dots inside and doped with two electrons. The electrons can tunnel through the quantum dots, but cannot

get out of the corrals that form the cells of the automaton. This architecture can propagate and process binary information with adequate control protocols [4]. The first experimental demonstration of the implementation of a QCA was published in 1997 [5]. A subsequent work also demonstrated an experimental method for the implementation of a logic gate [6], and a shift register was also reported [7]. These results provide good agreement between theoretical predictions and experimental outcomes at low temperatures. Implementation at room temperature requires working at a molecular level, and in the context of molecular cellular automata there are also important contributions at the experimental level [8]. In the molecular case, the quantum dots correspond to oxide-reduction centers, and as in the case of metallic quantum dots or semiconductors, are operated with electrical polarization. The implementation of this cellular automata architecture is achieved with an extremely small chain of molecules [8], supported in a chemically inert substrate. Another implementation at room temperature corresponds to an array of magnetic quantum dots propagating magnetic excitations to process digital information [9]. These systems use the magnetic dipolar interaction among particles whose size is at the submicrometer scale. A theoretical study was recently published about the behavior of cellular automata composed of an array of polycyclic aromatic molecules [10], using the polarization of the electronic spin. In that paper is established that by increasing molecules along one direction on the plane, forming graphene nanoribbons, binary information can be transmitted at room temperature. In this study we propose a molecular wire with graphane (hydrogenated graphene) nanoclusters to propagate and process digital information. We intend to

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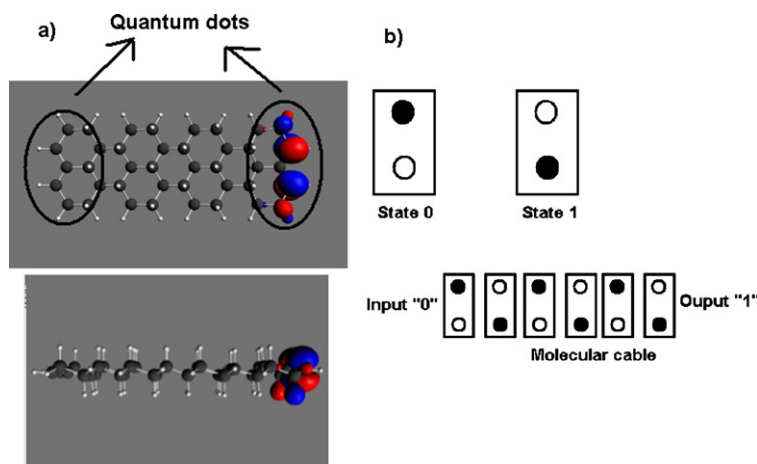


Fig. 1. a) Graphane molecules studied in this work. These molecules have a minimum energy state with the charge located in one of the quantum dots. b) Schema of the defined logical states, and the molecular wire formed with these molecules.

verify theoretically that the proposed system is scalable and that binary information can be stored, propagated and processed at room temperature.

1.1. Graphane

In 2004 the group of Kostya Novoselov [11] succeeded in isolating a simple layer of carbon atoms (graphene) using a technique by mechanical exfoliation of graphite. This work represented the beginning of many theoretical and experimental studies and their potential applications to systems derived from graphene [12,13]. A theoretical investigation in 2007 [14] predicted a new form of graphene totally saturated with hydrogens. The authors of this Letter gave the name “graphane” to this new form derived from the graphene. The shape of this new structure is similar to graphene, with the carbon atoms in a hexagonal lattice and alternately hydrogenated on each side of the lattice. In January 2009, the same group that isolated graphene in 2004, published a paper in Science magazine reporting the hydrogenation of graphene and the possible synthesis of graphane [15]. Since then there has been growing scientific interest in the study of hybrid graphene–graphane systems and their potential applications.

In this Letter, we study a molecular wire formed by clusters of graphane. The role of quantum dots in the studied nanostructures will be played by redox centers. These centers will be obtained by leaving two regions, on opposite edges, with three unhydrogenated carbon atoms. As a result of this, the free electrons will locate themselves in one of the quantum dots if an external electrical field is applied.

2. Electronic properties of graphane nanoclusters

The dynamic properties of molecular wire depend on the electronic properties of individual cells. The molecules studied in this work are structure similar to polycyclic aromatic molecules (PAHs), saturated with hydrogen atoms, except at the ends (quantum dots). In those ends there are two unpaired electrons in each quantum dot and in the case of the molecular cation, there is an unpaired electron that can be located in a quantum dot or in the other. Our results obtained using methods based on first principles calculations, show that the molecular cation has a state of minimum energy with the electron located in one of the quantum dots and it has an excited state when the electron is in the quantum dot at the other end (the technical details of our calculations will be given in Section 2.1). Fig. 1(a) shows the structure of the molecules studied.

We will use cell- nm to denote these molecules, where n represents the number of carbon atoms of the armchair edge and m is the number of carbon atoms of the zigzag edge of the molecule. The figure shows two quantum dots at the ends and the iso-surface of the HOMO of cation cell-82. Due to these molecules have two states with the charge localized in the quantum dots, they can be defined as the cells that form the automaton (molecular wire). The polarization of the charge and the Coulomb interaction between cells are used to transmit binary information from one cell to the next. A scheme of the logical states defined for each cell and how the molecular wire would operate are shown in Fig. 1(b).

