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Implication of Quantum Chemical Methods in Future Storage Devices-Molecular Quantum Dot Cellular Automata

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ABSTRACT

Now-a-days, scaling down, that is increasing the element density on the wafer plays predominant rolee in electronic industries. The Scaling down of complementary metal oxide semiconductor CMOS circuits has its limitations. So to get rid of these constrains, one promising approach is Quantum-dot cellular automation (QCA), an up-coming nanotechnology in the area of Nano electronics. It has attractive features such as faster speed, smaller size, and low power consumption compared to transistor-based technology. Though many researchers implemented many digital QCA based circuits by QCA Designer and simulated the design, the practical approach towards QCA and the characterization of quantum cell is less. This paper provides crucial part of ab initio quantum chemical calculations in the construction and operationof quantum cells .

Keywords: ab initio methods,CMOScircuits,Potenial well, Potenial Energy, QCA.

I.INTRODUCTION

Since the conventional CMOS technology has several limitations such as physical, material, Power-thermal, technological limitations, we need to approach a non-CMOS devices [1]. Quantum Cellular Automata (QCA) is a nanotechnology that has recently been recognized as one of the top six emerging technologies with potential applications in future computers. The main difference between QCA and transistor is, QCA does not operated by the transport of electrons. As the name implies, QCA consists of a quadratic cell. The square has four or five potential well in the four corners of the QCA cell. Out of four well, two electrons will be locked in two potential wells. The two electros try to occupy the diagonal due to columbic repulsive forces. Depending upon the occupation on these two electrons in the diagonal, the particular binary logic “0” or “1” can be implemented[2,3]. To implement the QCA in practice, many researchers engineered various semiconductor heterostructures. The main operation of QCA depends on the polarization of one cell to the induced polarization of a neighbouring cell. The quantum chemical calculations are well suited for the construction and in the functioning of QCA.

The underlying principle behind the quantum-dot cellular automata (QCA) cell is it do not conduct current at all, its functionality includes charge localization, bistable charge switching within the cell and electric field coupling between one molecular cell and its neighbour. The combination of these effects can be examined using the cell–cell response function which relates the polarization of one cell to the induced polarization of a neighbouring cell. The response function can be obtained by calculating the molecular electronic structure with *ab initio* quantum chemistry techniques[4].

II. QUANTUM DOT CELLULAR AUTOMATA (QCA)

Quantum-dot Cellular Automata (QCA) technology is a promising potential alternative to CMOS technology. The Quantum Dot Cellular Automata is a paradigm having arrays of interlinked quantum dots to execute Boolean logic functions. A basic QCA cell consists of four or five quantum dots in a square array coupled by tunnel barriers for the electrons to move[5] as shown in Fig.1. The QCA uses electrons in the cell to store and transmit data. Electrons move between different positions via electron tunnelling. The logic functions are performed by columbic interactions [6].

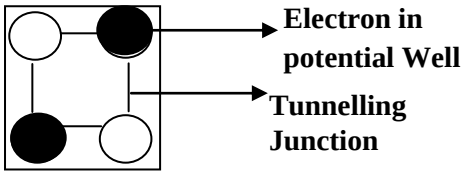

Fig. 1 (a). QCA Cell

Fig.1.(b). Logical functions by columbic

III. TYPES OF QCAS

There are four QCA implementing technology known as metal-Island QCA, semiconductor QCA, molecular QCA and magnetic QCA. In metal-Island QCA[7, 8], the 1mm dimension of metal Islands are prepared by aluminum and aluminum oxide tunneling Junction. The type of QCA, which uses semiconductors such as GaAs / AlGaAs as quantum dots are known as semiconductor QCA [9,10]. The molecular QCA can be implemented by induced electrons switching between four ferrocene groups due to electrostatic interactionsand the cobalt group in the centre of the group acts as the tunneling path [11-14]. In magnetic QCA cell consists of a nanomagnet, the binary information is based on the dipole moment alignment in particular domain [15,16].

IV. THE SIGNIFICANCE OF QUANTUM DOTS IN QCA

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The Quantum Dot plays a predominant role in the QCA cell. The function of this dot is to confine the charge of the electron. The quantum dot has high potential barrier surrounding area to provide quantized energy to the electron .The electron will be well trapped inside the dot as shown in fig.2. The barrier can be altered in order to make the electrons to tunnel through them during switching.

