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Nanocomputing Memory Devices Formed from Carbon nanotubes and Metallofulleres

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***Abstract*—**In this paper, we summarize recent work of the authors on nanocomputing memory devices. We investigate two memory devices, each comprising a charged metallofullerene and carbon nanotubes. The first device involves two open nanotubes of the same radius that are joined by a centrally located nanotube of a smaller radius. A metallofullerene is then enclosed inside the structure. The second device also involves a metallofullerene that is located inside a closed carbon nanotube. Assuming the Lennard-Jones interaction energy and the continuum approximation, for both devices, the metallofullerene has two symmetrically placed equal minimum energy positions. On one side the metallofullerene represents the zero information state and by applying an external electrical field, it can overcome the energy barrier, and pass from one end of the tube to the other, where the metallofullerene then represents the one information state.

***Keywords*—**Carbon nanotube, Continuous approach, Energy barrier, Lennard-Jones potential, Metallofullerene, Nanomemory device

I. Introduction

In the past 36 years, the computer industry has followed Moores' law [1] that every two years the complexity of integrated-circuit chips doubles solely by shrinking the size of transistors, so that electrical signals travel less distance and process information faster. However, this will soon reach a barrier as transistors become so small that the current fabrication technology and the basic physical laws pose severe limitations on further miniaturization [2], [3]. For example, the present smallest commercial transistors are only 32 nanometers (nm) wide but it would be extremely difficult to fabricate transistors less than 22 nm using present lithography techniques [4], [5]. Nanotechnology has brought many revolutionary advanced materials, which at the nanometer scale display exceptional physical characteristics, such as their mechanical and electronic properties [6], and these properties can be quite different as compared to those at the micro and nano scales. Accordingly, nano scaled components might be one possible solution for future computer design. Since the first carbon nano-materials were discovered [7], carbon nanotubes and fullerenes have been examined for possible use as memory devices either experimentally [8], theoretically [9]-[12] or computationally (molecular dynamics studies) [8]-[11], [13].

Here, we summarize recent work of the authors presented in [12], [14] where we propose potential two-state memory devices each comprising a charged metallofullerene and carbon nanotubes. The first proposed device shown in Figure 1(a) involves two open host nanotubes of the same radius that are joined by an open nanotube, which is centrally located between the host nanotubes but has a smaller radius. A metallofullerene is then placed inside the structure to represent a bit information and is originally located inside one of the host nanotubes. The second proposed shuttle memory device shown in Figure 1(b) also involves a metallofullerene that is located inside a single closed carbon nanotube. In the following section, we introduce the method for the calculation using the Lennard-Jones potential function which gives rise to the forces operating in each system. Some numerical results are presented and discussed, and some overall concluding remarks are made in the final section of the paper.

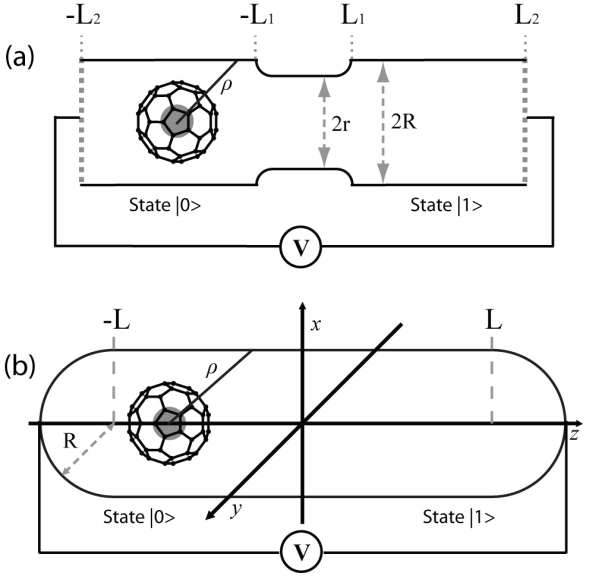

Fig. 1 Two two-state memory devices.