2.1. Analysis of the hybrid methods

A very important parameter to determine the dynamic properties of molecular wire, is the energy of tunneling between quantum dots of the molecule. For molecular cations we can define this energy as $\gamma = \frac{E(\text{LUMO}) - E(\text{HOMO})}{2}$. The dynamic response of the automaton is very sensitive to this parameter, so we will detail the methodology used to determine its value from first principles. The study of cations and neutral molecules, using these methods, presents a difficulty in relation to the localization of the charge. The Hartree–Fock method overestimates this localization and the DFT method underestimates it [16–19]. By other hand the method of Complete Active Space Self-Consistent Field (CASSCF), which uses the excited states in the base, is efficient to predict the correct charge localization, however it is completely impractical for systems with many atoms. For this reason in this research we use methods hybrids that combine the HF and DFT methods. In order to choose the appropriate hybrid potential, we study known structures that are similar to the structures proposed in this work, with several potentials. First we show a study of the neutral hydrocarbon HOMO–LUMO gap which is known experimentally, with the hybrid method that we use in our research. The molecules studied are benzene, naphthalene, tetracene, and anthracene that correspond to hydrocarbons formed with benzene rings. In all our calculations the structure is relaxed by means of the method “Quasi-Newton Approach” [23] and we adopt Slater type orbitals and double zeta polarized basis (DZP), by using the ADF software [21]. The results obtained are shown in Table 1, this table also includes the corresponding experimental values [22]. We observe that the methods hybrids O3LYP, B3LYP and B3LYP* present a good fit with experimental data. The graph of Fig. 3(a) shows the gap in eV plotted as a function of the number of benzene rings of the molecule. Only the hybrid methods of interest have been plotted.

Table 1
Gap obtained for 4 molecules, using different methods hybrids.

Method	% HF	Benzene gap (eV)	Naphthalene gap (eV)	Anthracene gap (eV)	Tetracene gap (eV)
GGA-PBE	0	5.28	3.24	2.12	1.45
O3LYP	12	6.19	4.05	2.81	2.06
B3LYP*	15	6.44	4.28	3.01	2.24
B3LYP	20	6.82	4.60	3.30	2.51
B1LYP	25	7.20	4.93	3.58	2.78
MPW1PW	43	7.21	4.94	3.58	2.78
BHandH	50	9.10	6.57	5.03	4.11
Hartree–Fock	100	12.78	9.84	7.96	6.85
Experimental		6.20	4.51	3.31	2.63

Table 2
Results obtained for the parameters γ and L .

Method	Cell-42 γ (eV)	Cell-62 γ (eV)	Cell-82 γ (eV)
GGA-PBE	0.027	0.019	0.018
O3LYP	1.329	0.327	0.254
B3LYP*	1.627	0.759	0.412
L (Å)	6.60	10.78	15.22

Additionally we performed calculations with charged molecules to verify the behavior of these hybrid methods with cations. In the work of Lu and Lent [20], it is performed a study with an alkyl-diene cation using the CASSCF method to determine the difference in energy between the ground state (with the charge located at one end) and the first excited state (with the charge on the other end). The alkyl-diene molecule consists of two ethylene groups connected by an alkyl bridge.

Fig. 3(b) shows results for the unrestricted Hartree–Fock, DFT GGA-PBE and the different hybrid methods of interest. These results correspond to 4 molecules with the structure of alkyl-diene differing in the number of elements CH_2 composing the alkyl-bridge and therefore, in the distance separating the two quantum dots. Also included on the graph are the results obtained by Lu and Lent using the CASSCF method [20]. In this graph x axis represents the distance separating the quantum dots (edge) in the molecule. Our relaxation calculations did not coincide with those reported by the authors of work [20] and that is the reason for the difference in position of the points in the plot. In all our calculations we relax the structure doped with $Q = +1$ and we use the same level of theory that for the neutral molecules. Our results show that hybrid methods B3LYP* and O3LYP show good agreement with the CASSCF method for these small molecules.

By the analysis of the results we establish that the O3LYP and B3LYP* are very good methods to determine the gap of neutral and charged molecules, and therefore we will adopt them to determine the parameter γ of our molecules.

2.2. Electronic properties of graphane-like molecules

Using hybrid methods and the level of theory described in the previous section, we calculate the electronic spectrum for cations cell-42, cell-62 and, cell-82. These structures (type graphane) are shown in Fig. 4 and the corresponding parameters γ and L are shown in Table 2. The parameter L is obtained by relaxing each structure and the γ value was obtained with the methods listed in Table 2.

