

Design of a Two-State Shuttle Memory Device

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Abstract: In this study, we investigate the mechanics of a metallofullerene shuttle memory device, comprising a metallofullerene which is located inside a closed carbon nanotube. The interaction energy for the system is obtained from the 6-12 Lennard-Jones potential using the continuum approximation, which assumes that a discrete atomic structure can be replaced by an average atomic surface density. This approach shows that the system has two equal minimum energy positions, which are symmetrically located close to the tube extremities, and therefore it gives rise to the possibility of being used as a two-state memory device. On one side the encapsulated metallofullerene represents the zero information state and by applying an external electrical field, the metallofullerene can overcome the energy barrier of the nanotube, and pass from one end of the tube to the other end, where the metallofullerene then represents the one information state. By appropriately selecting different nanotube geometries, the memory device can be designed to have various data transfer rates. In particular, design parameters are presented for the optimization of the data transfer rates and the stabilization of the data storage. The former involves optimization of the nanotube length and the applied electric field, while the latter involves the nanotube radius and the choice of metallofullerene.

Keywords: Carbon nanotubes, metallofullerenes, Lennard-Jones potential, nanomemory device.

1 Introduction

Moore (1975) suggested that the complexity of integrated-circuit chips would double every two years by solely shrinking the size of transistors, so that electrical signals could travel less distance in order to process the information faster. The trend for modern computer devices is towards decreasing in size Moore (1975) to

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improve speed and capacity, by reducing the energy and the heat generated. However, physicists and engineers have already predicted that this trend 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 Arden and Muller (1987); Harriott (2001). 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 Bloomstein, Marchant, Deneault, Hardy and Rothschild (2006); Thompson and Parthasarathy (2006). For the smaller transistors, the heat released is a significant issue and the processing might become unstable and the speed might not be improved. To overcome such difficulties, the central processing unit (CPU) industry has already squeezed several processors into a single unit such as 2, 4, 6 or multi cores Kumar, Zyuban and Tullsen (2005) in a single chip and they have adopted parallel computing such as cloud computing or multi threads to raise the computational speed. Nanotechnology has brought many revolutionary advanced materials, for which the physical size of the smallest components have reduced from the micrometer scale to the nanometer scale. Many materials at the nanometer scale display exceptional physical characteristics such as their mechanical and electronic properties Kamat and Liz-marzan (2003), and these properties can be quite different compared to those at the micro-scale. Therefore, nanotechnological components might be one possible solution for future computer design.

Both carbon nanotubes and fullerenes are particular types of a carbon isomer. Carbon nanotubes were first discovered by Iijima Iijima (1991), and are conceptualized by beginning with a two dimensional carbon sheet which is then rolled into a right circular seamless cylinder Dresselhaus, Dresselhaus and Saito (1992, 1995); Jishi, Dresselhaus and Dresselhaus (1993). A closed carbon nanotube has ends which are each closed by a half-fullerene. A fullerene is a spherical carbon cage with a structure resembling a soccer ball with an empty center David, Ibberson, Mattewman, Prassides, Dennis, Hare, Kroto, Taylor and Walton (1991), but which might contain an additional atom, such as F^- , Ne, Na^+ , Mg^{2+} or Al^{3+} , which are then called endohedral fullerenes Cioslowski and Fleischmann (1991). If the additional atom is a metal, then it is called as an endohedral metallofullerene or simply a metallofullerene, and which may have large electric dipole moments ranging between 3 and 4 Debye Bethune, Johnson, Salem, de Vries and Yannoni (1993); Laasonen and reoni and Parrinello (1992). The metal at the center of the fullerene has been found to shift from the fullerene center with charge transfer to the cage Li, Sabirianov, Lu, Zeng and Mei (2008). The intermolecular interactions of $M@C_n$ are dominated by strong dipole interactions, where the symbol M is used to denote the additional metal atom inside the fullerene, and n indicates the total number of

carbon atoms in the cage. The endohedral fullerene size is based on the number of carbon atoms n which ranges from 60 to 100. For the standard fullerene C_n , C_{60} and C_{70} are the most abundant. However, $M@C_{60}$ such as $La@C_{60}$ and $Ca@C_{60}$ metallofullerenes are unstable in air Shinohara (2000), and the most abundant stable metallofullerenes are the $M@C_n$ class ($n=80, 82, 84$), such as $Ca@C_{82}$, $Sc_3N@C_{80}$, $Tb@C_{82}$, $Dy@C_{82}$, $La@C_{82}$, $Sc_2@C_{84}$ Shinohara (2000). Beck, Weis, Rockenberger, and Kappes (1996); Beck, Weis, Rockenberger, Michel, Fuchs, Benz and Kappes (1996) report structures with ions embedded in a “giant” fullerene such as $La_2@C_{100}$ and $Ce_2@C_{100}$.

