PERFORMANCE ANALYSIS –A PARADIGM APPROACH TO MOLECULAR COMPUTING

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ABSTRACT

The objective of the proposed research is to analyze the performance of designing a molecular computer. The performances are analyzed starting from molecular diodes to transistors, integrated chip, and very large scale circuit design with different organic materials. It overviews the properties like material compatibility, chemical registrant, dimension, temperature variation, specific heat, hybridization property, moulding shrinkage and tunneling effect etc. affect the performance in compare to our silicon level design. Further it enhance to DNA level design and analyze the advantages, disadvantages of various techniques of designing an optimum and powerful molecular computer with high speed and accuracy. Another objective of this research work to go for a total bench mark analysis to silicon based computer, organic molecule based computer and biological based DNA Computer with a paradigm approach to performance factors. It reflects a standard formula to go for a speed, accuracy and memory of processor taking into different performance factors.

Keywords: *Molecular Computing, DNA (Deoxyribonucleic Acid), Organic Molecule, Performance Factors*

1. INTRODUCTION

The present computers use switches made of silicon, But future computers might use molecules or clusters of atoms. It implies that molecular electronics - or moletronics - could replace transistors, diodes and conductors in conventional silicon based microelectronic circuitry. Even the industry projections suggest that silicon transistors may shrink to about 120 nanometers in length, but still be more than 60,000 times larger in area than molecular electronic devices. The future is predicting about the atomic and molecular computing .The Molecular computer would consume very little power as an advantage of size. It also predicts to acquire a very faster and reliable computing power. The innovation in initial stages of development and estimate the technology could be commercialized as such a speculation. Not only with size, the material contents with a molecule carrying at a time with different chemical combinations which in other hand have different chemical properties giving rise to more speed to our molecular processor design. The accuracy will obviously will increase as we are finding different material combination with different energy level and with different chemical structures. The computing power or speed will be within nanosecond with latest design of robust computing algorithm taking in to consider the high throughput concepts.

2. METHODOLOGY

To proceed with our methodology approach to have a benchmark analysis to silicon, molecular and DNA computer the idea of periodic table must be in our sight to study the metals, atoms, molecules and compounds which take vital part in our study.

2.1. Analysis to silicon computer design

The design of silicon computer started with the revolution from Diode design, Triode design,

Transistor design and later progress to integrate circuit design and VLSI design. Similarly to find out All these, still it is taking more space for physical existence and also the memory and speed of computing of these is not so fast for large data and more even complicated computing can not be done at mean the time. To understand the functions it is necessary to understand the basic structure of all semiconductor devices.

2.2 Analysis of molecular computer design

Molecular computation in particular focuses on the computational power of molecules with specific to that made of organic molecules and attempts to realize information processing .By using molecules, We expect to go for information processing in a faster parallel processing, smaller in size and efficient-energy-saving. So we are expecting the emerging of a brand-new technology in terms of a new model of computation. An organic molecule as devices mainly focuses on Polyphenylene-based molecular-scale electronic devices, conjugated aromatic organic molecules as conductors or wires and aliphatic organic molecules as insulators.

2.2 Analysis to DNA computer design.

The primary molecule that could be used as potential basis for carrying out symbolic computation is DNA (Deoxyribonucleic Acid). Biological molecules as devices considered as DNA based Electronic Devices and Oligo nucleotides which generates a signal representations in DNA computing paradigm.

3. PERFORMANCE FACTORS

3.1 Material Effect

We come across with our design concept of silicon, Molecule and DNA Diode, Transistor and IC, VLSI circuit design. We will now analyze how different materials affect the Performance of these three types of design. As you know we can take different metal oxide, conducting material and insulation material, the energy and electrical flow also affect on the performance of computer. As per example with silicon computer presence of silicon, and argentenium affect the performance, similarly in molecular computer the presence of alkali, organic, aliphatic also affect the performance. So as if we consider in the gene level and taking a known sequence where conducting chemicals are there, and as the biological activity given by particular gene, our electronic design will also give such kind of electronic properties that will use full for designing DNA Diode, Transistor, IC, and VLSI.