II. Method

Figure 1 shows the two proposed two-state nanomemory devices comprising two non-bonded molecules, namely a charged metallofullerene and carbon nanotubes. The total interaction energy for non-bonded molecules using the continuum approximation is obtained from the double surface integral, $E = \eta_1\eta_2 \int_{S_2}\int_{S_1} \Phi(\rho) dS_1 dS_2$, where $\Phi(\rho)$ is the potential energy for two non-bonded atoms, η_1 and η_2 denote the mean atomic surface densities of each molecule and ρ denotes the distance between two typical surface elements dS_1 and dS_2. The 6-12 Lennard-Jones potential for two non-bonded atoms at a distance ρ apart is given by $\Phi(\rho)=4\varepsilon[-(\sigma/\rho)^6+(\sigma/\rho)^{12}]$, where σ is van der Waals diameter and ε is the well depth [15]. The van der Waals diameter σ_{ab} and the well depth ε_{ab} for two different materials, say materials a and b, are usually found from the empirical combining rules

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$\sigma_{ab}=(\sigma_a+\sigma_b)/2$ and $\varepsilon_{ab}=(\varepsilon_a\varepsilon_b)^{1/2}$ [15]. The van der Waals interaction force F_{vdW} is determined by differentiation of the total internal energy, thus $F_{vdW}=-\nabla E$.

The interaction energy $E_m(\rho)$ for the metal atom with one carbon atom, and the energy $E_f(\rho)$ for the fullerene with one carbon atom, as derived in Cox *et al.* [16], are given by

$$E_m(\rho)=4\varepsilon[-(\sigma/\rho)^6+(\sigma/\rho)^{12}] \quad (1)$$

$$E_f(\rho)=\frac{4\varepsilon\eta_c\pi b}{\rho}\left\{\begin{array}{l}\dfrac{\sigma^6}{2}\left[\dfrac{1}{(\rho+b)^4}-\dfrac{1}{(\rho-b)^4}\right]\\ -\dfrac{\sigma^{12}}{5}\left[\dfrac{1}{(\rho+b)^{10}}-\dfrac{1}{(\rho-b)^{10}}\right]\end{array}\right\} \quad (2)$$

where the numerical values of the Lennard-Jones constants are as shown in Table 1. The Lennard-Jones constants, ε and σ for equations (1) and (2) have two different values and the numerical values of these constants are as shown in Table 1. Goddard III *et al.* [17] propose that a potassium metal ion K could be ionized to K^+, and then the corresponding negative charge on the single walled carbon nanotube is uniformly distributed, and the Lennard-Jones potential equation can still be used for the internal energy of the system.

A. Energy for the first memory device

For an axially symmetric problem, using cylindrical polar coordinates (r,θ,z), any atom of the memory device can be represented simply by (R,z) for the left and the right carbon nanotubes; (r,z) for the central carbon nanotube; (0,Z) for the center of the metallofullerene as shown in Figure 1(a), where r and R are the different radii of the nanotubes, L_1 is the half length of the central nanotube and L_2-L_1 is the length of the host nanotubes. The total internal energy E_{vdW} can be calculated from $E_{vdW}=E_{m\text{-}T1}+E_{m\text{-}t}+E_{m\text{-}T2}+E_{f\text{-}T1}+E_{f\text{-}t}+E_{f\text{-}T2}$, where m, f, T1, t and T2 indicate the metal, fullerene, left, central and right nanotubes, respectively [12].

