Three-Dimensional-Topology Processing and Memory Cells

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ABSTRACT

This paper researches an innovative fundamental concept and proposes a practical solution for envisioned molecular processing platforms (^{M}PPs). At the device level, we report three-dimensional (3D) topology multi-terminal molecular processing primitives (^{M}primitives) which exhibit electrochemomechanical transitions ensuring functionality. These ^{M}primitives can be utilized as logic gates. Aggregated ^{M}primitives comprise neuronal hypercells ($^{\aleph}$hypercells). The networked $^{\aleph}$hypercells form ^{M}PPs within 3D system organization.

Keywords: molecular primitive, neuronal hypercell, polypeptide, processing platform

1. INTRODUCTION

High-performance processing and computing, as forefront challenging areas, have been widely examined in the literature. Electronic, electrical, mechanical, chemical and other logic devices were proposed, studied and utilized in various data processing, computing and memory platforms. Tremendous progress has been achieved by utilizing complementary metal-oxide semiconductor technology to fabricate integrated circuits (ICs) designed using very-large-scale integration methodology. However, emerging fundamental problems and technological limits, associated with solid-state microelectronics and ICs, cannot be overcome, or solutions are unknown [1, 2]. Departing from conventional concepts, we study alternative solutions.

Various *solid* and *fluidic* molecular processing, logic and memory devices (^{M}devices) have been studied [3-7]. Only a few ^{M}devices were synthesized, tested and characterized [3-8]. The major challenges encountered are:

1. Device physics soundness;
2. Synthesis and assembly;
3. Aggregation, integration and compatibility;
4. Testing, evaluation and characterization.

Though some devices promise to exhibit meaningful phenomena and ensure functionality, these devices still pending as long as the aforementioned tasks are performed proving overall device soundness.

The processing (computation) can be accomplished by means of electron transport, conformational changes and other electrochemomechanical transitions. These transitions can be accomplished by molecules or molecular complexes which form ^{M}primitives. The device-level functionality, which is predefined by the device physics, should be supported by synthesis feasibility. We propose to engineer ^{M}primitives using the following innovations:

1. Use the polypeptide backbone as a structural skeleton with side groups which exhibit electro-chemomechanical transitions and interaction ensuring combinational logics (logic functions) and memory storage;
2. Aggregate the side groups of neighboring primitives forming $^{\aleph}$hypercells.

This solution mimics, to some extent, a *natural biomolecular hardware*. However, this does not imply that we mimic or approach *natural* information processing, data processing or memory storage. We study *engineered* ^{M}primitives, $^{\aleph}$hypercells and ^{M}PPs which inherently possess 3D topology and 3D organization features. In general, ^{M}PPs integrate a large class of computing, memory and processing solutions and systems. For example, if the electron transport ensures the device functionality, ^{M}primitive can be classified as a molecular electronics device (^{ME}device), implying that a ^{M}PP can be designed utilizing molecular integrated circuits (^{M}ICs).

2. MOLECULAR PROCESSING

Among the key challenges in devising and the design of ^{M}primitives, the major ones are:

- Device physics, functionality, and processing capabilities;
- Synthesis, e.g., technological feasibility, practicality, yield, etc.;
- Aggregability and integration (assembly, interfacing, compatibility, compliance, interactability, matching, packaging, etc.).

The technological soundness can be achieved by using ^{M}primitives implemented as organic or inorganic molecules (molecular complexes) within the structural backbone formed by polypeptides [8]. It is known that polypeptides are used to form very-complex functional *natural*, organic and hybrid molecular organelles and assemblies such as various proteins, enzymes, hormones and other biological polymers. Though a significant progress has been documented for biomolecules and proteins, there is a need to depart from the attempt to blindly prototype *natural*

biomolecular hardware due to immense unsolved fundamental and synthesis problems. For example, one may not be able to utilize *natural* biomolecular and protein functionality, transitions, mechanisms, etc. Our objective is to design *synthetic* ^{M}PPs, including ^{M}ICs, which are entirely distinct as compared to biosystems. The peptide synthesis, custom biosynthesis and wide range of possible structural modifications provide the designer with a needed flexibility and multiplicity maintaining the specificity and soundness. In ^{M}primitives we propose to utilize side groups which must ensure and exhibit:

- Desired device functionality, capabilities and characteristics (for ^{ME}devices, controlled electron transport, switching characteristics, *IV* characteristics, energetics, etc.);
- Assembling, interfacing, networking and interconnecting features.

3. ^{M}PRIMITIVES AND $^{\aleph}$HYPERCELLS

We study envisioned ^{M}PPs which are comprised from networked $^{\aleph}$hypercells formed as aggregated ^{M}primitives. Each ^{M}primitive is engineered utilizing:

- Polypeptide backbone $(–N–C–C–)_n$ which forms structural skeleton;
- Side groups (S_{ijk}).

Consider a 3D-cube-topology $^{\aleph}$hypercell which consists of ^{M}primitives, as depicted in Figure 1. Here, side groups S_{ijk} and the polypeptide backbone $(–N–C–C–)_n$ comprise ^{M}primitives $^{M}P_{ijk}$.

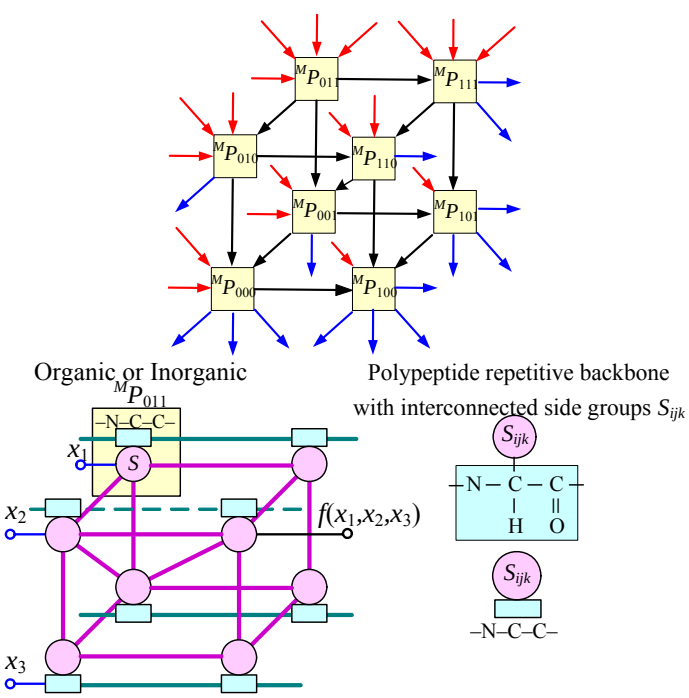

Figure 1. 3D-topology $^{\aleph}$hypercell comprised from ^{M}primitives $^{M}P_{ijk}$ formed by the polypeptide backbone and side groups S_{ijk}

The $(–N–C–C–)_n$ chains provide a structural skeleton (mechanical structure), while side groups S_{ijk} must guarantee the overall functionality within the device physics. Each S_{ijk} may integrate multi-terminal and multi-functional ^{M}devices engineered from organic or inorganic molecules. As shown in Figure 1, the 3D-topology interconnect is accomplished by S_{ijk}. $^{\aleph}$Hypercells can be clustered to form macrocells, thereby forming ^{M}PPs.

Engineered and Natural Processing Platforms – The proposed concept, in general, cannot be manifested to be biomimetic-centered because it is highly unlikely that ^{M}primitives guarantee the functionality and operationability equivalence to biomolecules and *natural* biomolecular aggregates. That is, ^{M}PPs' and *natural* biomolecular platforms' functionality, capabilities, hardware, software and other basic features are entirely distinct. However, we typify the *natural biomolecular hardware*. A significant departure from conventional concepts is achieved providing a viable sound alternative.