3.2 Bond effect

Different kinds of bonds exist when we consider which material is fit for what and which will make a conductor or insulator in designing a Silicon Diode, Molecular Diode, and DNA Diode. Basically we have two categories of bonds, they are I) intramolecular bond (bonds within the molecule) and II) intermolecular bond (Bonds between the molecules).Intramolecular bond contains covalent bond, ionic bond and metallic bond.

3.3 Tunneling Effect

Tunnel effects come when two molecules approaching towards each other their atoms come in contact with other different molecule which is closest. At this point of approaching, the nature of the electrons surrounding the atoms is slightly changed; each reflects some characteristics of the other. Some of the characteristics of tunnel effect are 1) where energy finds difficult to appear, but particles can appear easily 2) The wave nature of particles produce tunnel effect. 3) The tunnel effect can be applied to various fields.

3.4 Particle effect

Different Atomic and subatomic particles are existing which play a major role with their valence and energy in the designing and analysis process of silicon, Molecular and DNA Computer Design. An atom generally consists of a nucleus with positively charged protons and neutral neutrons surrounded by negatively charged electrons.

3.5 Size Effect

Because atoms and molecules are so small, it is difficult to determine their sizes. Special instruments are normally needed for such measurements. As electrons move around nucleus, it is reasonable that the size of an atom depends on valence electrons in outermost orbit.

The atom seems very small in size, if electrons are very close to the nucleus.

3.6 Surface Effect

Electric current measures by ejecting electrons from a sodium metal surface .The opposing voltage need to stop all the electrons indicates a measure of the maximum kinetic energy in electron volts and the minimum energy is called photoelectric work function to eject an electron from the surface.

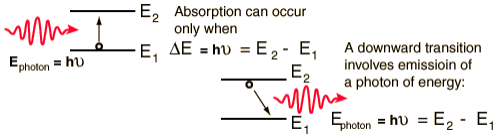

Fig.1 Energy Band

3.7 Structure effect

Depending on structure of atomic materials and their energy levels in orbital, similarly the different chemical structure of the molecule depending on the positions of atoms the structure varies so as the energy also. In Organic molecules the structure matters much than the simple molecules. So Structure effect plays a very major role in energy and intensity level study. Atom generally is the smallest building block of matter made of neutrons, protons and electrons.

3.8 Chemical Registrants

Every electrical component is identified by register and used in many varied ways. Registers are the components manufactured in many types and sizes. The resistors which are made of Chemical molecule show different types of resistivity factors which are responsible in designing molecular diode, Transistors.

3.9 Conductance

Conductance is the opposite of opposite of resistance .The ability of a material to pass electrons is determined by conductance. The magnitudes of conductance factors are exactly the same as resistance, but they affect conductance in the opposite manner. Conductance is directly proportional to area, and inversely proportional to the length of the material. Material temperature is definitely a factor, but in a constant temperature, the conductance of a material can be determined.

3.10 Specific heat

The heat per unit mass required to raise the temperature by one degree Celsius is called as specific heat. The relationship between heat, temperature and specific heat shown as $Q=cm\Delta T$, where Q=Heat, c=specific heat, m=mass and ΔT=change in temperature. If phase change is encountered the above relationship does not hold good as phase change does not change the temperature even if you add or remove heat.

3.11 Hybridization property

Mixing of atomic orbitals to form new orbitals by atomic boding properties is called as hybridization. Taking into consider hybrid orbital, we use to describe the process of hybridization as change from atomic orbitals to bonding orbitals.These orbitals are helpful in determining the shape of molecules orbitals for molecules.

3.12 Moulding shrinkage

Packaging is the major factor when we design any microchip for computer design. If we use plastics, it has profound shrinkage behavior. This leads to the fact that the molded thermoplastic parts are smaller in dimensions than producedmold. The total shrinkage is calculated by taking into consider after shrinkage condition. The part begins to shrink in the injection mold as it goes on cool. This process may also continue after demolding.