The distances from the center of the metallofullerene to the host nanotubes and to the central nanotube are given respectively by

$$\rho_T^2=R^2+(Z-z)^2, \quad \rho_t^2=r^2+(Z-z)^2 \quad (3)$$

Based on the above equations (1), (2) and (3), the total internal interaction energy for the metallofullerene interacting with the nanotube structure is given by

$$E_{vdW}(Z)=2\pi\eta_t\left[\begin{array}{l}r\int_{-L_2}^{-L_1}E_{m+f}(\rho_T)dz+R\int_{L_1}^{-L_1}E_{m+f}(\rho_t)dz\\ +r\int_{L_1}^{L_2}E_{m+f}(\rho_T)dz\end{array}\right]$$

where the function $E_{m+f}=E_m+E_f$ and ρ_T and ρ_t are as given in equation (3) and the numerical values of the constants r, b, η_c and η_t are as shown in Table 1. Owing to the symmetry, we are only concerned with the force in the axial *z*-direction given by $F_z=-dE_{vdW}/dZ$.

B. Energy for the second memory device

As for the first memory device, using cylindrical polar coordinates (r,θ,z), any atom of the system can be represented simply by (R,z) for the carbon nanotube; (0,Z) for the center of the metallofullerene; $([R^2-(z+L)^2]^{1/2}, z)$ for the left cap and $([R^2-(z-L)^2]^{1/2}, z)$ for the right cap as shown in Figure 1(b), where R is the radius of the nanotube and the hemi-spherical caps, and L is the half length of the nanotube. The total internal energy E_{vdW} can be calculated from $E_{vdW}=E_{m\text{-}c1}+E_{m\text{-}t}+E_{m\text{-}c2}+E_{f\text{-}c1}+E_{f\text{-}t}+E_{f\text{-}c2}$, where m, f, t, c1 and c2 indicate the metal, fullerene, nanotube, left cap and right cap, respectively [14].

The three distances from the center of the metallofullerene to the left cap, to the nanotube and to the right cap are given respectively by

$$\rho_{c1}^2=R^2-(z+L)^2+(Z-z)^2,\ \rho_T^2=R^2+(Z-z)^2,\ \rho_{c2}^2=R^2-(z-L)^2+(Z-z)^2. \quad (4)$$

Based on the above equations (1), (2) and (4), the total internal interaction energy for the metallofullerene interacting with the closed nanotube is given by

$$E_{vdW}(Z)=2\pi r\left[\begin{array}{l}\eta_c\int_{-L-r}^{-L}E_{m+f}(\rho_{c1})dz+\eta_t\int_{-L}^{L}E_{m+f}(\rho_T)dz\\ +\eta_t\int_{L}^{L+r}E_{m+f}(\rho_{c2})dz\end{array}\right]$$

where the function $E_{m+f}=E_m+E_f$ and ρ_{c1}, ρ_T and ρ_{c2} are as given in equation (4) and the numerical values of the constants r, b, η_c and η_t are as shown in Table 1. Again from the symmetry, we are only concerned with the force in the axial *z*-direction given by $F_z=-dE_{vdW}/dZ$.

III. Results and Discussion

Figure 2 shows the total energy and the total force for the $K^+@C_{60}$ metallofullerene in (10,10) with length L_2-L_1=80Å and (9,9) carbon nanotubes of half length L_1=20Å. Figure 3 shows the total energy and the total force for the $K^+@C_{60}$ metallofullerene in a (10,10) carbon nanotube of half length L=20Å.

Both memory devices have an energy barrier in the middle of the strucutre as indicated in Figures 2(a) and 3(a), so that the metallofullerene stays in one of the minimum energy locations. The left minimum energy location represents the zero state information and the right location is the one state information.

The first nanomemory device has two symmetrically placed minimum energy locations which are inside the larger tubes as indicated in Figure 2(a). The second nanomemory device also has two symmetrically placed minimum energy locations which are close to the tube extremities as indicated in Figure 3(a). Since this is a symmetric system, the two minimum energy locations are such that $Z=\pm Z_{min}$, and they are found by differentiation or $F_{vdW}(Z)=0$. We find that the minimum energy positions are linearly dependent on the half length L such that we have the relationship $Z_{min}=L+r-\lambda$, where λ is a constant. The total energy at both ends tends to infinity because the distance of the hemi-spherical surfaces from the cap and the

metallofullerene are very small, and so there is a greater repulsive force. Numerical values for the constant λ, the minimum energy E_{min}, the energy gap E_{gap} and the critical force $|F_{critical}|$ are found to be 7.23Å, -4.39eV, 1.13eV and 0.469eV/Å, respectively.