4. FUNCTIONALITY OF ^{M}PRIMITIVES

Various quantum, electrostatic, electromagnetic, optical, mechanical and chemical phenomena and effects can be utilized to perform logic operations, implement switching functions and store information. The corresponding side groups must be engineered to guarantee the specified phenomena, effects and transitions. Though electron transport and bond formation/braking are due to electron transitions (transport, exchange, sharing, etc.), they are profoundly different. While the overall device functionality is defined by S_{ijk}, the soundness of spatial topology assembly (geometry and conformation) must be ensured through a coherent backbone–S_{ijk} aggregation.

Various electronic and quantum-effect devices have been utilized focusing the major thrust on the well-defined microelectronic paradigms. Different device-level solutions were examined and extensively investigated. Molecular electronics is within the most promising solutions. This direction affects not only engineering but also life science.

For ^{ME}devices, the expected characteristics and the controlled electron transport are examined by utilizing the methods of quantum mechanics [8]. We investigate various side groups engineered from organic and inorganic molecules which should ensure overall functionality and practicality of multi-terminal ^{ME}devices.

Consider a three-terminal ^{ME}device with the *input*, *control* and *output* terminals, as shown in Figure 2.a. The device physics of this ^{ME}device is based on quantum interactions and controlled electron transport. The applied $V_{\text{control}}(t)$ changes the charge distribution $\rho(t,\mathbf{r})$ and electric field intensity $\mathbf{E}_E(t,\mathbf{r})$ affecting the electron transport. This ^{ME}device operates in the controlled electron-exchangeable environment due to quantum transitions and interactions. The controlled super-fast potential-assisted electron transport may be ensured.

Consider the electron in the time- and spatial-varying metastable potentials $\Pi(t,\mathbf{r})$. The changes in the Hamiltonian result in:

- Quantum interactions due to variations of the charge distribution $\rho(t,\mathbf{r})$, $\mathbf{E}_E(t,\mathbf{r})$ and $\Pi(t,\mathbf{r})$;
- Changes of tunneling $T(E)$.

The device controllability is ensured by varying $V_{\text{control}}(t)$ that affects $\rho(t,\mathbf{r})$, $\mathbf{E}_E(t,\mathbf{r})$ and $\Pi(t,\mathbf{r})$ leading to variations of electron transport. Hence, the device switching, *IV*, *GV* and other characteristics are controlled.

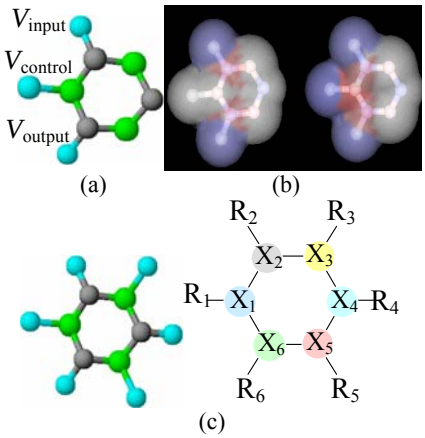

Figure 2.
(a) Side group S_{ijk}: Three-terminal ^{ME}device comprised from a monocyclic molecule with a carbon interconnecting framework; (b) Charge distribution $\rho(\mathbf{r})$; (c) Six-terminal ^{ME}device.

To study the device characteristics, we simplify S_{ijk} to 9 atoms with motionless protons with charges q_i. The radial Coulomb potentials are

$$\Pi_i(r) = -\frac{Z_{eff\,i} q_i^2}{4\pi\varepsilon_0 r}.$$

For carbon, we have $Z_{eff\,C}$=3.14.

Using the spherical coordinate system, the Schrödinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right]$$
$$+\Pi(r,\theta,\phi)\Psi(r,\theta,\phi)=E\Psi(r,\theta,\phi)$$

should be solved.