4. EXPECTED RESULTS

4.1 A Proposed paradigm design:

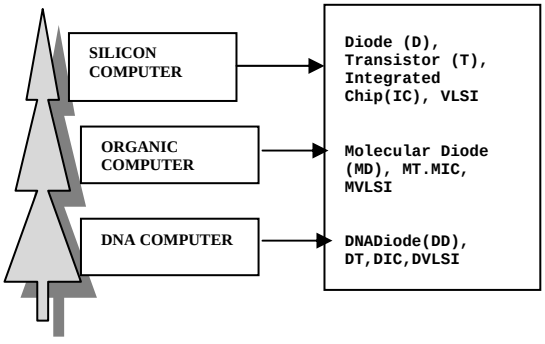

Fig2.Paradigm to Silicon, Molecule and DNA Computer

4.2 MSA (Memory-Speed-Accuracy) Model Design

Let us consider X, Y and Z are the silicon computer, organic molecule Computer and DNA Computer.

Let us take parameter M, S, A for Memory, Speed and Accuracy of three different types of Computers.

Let us notate our performance factors as follows
1) Material Effect (M_E)
2) Bond Effect (B_E)
3) Tunneling Effect (T_E)
4) Particle Effect (P_E)
5) Size Effect (S_E)
6) Surface Effect (Sr_E)
7) Structure effect (Str_E)
8) Chemical Registrants (CR_E)
9) Conductance (C_E)
10) Specific heat (SP_E)
11) Hybridization property (H_E)
12) Moulding shrinkage (MD_E)

4.3 Expected analysis:

The performance factor (P) can be calculated with the proposed mathematical derivation as

P (Memory) = P (X, Y, Z) * K_1
P (Speed) = P (X, Y, Z) * K_2
P (Accuracy) = P (X, Y, Z) * K_3

Where K_1, K_2, K_3 are the performance factors responsible for memory, speed and accuracy of different level of design. K_1, K_2, K_3 will differ as some of the performance factors will not come for all types of material, second as the material is combination of so many types of atoms it will differ. Similarly the organic structure will also differ, so also their angle, so give rise to different structure effect and orbital energy vale.

$P(X, Y, Z)_{memory} = \sum K_1 * (L_1)$,
Where $L_1 = M_E , B_E, T_E, P_E, S_E, Sr_E, Str_E, CR_E, C_E, SP_E , H_E, MD_E$
$P(X, Y, Z)_{Speed} = \sum K_2 * (L_2)$,
Where $L_2 = M_E , B_E, T_E, P_E, S_E, Sr_E, Str_E, CR_E, C_E, SP_E , H_E, MD_E$
$P(X, Y, Z)_{Accuracy} = \sum K_3 * (L_3)$,
Where $L_3 = M_E , B_E, T_E, P_E, S_E, Sr_E, Str_E, CR_E, C_E, SP_E , H_E, MD_E$

L_1, L_2, L_3 will again vary depending on Diode, Transistor, IC, VLSI Category.

Diode: $L_{1\,(D,MD,DD)} = \sum L_1(X,Y,Z)$, $L_{2\,(D,MD,DD)} = \sum L_2(X,Y,Z)$, $L_{3\,(D,\,MD\,,\,DD)} = \sum L_3(X,Y,Z)$.

Transistor: $L_{1\,(T,MT,DT)} = \sum L_1(X,Y,Z)$, $L_{2\,(T,MT,DT)} = \sum L_2(X,Y,Z)$, $L_{3\,(T\,,\,MT,\,DT)} = \sum L_3(X,Y,Z)$.

Integrated Chip: $L_{1\,(IC,\,MIC,\,DIC)} = \sum L_1(X, Y, Z)$,$L_{2\,(IC,MIC,DIC)} = \sum L_2(X,Y,Z)$, $L_{3\,(IC\,,\,MIC\,,DIC)} = \sum L_3(X,Y,Z)$

VLSI: $L_{1\,(VLSI,MVLSI,DVLSI)} = \sum L_1(X,Y,Z)$, $L_{2\,(VLSI,MVLSI,DVLSI)} = \sum L_2(X,Y,Z)$,
$L_{3\,(VLSI,MVLSI,DVLSI)} = \sum L_3(X,Y,Z)$

The L1, L2, L3 plays a major role in calculating the performance factors depending on silicon, organic or DNA string material.