Since the first carbon nano-materials were discovered, carbon nanotubes and fullerenes have been examined for possible use as memory devices either experimentally Kwon, Tománek and Iijima (1999), theoretically Xiao and ersen and Yang (2008); Lee, Kim, Kahng, Kim, Son, Ihm, Kato, Wang, Okazaki, Shinohara and Kuk (2002); Kang and Hwang (2005, 2004b); Chan, Lee and Hill (2010) or computationally (molecular dynamics studies) Kwon, Tománek and Iijima (1999); Xiao and ersen and Yang (2008); Lee, Kim, Kahng, Kim, Son, Ihm, Kato, Wang, Okazaki, Shinohara and Kuk (2002); Hwang, Byun, Lee and Kang (2005); Kang and Hwang (2004a, 2005, 2004b). Recent, memory devices based on boron-nitride nanotubes have been investigated because fullerenes are found to be more easily sucked into boron-nitride nanotubes than into carbon nanotubes Hwang, Choi and Kang (2005); Choi, Kang and Hwang (2004).

In this study, we propose a two data storage state memory device comprising a metallofullerene situated inside a closed single wall carbon nanotube as indicated in Figure 1. Although Hwang, Choi and Kang (2005); Choi, Kang and Hwang (2004) report that the best host material is boron nitride, in this study we adopt a carbon nanotube because it has been most thoroughly investigated, and it would be a simple matter to undertake a corresponding analysis for boron nitride. The metallofullerene is encapsulated on one side, due to the van der Waals forces, and represents the zero state, and then we apply an external electric field to the system to initiate the metallofullerene with an initial kinetic energy which is sufficiently large so as to escape the energy well and pass to the other side. The metallofullerene is then encapsulated on the other side and represents the one state. Such a nano-memory device might be used either as a static random access memory, or a dynamic random access memory, or a solid-state drive.

In this study, using applied mathematical modelling we formulate the design rules for such a two-state nano-memory device. In the following section, we introduce the method for the calculation of the potential function giving rise to the forces for this system. The potential energy of the 6-12 Lennard-Jones potential function is then introduced and the continuum approximation, which assumes that a discrete

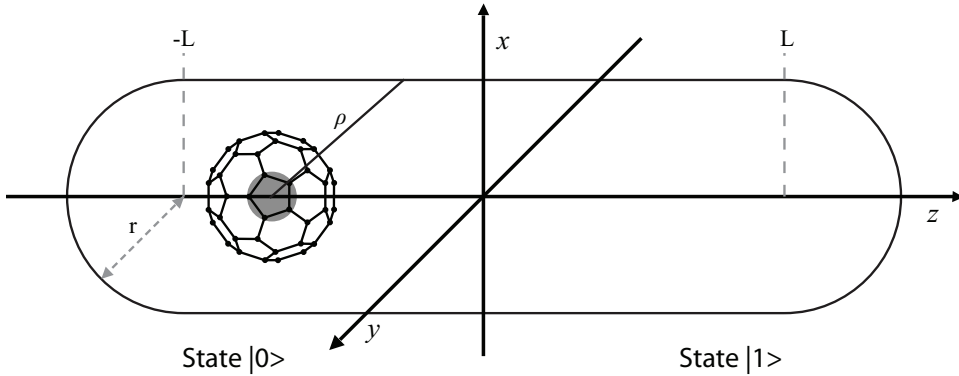


Figure 1: Two-state memory device.

atomic structure can be approximated by an average constant atomic surface density. In Section 3, some numerical results are presented and discussed and some overall concluding remarks are made in Section 4.