There exists an energy barrier between the two minimum energy locations, and in order to change states, the metallofullerene needs an external force F_{ext} to overcome the energy barrier to change state from the left (state zero) to the right (state one). In order to reverse the states, the same applied force is necessary but in the negative direction, so that the metallofullerene overcomes the energy barrier from the right to the left. The external force produced from an electrical field is given by $F_{ext}=qE$ where q is the total charge of the metallofullerene and E is the magnitude of the applied external electrical field, and an equal and opposite force is produced simply by reversing the direction of the external electrical field.

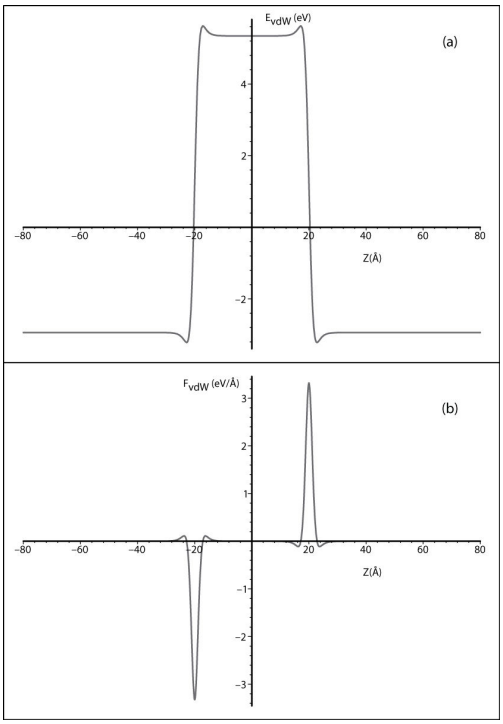

Fig. 2 First memory device (a) Internal energy E_{vdW} (eV) and (b) internal force F_{vdW} (eV/Å) for $K^+@C_{60}$ in (10,10) and (9,9) carbon nanotubes with L_1=20Å

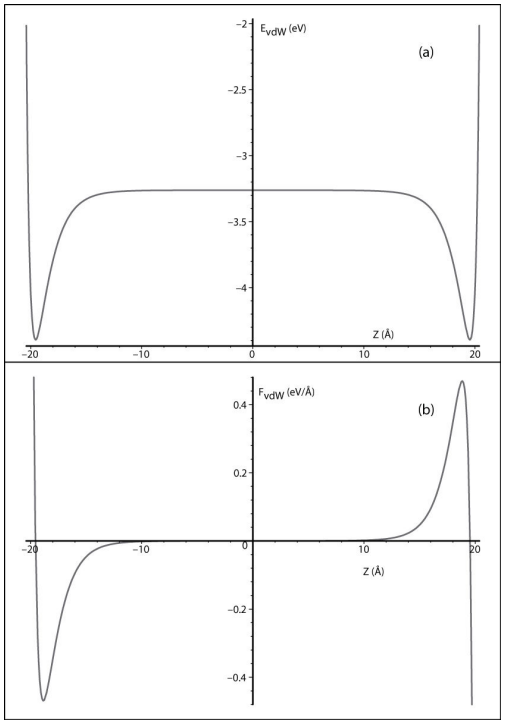

Fig. 3 Second memory device (a) Internal energy E_{vdW} (eV) and (b) internal force F_{vdW} (eV/Å) for $K^+@C_{60}$ in (10,10) carbon nanotube with L=20Å

TABLE I
NUMERICAL VALUES USED IN THE MODEL.