3. Dynamics and thermal behavior of the molecular wire

In this section we analyse the dynamic response of the automaton when binary information is transmitted from one extreme to

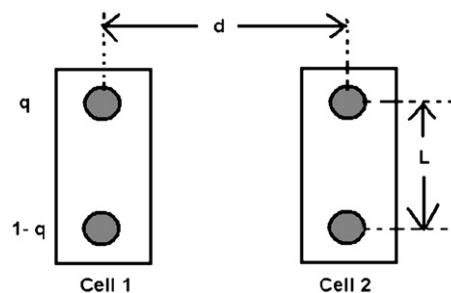


Fig. 2. Interaction between neighboring cells.

the other of the molecular cable. Let us consider a system consisting of N cells, as shown at the bottom of Fig. 1(b). The first cell acts as a driver and its polarization is externally manipulated. For the remaining $N - 1$ cells, we solve the time-dependent Schrödinger equation using the occupation number Hamiltonian. Most of the work which exists in the literature on multiple quantum dot systems is based on occupation number (Hubbard-like) formalism [27–29]. This type of Hamiltonian is rather straightforward to implement and requires very limited computational resources. Each quantum dot and its interaction with the other dots are described by means of a few phenomenological parameters, such as the tunneling energy, the dot confinement energy, the on-site electrostatic interaction. Such descriptions are successful in capturing the overall behavior of the system, and in providing a qualitative understanding of the underlying physics. For the i -cell in the automaton, the Hamiltonian can be written:

$$H = V_\alpha \hat{n}_\alpha + V_\beta \hat{n}_\beta - \gamma (\hat{a}_\alpha^\dagger \hat{a}_\beta + \hat{a}_\beta^\dagger \hat{a}_\alpha) \quad (1)$$

In this equation the subscripts α and β denote the upper and lower quantum dot respectively (Fig. 2). The terms \hat{n} , \hat{a}^\dagger and \hat{a} correspond to the number, creation and annihilation operators, respectively. The parameter γ corresponds to the tunneling energy between the quantum dots of the molecule and it was defined in the previous section. The terms V_α and V_β represent the Coulomb interaction between the charge in the dot α or β and the other cells. These terms take into account the interaction with neighboring. The vector representing the state of the i -cell is written as:

$$|\Psi(t)\rangle = c_\alpha(t)|\alpha\rangle + c_\beta(t)|\beta\rangle \quad (2)$$

where $|\alpha\rangle$ and $|\beta\rangle$ are the charge wave functions as it is in the upper quantum dot and in the lower, respectively. Using the Hamiltonian given by Eq. (1), the dynamics is obtained from the equation:

$$i \frac{\partial |\Psi(t)\rangle}{\partial t} = H |\Psi(t)\rangle \quad (3)$$

By replacing the wave vector (2) in the Schrödinger equation (3), a system of differential equations for the coefficients are obtained

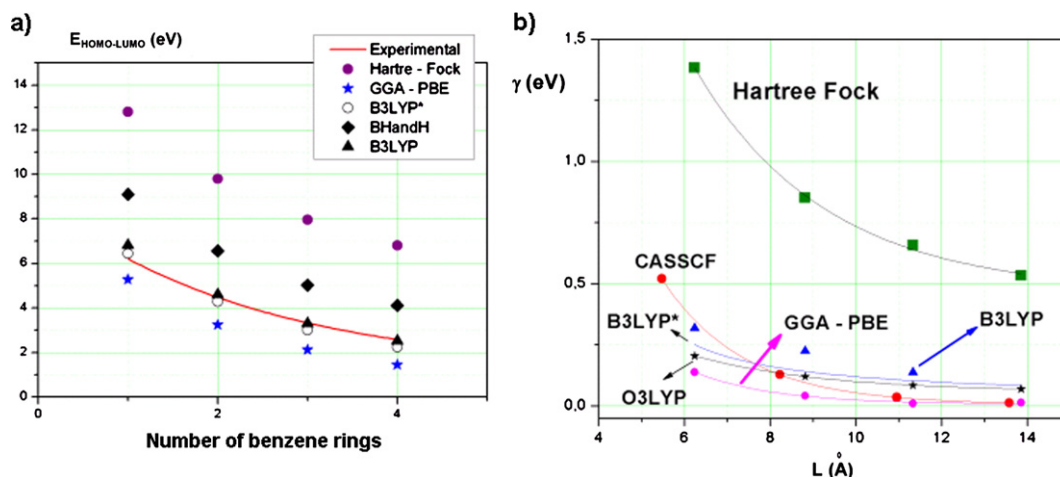


Fig. 3. a) Results of the gap HOMO–LUMO, obtained using different methods. b) Study alkyl-diene cation.