2 Methods

A two-state nano-memory device as shown in Figure 1 has a metallofullerene and a carbon nanotube which comprises two non-bonded molecules, and the total interaction energy is obtained by the superposition principle, by summation of the interaction energy for each non-bonded atomic pair, thus $E = \sum_i \sum_j \Phi(\rho_{ij})$, where $\Phi(\rho_{ij})$ is the interaction potential energy for non-bonded atoms i and j at a distance ρ_{ij} apart. For the continuum approximation, we assume that the total potential energy can be approximated by the double surface integral, $E = \eta_1 \eta_2 \int_{S_2} \int_{S_1} \Phi(\rho) dS_1 dS_2$, where 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 .

Generally, the 6-12 Lennard-Jones potential is used to find the van der Waals interaction force for two non-bonded molecular structures and the classical 6-12 Lennard-Jones potential for two atoms at a distance ρ apart is given by $\Phi(\rho) = -(A/\rho^6) + (B/\rho^{12})$, where A and B denote the attractive and the repulsive constants, respectively Girifalco, Hodak and Lee (2000). This equation can also be rewritten as $\Phi(\rho) = 4\varepsilon[-(\sigma/\rho)^6 + (\sigma/\rho)^{12}]$, where $\rho_0 = 2^{1/6}\sigma = (2B/A)^{1/6}$ is the equilibrium distance, σ is van der Waals diameter and $\varepsilon = A^2/(4B)$ is the well depth Girifalco, Hodak and Lee (2000). The van der Waals diameter σ_{ab} and the well depth ε_{ab} for two different materials, say materials a and b , can be found from empirical combining rules $\varepsilon_{ab} = (\varepsilon_a \varepsilon_b)^{1/2}$ and $\sigma_{ab} = (\sigma_a + \sigma_b)/2$ where the labels a , b and ab refer to the interactions between a material, b material and ab materials,

respectively Girifalco, Hodak and Lee (2000). The van der Waals interaction force F_{vdW} is found by differentiation of the total internal energy, thus $F_{vdW} = -\nabla E$, and the numerical values used for the 6-12 Lennard-Jones constants for carbon nanostructures and potassium are as shown in Table 1.

For an axially symmetric problem, using cylindrical polar coordinates (r, θ, z) , any atom of the system can be represented as (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, where r is the radius of the nanotube and the caps, and L is the half length of the nanotube. From the superposition principle, the total internal energy E_{vdW} and the total internal force F_{vdW} can be calculated from $E_{vdW} = E_{m-c1} + E_{m-t} + E_{m-c2} + E_{f-c1} + E_{f-t} + E_{f-c2}$ and $F_{vdW} = F_{m-c1} + F_{m-t} + F_{m-c2} + F_{f-c1} + F_{f-t} + F_{f-c2}$, where m , f , t , $c1$ and $c2$ indicate the metal, fullerene, nanotube, left cap and right cap, respectively. 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

$$\rho_{c1}^2 = r^2 - (z + L)^2 + (Z - z)^2, \quad \rho_t^2 = r^2 + (Z - z)^2, \quad \rho_{c2}^2 = r^2 - (z - L)^2 + (Z - z)^2. \quad (1)$$

The energy $E_m(\rho)$ for the metal atom with one atom and the energy $E_f(\rho)$ for the fullerene with one atom are derived in Cox, Thamwattana and Hill (2007a,b) and they are given by

$$E_m(\rho) = -A/\rho^6 + B/\rho^{12}, \quad (2)$$

$$E_f(\rho) = \frac{\eta_c \pi b}{\rho} \left\{ \frac{A}{2} \left[\frac{1}{(\rho + b)^4} - \frac{1}{(\rho - b)^4} \right] - \frac{B}{5} \left[\frac{1}{(\rho + b)^{10}} - \frac{1}{(\rho - b)^{10}} \right] \right\}, \quad (3)$$

where the numerical values of the 6-12 Lennard-Jones constants are as shown in Table 1. The Lennard-Jones constants, A and B for equations (2) and (3) have two different values for each equation, arising from metal with cap; metal with graphene; fullerene with cap and fullerene with graphene. Based on the above equations (1), (2) and (3), the total internal energy for the metallofullerene with the closed nanotube is given by

$$E_{vdW}(Z) = 2\pi r \left[\eta_c \int_{-L-r}^{-L} E_m(\rho_{c1}) dz + \eta_t \int_{-L}^L E_m(\rho_t) dz + \eta_c \int_L^{L+r} E_m(\rho_{c2}) dz \right. \\ \left. + \eta_c \int_{-L-r}^{-L} E_f(\rho_{c1}) dz + \eta_t \int_{-L}^L E_f(\rho_t) dz + \eta_c \int_L^{L+r} E_f(\rho_{c2}) dz \right],$$

where ρ_{c1} , ρ_t and ρ_{c2} are given by equation (1) and the numerical values of the constants r , b , η_c and η_t are as shown in Table 2.