4.4 Results with Memory, Speed & Accuracy

With the above proposed paradigm, we are hoping to find out the performance level with below prediction or more than this. As different calculations will come for silicon, organic and DNA material, we hope it will more way effect to the performance with below level. The atomic mass and atomic number with its orbital and angle view produce different level of energy stage which not only restricted to crystal level but with a vision to go for minute level of particle study like meson, phonon and quark study .The nuclear magnetic radiation material will play a major role to studying molecular computing in Large Computing environment with enterprise level implications.

For the time being hoping to get, n^n bits in a organic or molecular computer, and n^L taking in to consider the n-bits for access of memory. Similarly n^{l-R} bits of speed with molecules, where l=number of carbon molecules and R=Residue factors and with DNA string n^L speed. If we are considering the accuracy level it will be n, (n+1-R) and (n+1)*L percentage for Silicon, Molecular and DNA computing level respectively. This calculation is in bit level, which we will consider for hertz level after finding a concrete formula for the performance factors.

Types	Memory	Speed	Accuracy
X (Silicon Computer)	n%	n-bits	n-bits at instant
Y (Molecule Computer)	(n+1-R)%	n^n	n^{l-R} bits
Z (DNA Computer)	(n+1)* L %	n^L Bits	n^L = at instant

Table1: A Prediction in Bit-Level

Considering n-bits of memory

l=no. of Carbon molecule,

L=Length of DNA strand or Polyphenylene chain and R-Residue.

5. IMPLICATIONS FROM INDUSTRY AND RESEARCH PERSPECTIVE

I am designing a CAD tool which will take help of *Cheminforamtics* to acquainted with all atoms, molecules available in the periodic table and generally available materials. This tool will contain the database of atomic mass, atomic number and all the factors necessary for performance. It will show all the chemical structures with all options like rotating, tilting, angle elevation, visual image of any surface for designing a computer and its compatibility. It will show depending upon particular design of silicon, molecular and DNA material where the computing giving reliable designs taking the same type of material.

This tool takes the help of Bioinformatics to have Chemo informatics knowledge to go for a gene level study of organic and biological material, so that we can go for a design of DNA computer which will act like human, but with more accuracy, speed and memory. As day to day new material properties are realized, it is a hope that organic electronics may replace the traditional technologies and manufacturers in next years to come ahead.

6. FUTURE PERSPECTIVE

With our performance analysis factors, I am hoping to get more accuracy, speed, and memory than the so far study happening to Molecular computing which is in midway between Silicon and High through put computing. We have analyzed different kinds of Chemical materials which are helpful in designing the molecular Computer and we need to test the Performance. The future perspective after the study of silicon, molecular and DNA computer design lies entirely on quantum computer, where we will take sub-atomic world as the basic of study with help of quantum physics. This field is in starting stage of research for quantum computing.

7. CONCLUSION

This research work is trying to bring out a performance level software like Cad tool where every researcher and scientist through out the world can find out every information about chemi-informatics and the use of it especially in Molecular Computer design which will lead a way to High throughput computing and designing of Software engineering concepts to this field in a later stage.

I can say more over my work will be concentrate to three things Systematic, Cybernetics and Informatics.Systematics will concern to my system level study and designing level study to different silicon computer, molecular computer and DNA level computer .From Cybernetics points of view I have to go for a study to Algorithms and mathematical model need for performance level study. From informatics point of view, I have to develop a CAD tool which will give all information about molecular design and performance factors checkout information before somebody take any molecule or material to design a Molecular Computer. The more study will spread to nano-level study to my present work and develop a paradigm which will go on enhanced version day by day.

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BIOGRAPHY

Mr.Manas Ranjan Pradhan received M.Sc (Physics-X-rays) from Regional Engineering College (presently called National Institute of Technology), Rourkela, India and Master in Technology (Computer Science) from Utkal University; Bhubaneswar, India He is currently a PhD scholar in computer science under University of Mysore, India. Currently he is working as faculty member in IBS, Hyderabad, India. His research interests are Bioinformatics, Speech recognition nano computing and business process simulation.

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