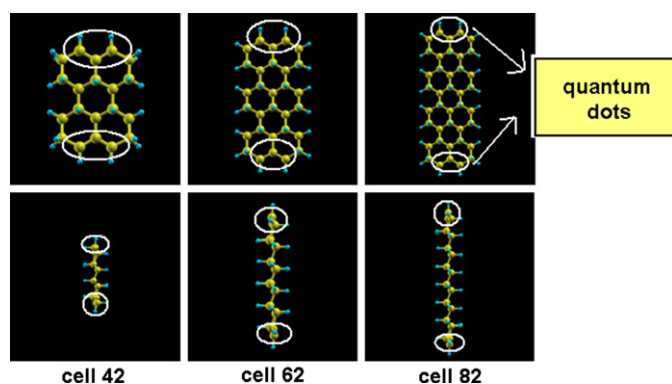


Fig. 4. Molecules studied. Top: top view of the system. Bottom: lateral view of the system.

which we solve numerically with given initial conditions. In our study, the value of polarization $P = +1$ (in atomic units) means the hole (positive charge) is in the upper quantum dot and $P = -1$, means it is on the lower quantum dot. First we study the dynamical response of a system consisting of 2 cells. The polarization of cell 1 (driver) is linearly changed from one state to other in a given time interval. We solve Eq. (3) for cell 2 and verify the temporal behavior of the polarization.

Fig. 5 shows results obtained for the molecule cell-82 with the parameter $\gamma = 254$ meV obtained with the method O3LYP and $L = 15.22$ Å for different values of separation between the cells. It was considered a time interval of 40×10^{-15} seconds (τ). The initial state of the cells 1 and 2 is $[-1, +1]$. In the time interval $0 \leq t \leq \frac{\tau}{4}$ the polarization of the cell 1 remains in the state $P_1 = -1$, then in the interval $\frac{\tau}{4} \leq t \leq \frac{3\tau}{4}$ the polarization of the cell 1 changes linearly from the -1 state to the $+1$ state and finally in the interval $\frac{3\tau}{4} \leq t \leq \tau$, the polarization of the cell 1 remains in the state $+1$. We can observe in Fig. 5(a), that when the molecules are far apart, the polarization of cell 2 oscillates between the values -1 and $+1$, with a frequency given approximately by $\nu \approx \frac{2\gamma}{\hbar}$ and therefore it would not be coupled to the first cell. As the distance decreases, the polarization of the molecule 2 responds to the driver changes. This distance has a minimum due to the interaction between neighboring atoms. Fig. 5(d) shows that the polarization of cell 2 changes the state $+1$ to state -1 , in a time interval of around 10×10^{-15} seconds and then it stays (with small oscillations) in the -1 state. This change in polarization is nonlinear and therefore has the desired requirements for bistability of such systems.

In what follows we study the dynamical response of a 5 cells chain (the first being the driver). The initial state of the chain is $[-1, +1, -1, +1, -1]$. We study a time interval τ , so that in the range $t \leq \frac{\tau}{4}$ the driver polarization changes linearly from the -1 to the $+1$ state and it remains there the rest of the time. We solve the Schrödinger equation for the remaining 4 cells, using the Hamiltonian (1). Fig. 6 shows results for 4 molecular wires of 5 cells. Fig. 6(a) corresponds to a cable formed with cell-42, Fig. 6(b) for cell-62, Fig. 6(c) for cell-82 and Fig. 6(d) for cell-hyp, a hypothetical molecule whose separation between the quantum dots is 20 Å and whose parameter γ is obtained by extrapolating the data in Table 2 with a function that decays exponentially. All calculations for parameter γ are obtained with the method O3LYP and the separation distance between the cells is of 7.5 Å. Each one of the four figures shows the polarization of each cell that forms the cable as a function of time. In the vertical axis is plotted the polarization (in atomic units) and the horizontal axis represents the time in units of 10^{-15} (s). For the case shown in a) $\tau = 10 \cdot 10^{-15}$ (s) and for cases b), c) and d) $\tau = 40 \cdot 10^{-15}$ (s). It is observed, in the figure, that the cables formed by cell-62 and cell-82 are able to properly polarize the last cell in the time interval studied. Instead, for cell-42, the high value of the parameter γ , makes that each one of the 4-cells attached to the first be oscillating between the two states of polarization, with a frequency close to $\nu \approx \frac{2\gamma}{\hbar}$. On the other hand, for the case where the molecule has the quantum dots far apart (Fig. 6(d)), the last two cells do not change their state of polarization in the time interval studied. This part of the study would indicate that we can choose a set of adequate geometric parameters to spread binary information through a cable formed by these graphene molecules.

The thermal behavior of the molecular wire is studied using a stochastic algorithm which incorporates the system temperature in the molecular dynamics of the cable. We performed a study for a molecular wire formed by 5 cells whose initial state of polarization is $[-1, +1, -1, +1, -1]$. The first cell represents the driver and its state of polarization is changed in a similar form as the case shown in Fig. 6. In each step of the algorithm a cell is randomly selected from the rest of the 4 cells of the automata. For this cell, the state given by Eq. (2) is changed randomly, so that $|c_\alpha(t)|^2 + |c_\beta(t)|^2 = 1$. This modification in the state lets the cell in any superposition of the $|\alpha\rangle$ and $|\beta\rangle$ states. With this new charge configuration of the molecular wire the electrostatic energy is calculated and, the change is accepted with probability 1 if $\Delta E < 0$ and with probability $p = e^{-\beta\Delta E}$ if $0 \leq \Delta E$, where $\beta = \frac{1}{kT}$ and T the system temperature. In general in the case of stochastic algorithms (Metropolis or Glauber) it must be assigned