Owing to the symmetry of this system, we are only concerned with the force in the axial direction, $F_z = F_{vdW} \cdot (Z - z)/\rho$, where F_{vdW} is the van der Waals interaction force defined by $F_{vdW} = -dE_{vdW}/d\rho$. Each part of the total force in the axial direction for the metallofullerene with the closed nanotube is given by

$$\begin{aligned}
 F_{m-c1} &= \frac{\pi r \eta_c}{(Z+L)^2} \left\{ (-r^2 + (Z+L)^2)[E_m(\rho)] + \left[\frac{-3A}{2\rho^4} + \frac{6B}{5\rho^{10}} \right] \right\}_{Z+L+r}^{[r^2+(Z+L)^2]^{1/2}}, \\
 F_{m-t} &= 2\pi \eta_t r \left[\frac{-A}{\rho^6} + \frac{B}{\rho^{12}} \right]_{[r^2+(Z+L)^2]^{1/2}}^{[r^2+(Z-L)^2]^{1/2}}, \\
 F_{m-c2} &= \frac{\pi r \eta_c}{(Z-L)^2} \left\{ (-r^2 + (Z-L)^2)[E_m(\rho)] + \left[\frac{-3A}{2\rho^4} + \frac{6B}{5\rho^{10}} \right] \right\}_{Z-L-r}^{Z-L-r}, \\
 F_{f-c1} &= \frac{\pi r \eta_c}{(Z+L)^2} \left\{ (-r^2 + (Z+L)^2 + \rho^2)[E_f(\rho)] + 2\eta_c \pi b \times \right. \\
 &\quad \left. \left[\frac{A}{6} \left(\frac{1}{(\rho+b)^3} - \frac{1}{(\rho-b)^3} \right) - \frac{B}{45} \left(\frac{1}{(\rho+b)^9} - \frac{1}{(\rho-b)^9} \right) \right] \right\}_{Z+L+r}^{[r^2+(Z+L)^2]^{1/2}}, \\
 F_{f-t} &= 2\pi^2 \eta_t \eta_c r b \left[\frac{A}{2\rho} \left(\frac{1}{(\rho+b)^4} - \frac{1}{(\rho-b)^4} \right) \right. \\
 &\quad \left. - \frac{B}{5\rho} \left(\frac{1}{(\rho+b)^{10}} - \frac{1}{(\rho-b)^{10}} \right) \right]_{[r^2+(Z+L)^2]^{1/2}}^{[r^2+(Z-L)^2]^{1/2}}, \\
 F_{f-c2} &= \frac{\pi r \eta_c}{(Z-L)^2} \left\{ (-r^2 + (Z-L)^2 + \rho^2)[E_f(\rho)] + 2\eta_c \pi b \times \right. \\
 &\quad \left. \left[\frac{A}{6} \left(\frac{1}{(\rho+b)^3} - \frac{1}{(\rho-b)^3} \right) - \frac{B}{45} \left(\frac{1}{(\rho+b)^9} - \frac{1}{(\rho-b)^9} \right) \right] \right\}_{Z-L-r}^{Z-L-r},
 \end{aligned} \tag{4}$$

where ρ is replaced by the upper limit and the lower limit and therefore the total force $F_{vdW}(Z)$ is a function of Z and is the summation of each part of the force arising from the above equation (4).

3 Results and discussion

Figure 2 shows the total energy and the total force for the $K^+@C_{60}$ metallofullerene in a (10, 10) carbon nanotube of half length $L = 20\text{\AA}$. The nano-memory device has two minimum energy positions which are close to the tube extremities as shown in Figure 2(a). Since this is a symmetric system, the total energy and force will be an even function and an odd function, respectively, and therefore they have the properties, $E_{vdW}(Z) = E_{vdW}(-Z)$ and $F_{vdW}(Z) = -F_{vdW}(-Z)$ so that the two minimum energy positions, Z_{min1} and Z_{min2} , have the relationship, $Z_{min2} = -Z_{min1}$.