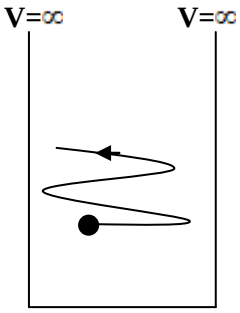

Fig.2. I-Dim potential Well with trapped electron

V. MECHANISM OF WORKING OF QCA

For understanding the working mechanism of a QCA, each quantum level of the electron must be studied. According to De-Brolgie concept, both light and matter show wave-like and particle like characteristics. When the particles are at rest, they behave like particles, and when they are in movement, they act as wave .Since the electrons are micro particles which are in motion, they act like wave, the energy possess by the electron can be calculated by Schrödinger's wave equation, which is given by

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} + \frac{8\pi^2 m(E-V)}{h^2}\Psi(x,t) = 0 \qquad \text{(1-Dim)} \qquad \text{----------(1)}$$

Where V is the potential acting on the electron, E = the energy of the electron and m is its mass.

A potential well is a barrier with infinite energy surrounding the electrons thus preventing electrons from tunneling. While the electron exits in this barrier, the wave function of the electron is given by Ψ(x), which is the probability of finding the electron in that well. This probability is proportional to |Ψ(x)2|. Where $\Psi(x)^2$ = Ψ×Ψ* (Ψ* is the conjugate of Ψ).

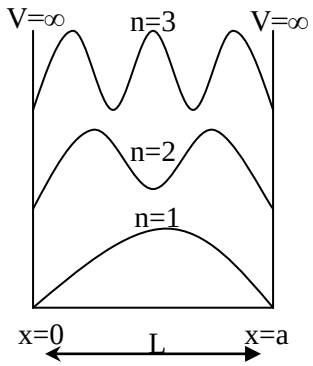

Fig.3. The infinite well which holds the electron with charge *e*−

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The boundary conditions of the system is

$$V(x)= \begin{cases} 0 & 0 \le x \le a \\ \infty & 0 \ge x \ge a \end{cases}$$

The solution to the Schr″odinger equation for a free electron which is moving inside the wellis (V(x) =0) is given as,

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} + \frac{8\pi^2 m(E)}{h^2}\Psi = 0 \qquad \text{----------(2)}$$

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} + k^2\Psi = 0 \text{ Where } K^2 = \frac{8\pi^2 mE}{h^2} \qquad \text{----------(3)}$$

$E_n = \frac{n^2 h^2}{8ma^2}$ Where n= 1,2,3,....

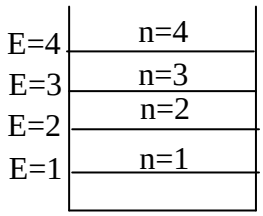

Fig.4.Eigen Values of Electron

From the above, it is clear that the electron possesses only discrete energy .The electron can only have certain discrete energies (E_n) known as Eigen Values. The spacing between adjacent energy levels depends on the width of the potential well. If we consider the height of the potential well to be finite, then there is a possibility for the electrons to tunnel out of the potential well. However in practice, it is not possible to get infinite potential, so if we consider the potential barrier is finite, the electrons couldtunnel freely between the quantum dots.While coming to the QCA ,each dot in a QCA cell behaves as a potential barrier for the electron and if the barrier lowered, then there is a probability for the electron to tunnel. If the potential barrier is lowered well enough, the electrons couldtunnel freely between the quantum dots[17].

VI.POLARIZATION IN QCA

Once the tunnelling is established by adjusting the barrier, and the electrons configure themselves by columbic repulsion, the barrier potential of the dots is raised again thereby trapping the electrons in their respective dots. So, the polarization of an electron can be altered by raising or lowering of potential barrier.

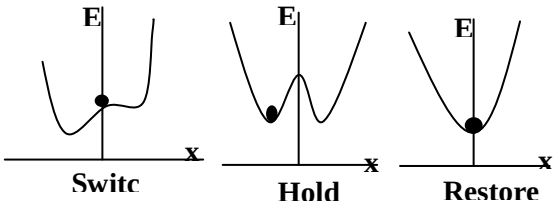

Figure5.Switching in QCA [8]

The modification in the tunnelling barriers can be controlled by the clockenergy and it is known as leakage power dissipation.The polarization of the electron reduces with increase in temperature, i.e. theelectrons are more likely to settle at higher energy level rather than at ground state**[17]**.

A stable arrangement of QCA cells can be obtained if the potential energies between them is minimum. The potential energy between two different cell electrons can be computed using the Eq. (4) [18,19]

$$U = \frac{kq_1q_2}{r} \quad \text{----------(4)}$$

$$kq_1q_2 = 9 \times 10^6 \times 1.6^2 \times 10^{-38} = 23.04 \times 10^{-19}$$

U is potential energy, q1 and q2 are electric charges, "r" is the distance between two electric charges.