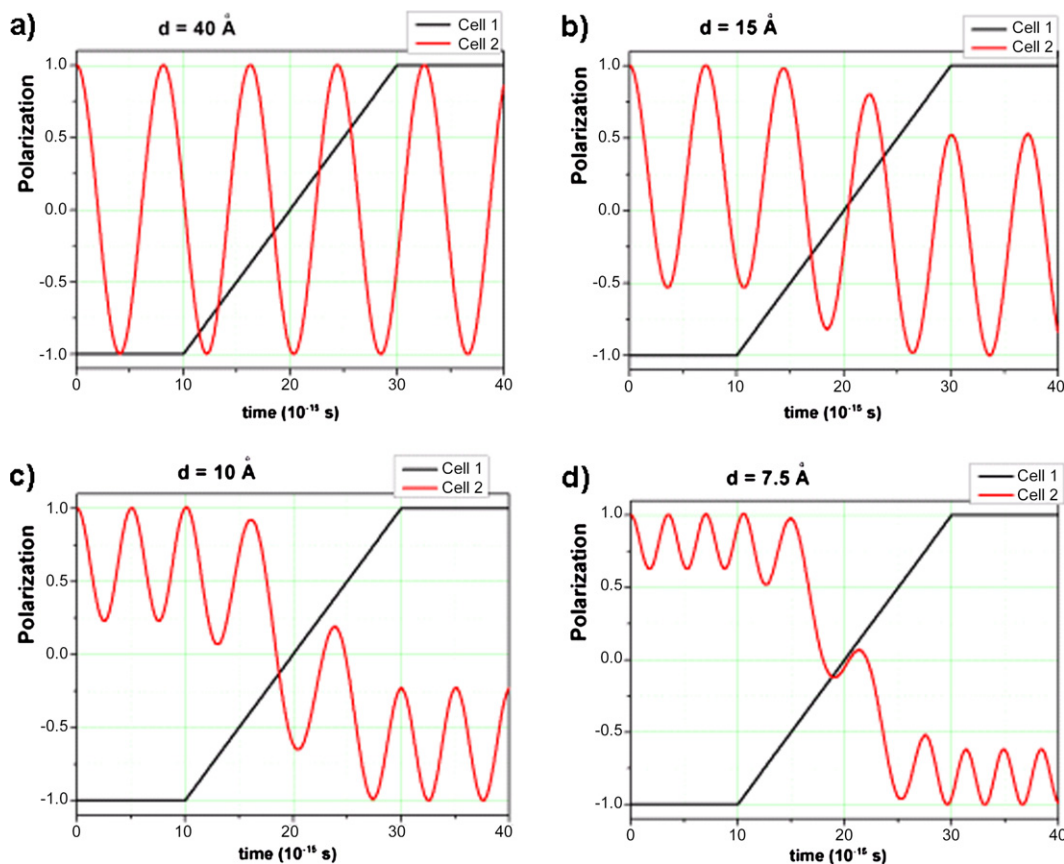


Fig. 5. Response of a system consisting of 2 cells as a function of the distance of separation of the cells.

a time interval to the step of the algorithm. One can use some phenomenological data, such as the energy difference between the two possible states of the cells [10], to estimate the time associated with each computational step. In our study this is not the case because in each step, the cell can take any value for $|c_\alpha(t)|^2$ and not necessarily to move to another state of polarization, i.e., it can stay in any superposition state. This implies that it takes several computational steps to go to another polarization state. Therefore we assign the same computational step used in the studies shown in Figs. 5 and 6 for valid comparisons. Fig. 7 shows simulation results for up to 4 cases where we are included the geometric parameters L of the molecule cell-42, cell-62, cell-82 and cell-hyp (Figs. 7(a), (b), (c) and (d), respectively). The separation distance is $d = 7.5 \text{ \AA}$ and the temperature is 40°C for the four cases.

The time interval that the driver takes to go from a polarization state -1 to a $+1$ is 5.0×10^{-15} (s) in the all cases. The results show a qualitatively similar behavior with those shown in Fig. 6 where the automata cell-62 and cell-82 are the best behaved. For the cases cell-42 and cell-hyp, the last cell achieves the proper polarization, but with much thermal noise, especially in the case of the automaton cell-42 (Fig. 7(a)). In this part we can conclude in a qualitatively way that the automaton can operate to the standard work temperature of the electronic devices.

4. Graphane nanoribbon

In this section we show the results for a molecular wire formed with the same structure as the molecules cell-42 (graphane structure), but on a continuum along the automaton axis. To perform first principles calculations to study a structure with one dimension which is considered large, we assumed it to be infinite. We

must form a periodic three-dimensional crystal, for which we define a unit cell repeating the structure along the axis of the ribbon (x axis), and also along the axis y and z . To simulate the behavior of an isolated nanoribbon we separate the ribbons along the axis y and z sufficiently so that the properties correspond to just one isolated ribbon. In our study, nanoribbons are separated 20 \AA axis along y (in the plane of the ribbons) and 10 \AA in the z axis. Fig. 8 shows a diagram of the unit cell used in this study, formed by four quantum dots with dimensions equivalent to the structure cell-42 ($L = 6.60 \text{ \AA}$, $d = 7.50 \text{ \AA}$) and charged with two positive charges.