Table 1: 6-12 Lennard-Jones constants used in the model and λ , minimum energy, energy gap and critical force for metal / ion in C₆₀ fullerene with (10, 10) carbon nanotube. λ is the constant arising in the equation $Z_{min} = L + r - \lambda$.

	ρ_0 (Å) ⁶	$ \epsilon $ (meV)	λ (Å)	E_{min} (eV)	E_{gap} (eV)	$ F_{critical} $ (eV/Å)
C-C Girifalco, Hodak and Lee (2000)	3.89	2.86	--	--	--	--
Graphene-Graphene Girifalco, Hodak and Lee (2000)	3.83	2.39	--	--	--	--
C ₆₀ -C ₆₀ Girifalco, Hodak and Lee (2000)	3.89	2.86	--	--	--	--
C ₆₀ -Graphene Girifalco, Hodak and Lee (2000)	3.86	2.62	--	--	--	--
K ⁺ -K ⁺ Chen, Guo, Karasawa and Goddard III (1993)	4.0010	3.0352	7.23235	-4.39478	1.13255	0.46929
F ⁻ -F ⁻ Hwang, Byun, Lee and Kang (2005)	2.495	0.403	7.23482	-4.36394	1.12464	0.46615
Pt-Pt Hilder and Hill (2008)	3.92	19.833	7.22848	-4.44309	1.14501	0.47424
Zn-Zn Babarao, Hu, Jiang, Chempath and Sandler (2007)	2.462	5.372	7.23408	-4.37292	1.12700	0.46708
Au-Au Pu, Leng, Zhao and Cummings (2007)	2.934	1.691	7.23423	-4.37119	1.12653	0.46690
Mg ²⁺ -Mg ²⁺ Callahan, Casillas-Ituarte, Roeselová, Allen and Tobias (2010)	0.7926	38.798	7.23466	-4.36577	1.12517	0.46635
Mg ²⁺ -Mg ²⁺ Callahan, Casillas-Ituarte, Roeselová, Allen and Tobias (2010)	0.9929	37.944	7.23454	-4.36724	1.12556	0.46651
Mg ²⁺ -Mg ²⁺ Callahan, Casillas-Ituarte, Roeselová, Allen and Tobias (2010)	1.0600	37.944	7.23449	-4.36783	1.12572	0.46657
Cl ⁻ -Cl ⁻ Callahan, Casillas-Ituarte, Roeselová, Allen and Tobias (2010)	2.4192	4.336	7.23422	-4.37120	1.12655	0.46691
Cl ⁻ -Cl ⁻ Hess, Holm and van der Vegt (2006)	4.40	4.332	7.23075	-4.41539	1.13776	0.47136
Cl ⁻ -Cl ⁻ Hess, Holm and van der Vegt (2006)	4.05	6.509	7.23093	-4.41263	1.13713	0.47111
Cl ⁻ -Cl ⁻ Hess, Holm and van der Vegt (2006)	4.45	4.622	7.23045	-4.41925	1.13873	0.47174
Na ⁺ -Na ⁺ Hess, Holm and van der Vegt (2006)	3.33	0.124	7.23478	-4.36449	1.12477	0.46620
Na ⁺ -Na ⁺ Hess, Holm and van der Vegt (2006)	2.43	2.031	7.23450	-4.36787	1.12568	0.46656
Na ⁺ -Na ⁺ Hess, Holm and van der Vegt (2006)	2.58	0.643	7.23472	-4.36524	1.12498	0.46628
Li ⁺ -Li ⁺ Perera and Berkowitz (1993)	2.224	13.429	7.23381	-4.37614	1.12787	0.46734
I ⁻ -I ⁻ Perera and Berkowitz (1993)	4.286	10.149	7.22895	-4.43797	1.14357	0.47367

Table 2: Constants used in the model.