Radius of (9,9)		r=6.093Å
Radius of (10,10)		R=6.766Å
Radius of C_{60}		b=3.550Å
Radius of C_{80}		b=4.200Å
Radius of C_{100}		b=4.660Å
Mean Surface density of C_{60}		η_c=0.379Å^{-2}
Mean Surface density of C_{80}		η_c=0.370Å^{-2}
Mean Surface density of C_{100}		η_c=0.366Å^{-2}
Mean Surface density of nanotube		η_t=0.3812Å^{-2}
L-J Constants for K^+ [17]	σ=3.564 Å	|ε|=3.0352meV
L-J Constants for C_{60} [15]	σ=3.466 Å	|ε|=2.86meV
L-J Constants for graphene [17]	σ=3.412 Å	|ε|=2.39meV

For both nanomemory devices proposed here the important parameters are the radii R and r, the length of the nanotube L or L_1, the composition of the metal M in the metallofullerene and the magnitude of the applied external force F_{ext}. Since the metallofullerene is assumed to be located on the nanotube axis, the radius of the nanotube R should be chosen to be as close as possible to 6.4Å, 7Å and 7.4Å for the $M@C_{60}$, $M@C_{80}$ and $M@C_{100}$ metallofullerenes, respectively and the radius of the nanotube r should be smaller than R so that the metallofullerene needs the applied external electrical field to change states. The data transfer rate for both memory devices depends on the length L or L_1 of the nanotube, the mass m of the metallofullerene and the external force F_{ext}. A shorter nanotube length improves the data transfer rate so that the length should be as short as is possible. However, the nanotube length cannot be less than 20Å because the energy gap does not provide a sufficient barrier for the two states, 0 and 1. In other words, the

metallofullerene can overcome the energy barrier without an applied external force if the length of the nanotube is less than 20Å. The metal in the metallofullerene can have two possible effects on the system. First, when the ion in the metallofullerene has two charges, the applied external electrical field can be reduced to half to give the same external force as that for a single charge ion. Second, a lighter metal or ion would tend to improve the data transfer rate. The external force F_{ext} should be greater than the critical attractive force $|F_{critical}|$ arising from the hemi-spherical caps and acting against the attractive force required to change state. For Figure 3(b), the critical attractive force for $K^+@C_{60}$ metallofullerene is 0.469eV/Å and the force necessary to change state from the left end to the right needs to be around 0.5eV/Å.

IV. Summary

We have presented a summary of the two-state nanocomputing memory devices formed from carbon nanotubes and metallofullerenes as proposed in [12], [14]. The internal energy for both memory devices are calculated assuming the continuous approach so that all the results are determined analytically, and can be evaluated by standard mathematical software packages such as Maple and Matlab. This approach has many advantages over molecular dynamics simulations, which require long computational times, while the present evaluations are virtually instantaneous. The energy barrier involves the binding energy that the fullerene needs to acquire to leave the host nanotube and the repulsive energy that it needs to overcome to enter the central nanotube.

The first nanomemory device comprises a charged metallofullerene and two open host nanotubes of the same radius that are joined by an open nanotube, which is centrally located between the host nanotubes but has a smaller radius. It has an energy barrier, due to the smaller radius of the central nanotube, and there are two minimum energy locations symmetrically situated in the larger radii nanotubes. For the second nanomemory device, a metallofullerene located inside a closed single walled carbon nanotube of half-length L and radius r also has two symmetrical minimum energy points Z_{min} and $-Z_{min}$ where Z_{min} is given by $Z_{min}=L+r-\lambda$ where λ is a constant.

For both memory devices, in order to change from state 0 to state 1, the charged metallofullerene needs an external force to overcome the attractive force arising from the van der Waals interactions. The external force must exceed the critical attractive force and it can be provided from an applied external electrical field. The lighter the atom at the center of the metallofullerene, the larger the external force, and the shorter the nanotube, are all important factors tending to increase the data transfer rate.

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