The electronic and magnetic properties of the systems are obtained by means of first principles calculations based on the pseudo-potentials method and by using the generalized gradient approximation Perdew–Burke–Ernzerhof with spin polarization [24]. All structures are relaxed using the Direct Inversion Iterative Subspace method [25] with a residual force criteria less than 10^{-4} Hartree/Bohr. Calculations were performed using the OPENMX Code [26]. In Fig. 9 it is shown the total spin density of the minimum energy state of the system. We see that in this minimum energy state the electron is in a quantum dot with spin up (red color), while the other is in the quantum dot of the other cell with spin down (blue).

Fig. 10 shows the density of states of this structure and a scheme of the real part of the wave function for different peaks in the density of states near Fermi level. Here, it can be seen that the minimum energy state for the spin up corresponds to the electron entirely located in the quantum dot, while the minimum energy state for the spin down corresponds to the electron located in the quantum dot of cell 2 and in a position that minimizes the electrostatic energy. The excited states of both spins correspond to the opposite quantum dots of each cell. By analysing the energy

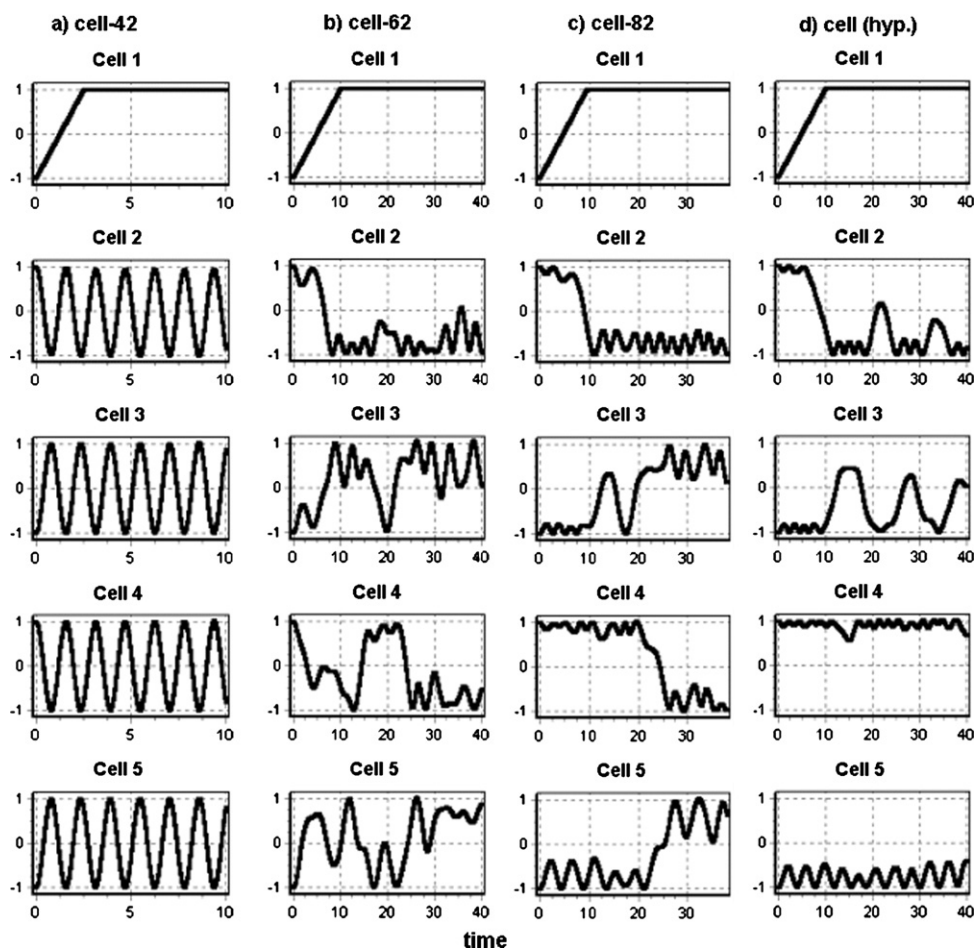


Fig. 6. Dynamic behavior of the polarization of a cable formed with 5 cells in which the first is the driver. Figures (a), (b), (c) and (d) show the simulation for cell-42, cell-62, cell-82 and cell-(hyp), respectively.

band diagram it was possible to determine a tunneling parameter γ_1 between quantum dots of the same cell (equivalent to the parameter γ in the study of molecules). The calculations gave a value of $\gamma_1 = 19.4$ (meV) close to the value obtained, using the same level of theory, for the isolated molecule cell-42. To verify the behavior of these structures considering the spin degree of freedom, we calculate the total energy of the unit cell for the minimum energy state and for two metastable states. The minimum energy state of the two cells (unit cell) corresponds to the polarization $[+1, -1]$, we call this state E_1 . The next state has a polarization $[+1, +1]$, we call this state E_2 and finally we analyse the state in which both electrons are in the same cell, leaving no net charge to the neighbor cell, this is the state of polarization $[0, 0]$ and energy E_3 . Using the same level of theory for the three states we find that $E_1 < E_2 < E_3$. This would be in agreement with the pure electrostatic calculations considering the same geometric parameters of the ribbon. Due to the Coulomb repulsion between the charges, each electron would be confined to its own cell and would tunnel between the opposite quantum dots.