Carbon-carbon bond length	$\sigma=1.440 \text{ \AA}$
Radius of (10,10)	$r=6.766 \text{ \AA}$
Radius of C ₆₀	$b=3.550 \text{ \AA}$
Radius of C ₈₀	$b=4.200 \text{ \AA}$
Radius of C ₁₀₀	$b=4.660 \text{ \AA}$
Mean surface density of C ₆₀	$\eta_c=0.379 \text{ \AA}^{-2}$
Mean surface density of C ₈₀	$\eta_c=0.370 \text{ \AA}^{-2}$
Mean surface density of C ₁₀₀	$\eta_c=0.366 \text{ \AA}^{-2}$
Mean surface density of a single layer graphene	$\eta_l=0.3812 \text{ \AA}^{-2}$
Mass of atomic mass	$1u=1.660540 \times 10^{-27} \text{ kg}$
Mass of atomic mass	$1u=931.49432 \times 10^6 \text{ eV}/c^2$
Speed of light	$c=2.99792458 \times 10^8 \text{ m/s}$
Mass of a single carbon atom, C	$m_C=12.011 \text{ u}$
Mass of a single C ₆₀ fullerene [$60m_C$]	$m_f=720.66 \text{ u}$
Mass of a single potassium atom, K	$m_K=39.102 \text{ u}$
Mass of a single fluorine atom, F	$m_F=19.00 \text{ u}$
Mass of a single platinum atom, Pt	$m_{Pt}=195.09 \text{ u}$
Mass of a single zinc atom, Zn	$m_{Zn}=65.38 \text{ u}$
Mass of a single gold atom, Au	$m_{Au}=196.97 \text{ u}$
Mass of a single magnesium atom, Mg	$m_{Mg}=24.31 \text{ u}$
Mass of a single chlorine atom, Cl	$m_{Cl}=35.453 \text{ u}$
Mass of a single sodium atom, Na	$m_{Na}=22.990 \text{ u}$
Mass of a single lithium atom, Li	$m_{Li}=6.941 \text{ u}$
Mass of a single iodine atom, I	$m_I=126.90 \text{ u}$

Based on this relationship, the minimum energy position will be denoted simply as Z_{min} . The minimum energy positions are found from the first derivative, $F_{vdW}(Z) = 0$. However, since the expression for the total force (4) is complicated, the minimum energy positions need to be found numerically, and Newton's method, using the initial values $-L$ and L for the two minimum energy positions, since these positions are close to the tube extremities is found to be effective. We may show that the minimum energy positions are linearly dependent on the half length L and we have the relationship $Z_{min} = L + r - \lambda$, where λ is a constant. The total energy at both ends goes to infinity because the distance of the two surfaces for the cap and the metallofullerene are very small, and so there is a greater repulsive force. Table 1 shows that the numerical values for constant λ , minimum energy E_{min} , energy gap E_{gap} and critical force $|F_{critical}|$ for different metals or ions are around $7.23 \pm 0.01 \text{ \AA}$, $-4.40 \pm 0.07 \text{ eV}$, $1.13 \pm 0.02 \text{ eV}$ and $0.47 \pm 0.01 \text{ eV/\AA}$, respectively. The minimum energy and energy gap are defined as $E_{min} = E_{vdW}(Z_{min})$ and $E_{gap} = E_{vdW}(0) - E_{min}$. The distance between the fullerene center and the cap surface is greater than the distance between the fullerene surface and the cap surface, so the material at the fullerene center does not contribute much to the potential energy of the system, and therefore the metal or ion in the fullerene is not a critical factor for creating the two-state memory device.

The nanotube provides an energy barrier between the two minimum energy positions which are close to the tube extremities, and in order to change the state, the metallofullerene needs an applied external force F_{ext} which should be greater than the critical attractive force $|F_{critical}|$ arising from the caps and acting against the attractive force. For Figure 2(b), the critical attractive force for $K^+@C_{60}$ metallofullerene is 0.46929 eV/\AA and therefore the external force necessary to change state from the left end to the right end needs to be around 0.5 eV/\AA . In order to reverse this state, the same applied force is necessary but in the negative direction, so that the metallofullerene overcomes the energy barrier from the right end to the left end. The external force produced from the electrical field is given by, $F_{ext} = qE$ where q is the total charge of the metallofullerene and E is the magnitude of external electrical field. When the ion in the metallofullerene has two charges, the external electrical field could be reduced to half for the same external force for a single charge ion. In the particular, the negative direction external force could be produced from a reverse external electrical field.