The total potential energy of a given structure is "U_T" and that can be calculated using Eq. (5).

$$U_T = \sum_{1=1}^{n} U_i \quad \text{----------(5)}$$

VII. MOLECULAR QCA

The redox centres are playing predominant role in QCA dots. Redox means reduction–oxidation reaction. In general, redox reactions involve the transfer ofelectrons between chemical species. The chemical species from which the electron is stripped is said to have been oxidized, while the chemical species to which the electron is added is said to have been reduced. Molecules with at least two redox centres, between which an electron can move are called mixed-valence compounds[20].Aviram[21]considered and studied a mixed-valence compound model with two allyl groups connected by an alkyl bridge.The allyl group isa 3-carbon complex with allow-lying non bonding orbital and act as a dot.Craig et.al[5] studied a three-dot molecule which could act as molecular QCA, composed of three allyl groups connected by alkyl bridges in a "V" shape of the three allyl group two are neutral and and one allyl group that has a positive charge. The transfer of electron is possible from the neutral allyl radical .A. Pulimeno et.al [22] studied a Bis-ferrocene molecule in which two ferrocenes are linked together by means of a carbazole central group. The ferrocene groups acts as dots for logic state encoding whereasthe carbazole acts as the central third dot.An alkyl-chain provides the binding of the Bis-ferrocene to the ending thiol (-SH) group. This end-group is responsible for the binding to the gold substrate, especially for the Self Assembled Monolayer formation.

VIII. THE SIGNIFICANCE OF THE FIRST PRINCIPLE METHODS IN MOLECULAR QCA STUDIES

Over the past three decades, ab initio quantum chemical methods become an essential tool in the study of atoms and molecules. The principle behind ab initio methods is to solve the electronic Schrodinger equation by considering the positions of a collection of atomic nuclei and total number of electrons. Under the ab initio methods Hatree-Fock(HF) and Density Functional Theory (DFT) are familiar[23]. Both methods are used to describe the quantum states of many-electron systems. The Hartree-Fock method assumes that the many-

electron wavefunction takes the form of a determinant of single-electron wavefunctionscalled a Slater determinant. It does not incorporate electronic correlation, whichresult in high energy values.

By means of HF or DFT methods[24], it is possible to calculate total energy of formation of the atom or the molecule from atomic nuclei or electrons. Thermodynamic properties such as enthalpies, entropies, Gibbs free energies or heat capacities are also possible. In addition to this, the geometryoptimization to find the stable configuration of molecules, Charges, dipole moments and electrostatic potentials can also be calculated. In addition to all the above, the candidate molecules designed to act as dots then it is important to carry out LUMO and HOMO analysis. In chemistry, **HOMO(**for "highest occupied molecular orbital") and **LUMO (**"lowest unoccupied molecular orbital") are types of molecular orbitals. The energy difference between the HOMO and LUMO is termed the**HOMO–LUMO gap**. The difference in energy between these two orbitals can be used to predict the strength and stability of transition metal complexes.

IX. HOMO -LUMO STUDIES IN QCA

Dey et.al[25]studied bio molecular Quantum dot Cell with two Adenine Nucleotide biomolecules along with one Carbazole and one Thiol group and showed the stability of the two polarization stated along with the null state. Through the density functional theory, Tokunaga[26]studied the dynamic behaviour of signaltransmission through metal complexes $[L_5M\text{-}BL\text{-}ML_5]^{5+}$ (M=Fe, Ru, Os, BL=pyrazine (py**)**, 4,4'-bipyridine (bpy), L=NH_3) and showed Bpy complexes have stronger signal amplitude and consume longer time for signal transmission than pycomplexes . John A. Christie [27] introduced a carborane cage between ferrocene and feerocenium in 7-Fc^+ -8-Fc-7,8-nido-$[C_2B_9H_{10}]^+$ (Fc^+ Fc $C_2B_9^-$) and studied the electron transfer with in Fc^+ Fc $C_2B_9^-$ by TD-DFT computational studies . The HOMO-LUMO study of zwitterionic by Yuhui Lu et. A [28]lconfirms the self-doping mechanismi.e the accepting of electron by monocarbaborate cluster from an allyl group to obtain a 2n +2 leading to the bistable configuration to encode binary information. Tokunaga[29] studied the signal transmission through Creutz–Taube complexes $[(NH_3)_5Ru\text{-}BL\text{-}Ru(NH_3)_5]^{5+}$(BL = pyrazine (py), 4,4′-bipyridine (bpy)) by UB3LYP and UHF and proved that signal amplitude (*A*) is strongly dependent on the position and charge of the input to the molecular QCA.

X.CONCLUSION

Quantum-dot cellular automata (QCA) is a new architecture for computation. It is based on encoding binary information in the charge configuration of quantum-dot cells. The binary information encoding in QCA will be done by means of the redox centres. From the above discussions it is clear that properties of differentmolecule candidates regarding their non-linear behaviour, bi-stable interactionbetween molecules on which the essential device performance depends, etc. ,are thoroughly be studied with the help of our quantum chemical methods. So the ab initio quantum chemical methods are playing crucial role is designing the future storage device, the quantum dot cellular automata.

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