The properties shown by the nanoribbons are similar to the automaton composed of molecules and therefore would be an alternative to the molecular wires discussed in the first part of this work.

5. Conclusions

In this work we have studied the electronic and dynamical properties of a molecular wire consisting of molecules with structures of graphane and with a graphane nanoribbon. The objec-

tive of this study was to verify the behavior of the molecular wire, transmitting binary information without electric current. The quantum dots in each cell of the automata correspond to areas of three carbon atoms without hydrogen passivation and that therefore would be redox centers. To study the dynamical properties of the automaton it is required to know a set of parameters which are obtained by studying the electronic properties of the isolated cells of the automaton, i.e., the molecules and a unit cell in the nanoribbon. In particular the energy separation between the HOMO and LUMO of the molecular cation is of vital importance for further study of the automaton, so we have made an exhaustive study of the possible methods, based on first principles, to achieve the best values. This study allowed us to verify that the hybrid methods O3LYP and B3LYP* give good values for this type of molecules. With the parameters obtained from the study based on hybrid methods, it was verified that for a chain of 5 cells the automaton binary information can be transmitted from one extreme to the other, for two of the molecules studied (cell-62 and cell-82). It was also carried out a study of the thermal behavior of the automaton, using the geometric parameters obtained from the geometric optimization of the nanostructures studied. In this study it was shown that the molecular wire can propagate the binary information at temperatures above the room temperature, in particular in this report it is shown results for the simulation for different molecules studied at a temperature of 40 °C, which is the typical work temperature of today information processors. Finally, the study of the electronic properties of a graphane nanoribbon shows that the charge carriers minimize the energy in a similar way to the automaton formed by the molecules. In summary,