In order to overcome the energy barrier, there must be an applied external force and the work done W on the metallofullerene by the net force, $F_{net} = F_{ext} + F_{vdW}$ is given by

$$W = \int_{-Z_{min}}^{Z_{min}} F_{net} dZ = \int_{-Z_{min}}^{Z_{min}} \left(F_{ext} - \frac{dE_{vdW}}{dZ} \right) dZ = 2F_{ext}Z_{min}$$

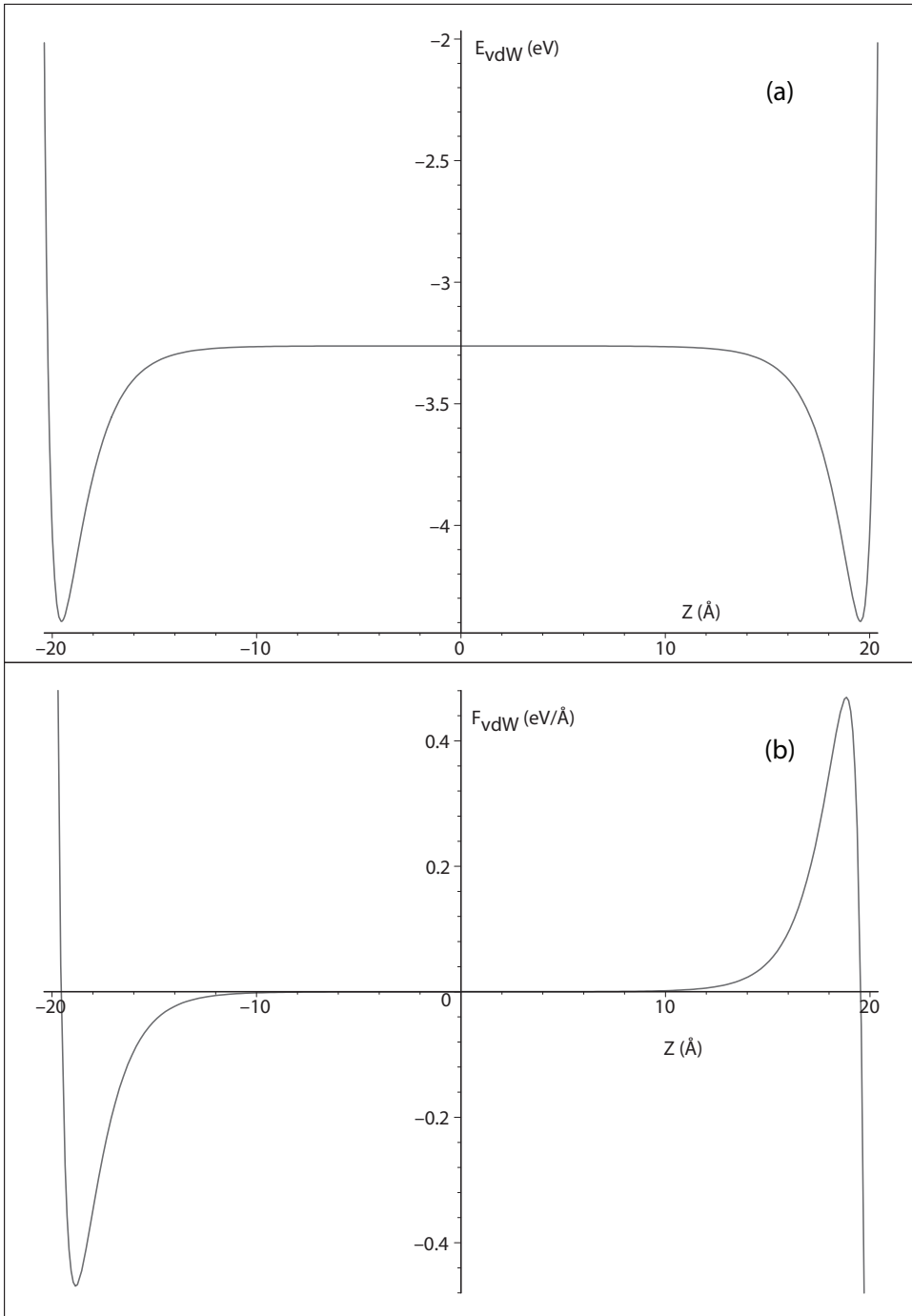


Figure 2: (a) Internal energy E_{vdW} (eV) and (b) internal force F_{vdW} (eV/\AA) for $\text{K}^+@C_{60}$ in (10,10) carbon nanotube with $L = 20\text{\AA}$.

Since the energy function is an even function, the last term of the integral becomes zero, and for a constant external electrical field the external force is also a constant. Since the initial velocity of the metallofullerene is zero, the final velocity of the metallofullerene v_f may be found from the work done, $W = mv_f^2/2$, where m is the mass of the metallofullerene.

The data transfer rate of this memory device is the inverse of the time taken for the metallofullerene to transfer from one state to the other. The data transfer rate is based on the length of the nanotube $2L$, the external force F_{ext} and the mass of the metallofullerene m . The transfer time is determined from Newton's second law, $F = ma$, where a is an acceleration which is given by dv/dt or d^2Z/dt^2 and m is a mass. The velocity of the metallofullerene is given by

$$v = \left\{ \frac{2}{m} [F_{ext} \cdot (Z + Z_{min}) - E_{vdW}(Z) + E_{min}] \right\}^{1/2},$$

where E_{min} denotes the minimum energy. For the final velocity, the metallofullerene is located at Z_{min} , therefore the final velocity v_f is $2\sqrt{F_{ext}Z_{min}/m}$ which is the same as the final velocity as determined from the work done. The metallofullerene transfer time t at the Z location is found from

$$t = \int_{-Z_{min}}^Z \frac{dZ}{v} = \left(\frac{m}{2}\right)^{1/2} \int_{-Z_{min}}^Z \frac{dZ}{[F_{ext} \cdot (Z + Z_{min}) - E_{vdW}(Z) + E_{min}]^{1/2}}, \quad (5)$$

and the total transfer time t_f is given by equation (5) with $Z = Z_{min}$. However, although the integral is clearly complicated, numerical values arising from such expressions may be readily evaluated using numerical packages such as MAPLE and MATLAB.

It turns out that an approximate but accurate value of the transfer time t_f may be determined by the following approximate equation (6)

$$t_f \simeq \left(\frac{m}{2}\right)^{1/2} \int_{-Z_{min}}^{Z_{min}} \frac{dZ}{[F_{ext} \cdot (Z + Z_{min})]^{1/2}} = \left(\frac{4mZ_{min}}{F_{ext}}\right)^{1/2} \quad (6)$$

This equation shows that the mass, the external force and the length of the nanotube are critical factors for the total transfer time t_f . Equation (6) shows that the heavy metals or ions give rise to increased transfer times, and the total transfer time decreases as the external force applied on the metallofullerene increases. However, the memory device will be destroyed if the metallofullerene receives an external energy which is larger than the disintegration force $2V/\text{\AA}$ for the carbon bond Kim, Lee, Nordlander and Tománek (1997); Lee, Kim and Tománek (1997). The minimum energy position Z_{min} involves the length of the nanotube, and therefore the

total transfer time increases for increasing length of the nanotube. In order to increase the data transfer rate, the factors which must be considered are the choice of a light center for the metallofullerene; a large external force and a short length of nanotube. The total transfer time is found to be 2.4933 ps for 0.5 eV/\AA external force and $2L = 27\text{\AA}$ for the nanotube length, and this gives a data transfer rate around 401 Gbit/s.

4 Summary

A metallofullerene located inside a single wall carbon nanotube has two symmetrical minimum energy points which can be exploited as a two-state memory device. The minimum energy positions Z_{min} and $-Z_{min}$ are found to be given by $Z_{min} = L + r - \lambda$ where λ is a constant. In order to change from state 0 to state 1, the 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 external electrical field. The lighter the atom at the center of the metallofullerene, the larger the external force, and the shorter the nanotube, the faster the data transfer rate. Since, the metallofullerene needs a charge in order to change states, every bit data would require at least one charge, and for large data storage, many metallofullerenes will be in close proximity. If all the metallofullerenes have the same charge polarity, then the total charges for the device would make it unstable. A possible extension of the device described here might be an endo-fullerene which has two metallofullerenes, one with a positive charge and one with a negative charge, which would replace the present metallofullerene, and since the total charge of the endo-fullerene is neutral, such a memory device would be more stable.

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