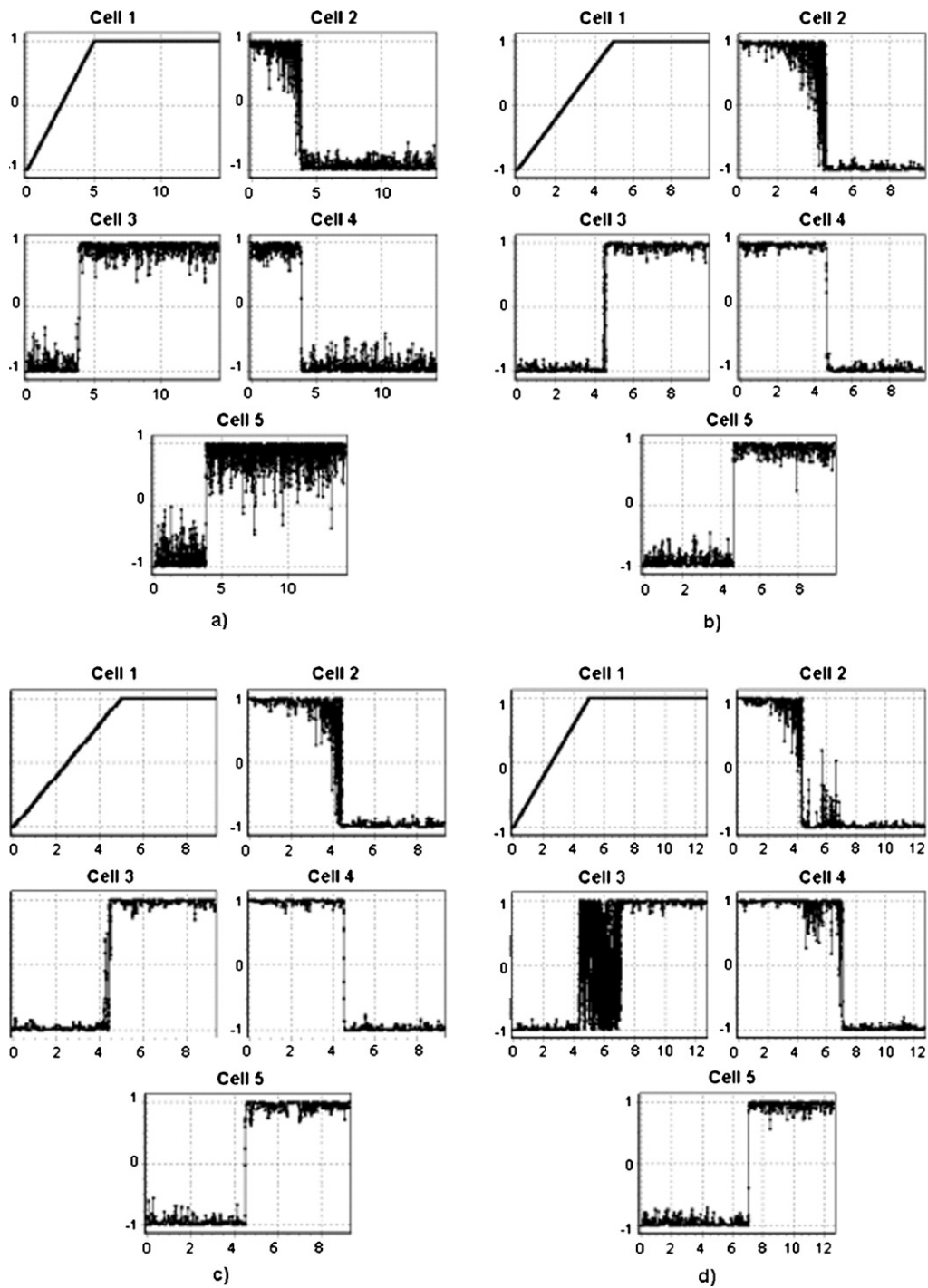


Fig. 7. Thermal study of a molecular wire formed by 5 cells. a) cell-42, b) cell-62, c) cell-82 and d) cell-(hyp). In all cases the system temperature is 40 °C.

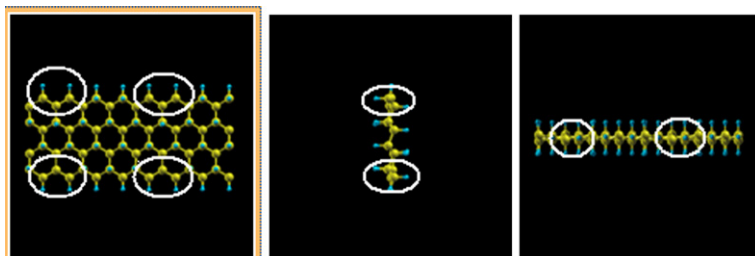


Fig. 8. Different views of the unit cell of the graphane nanoribbon.

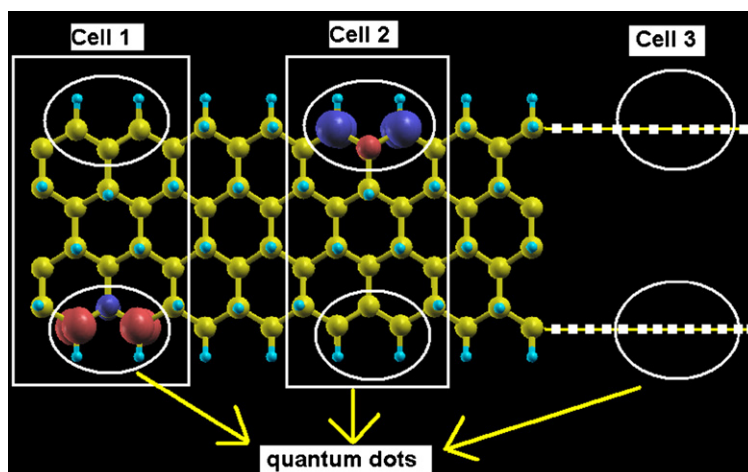


Fig. 9. Total spin density of minimum energy state of the system.

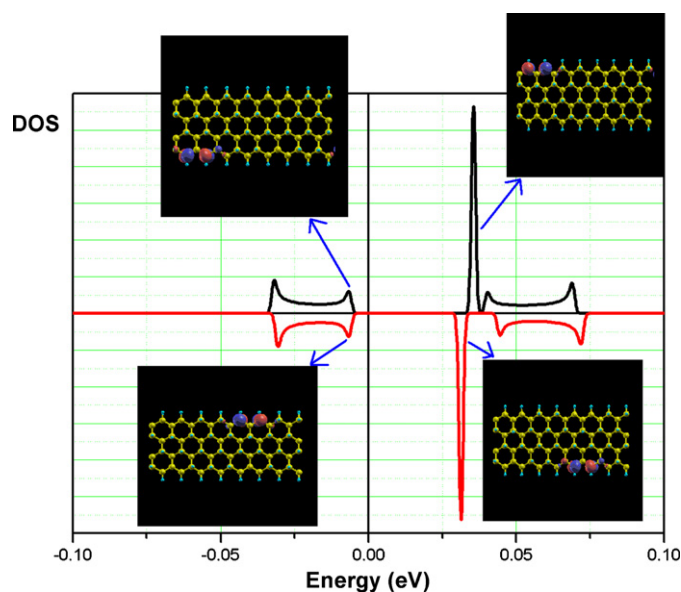


Fig. 10. Density of states as a function of energy for states near the Fermi level. It includes diagrams of the real part of the wave function for the peaks of interest. The red line (above zero in the DOS) corresponds to spin up and spin down the black line. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this Letter.)

this Letter shows theoretically that a molecular wire formed by graphane nanostructures has the desirable characteristics of bistability, operation at room temperature and times operation of the order of cents of picoseconds, to transmit binary information.

Acknowledgements

The authors acknowledge the financial support of FONDECYT program grants 1100672, 11100045 and USM 110971 internal grant.

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