One can represent the wave function as

$$\Psi(r,\theta,\phi)=R(r)Y(\theta,\phi)$$

in order to solve the radial and angular equations. We discretize the Schrödinger and Poisson equations to numerically solve these differential equations. The magnitude of the time-varying potential applied to the *control* terminal is bounded due to the thermal stability of the molecule, energetics and other limits. In particular, $|V_{\text{control}}|\le V_{\text{control max}}$, and $|V_{\text{control}}|\le 0.25$ V. Figure 2.b documents a three-dimensional charge distribution in the molecule for V_{control}=0.1 V and V_{control}=0.2 V.

The Schrödinger and Poisson equations are solved using a self-consistent algorithm in order to verify the device physics soundness and examine the baseline performance characteristics. To obtain the current density **j** and current in the ^{ME}device, the velocity and momentum of the electrons are obtained using

$$\langle p\rangle = \int_{-\infty}^{\infty}\Psi^*(t,\mathbf{r})\left(-i\hbar\frac{\partial}{\partial\mathbf{r}}\right)\Psi(t,\mathbf{r})d\mathbf{r}.$$

The wave function $\Psi(t,\mathbf{r})$ is numerically derived for distinct values of V_{control}. The *IV* characteristics of the studied ^{ME}device for two different control currents (0.1 and 0.2 nA) are reported in Figure 3 [8]. The results documented imply that the proposed ^{ME}device may be effectively used as a multiple-valued primitive in order to design enabling high-radix logics and memories.

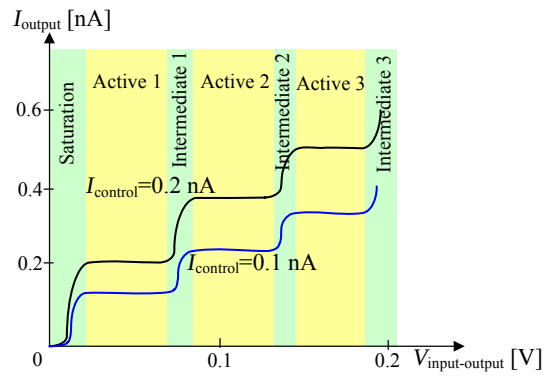

Figure 3. Multiple-valued *IV* characteristics

The traversal time of electron transport is derived using

$$\tau(E)=\int_{\mathbf{r}_0}^{\mathbf{r}_f}\sqrt{\frac{m}{2[\Pi(\mathbf{r})-E]}}d\mathbf{r}.$$

It is found that τ is ~5×10^{-15} sec. Hence, the proposed ^{ME}device ensures super-fast switching.

The reported monocyclic molecule can be used as a six-terminal ^{ME}device as illustrated in Figure 2.c. The use of the device's side groups R_i, shown in Figure 2.c, ensures the variations of the energy barriers, wells potential surfaces $\Pi(t,\mathbf{r})$, interatomic length, etc. The proposed carbon-centered molecular solution, in general,

- Ensures a sound *bottom-up* synthesis at the device, gate and hypercell levels;
- Guarantees assembly and aggregability features to form complex ^{M}ICs;
- Results in the experimentally verifiable and characterizable ^{ME}devices and ^{M}gates.

The studied ^{ME}devices can be utilized in combinational and memory ^{M}ICs. In addition, those devices can be used as routers. In particular, one may achieve a reconfigurable networking, processing and memory. The proposed ^{ME}device can be used as a *switch* or transmission device allowing one to design the neuromorphological reconfigurable ^{M}PPs.

5. TOWARDS MOLECULAR COMBINATIONAL LOGICS AND MEMORIES

A 2×2 array of SRAM cells is reported in Figure 4. The memories can be implemented using ^{M}NOR and ^{M}NAND gates which can be implemented by the proposed ^{M}primitives and ^{N}hypercells.

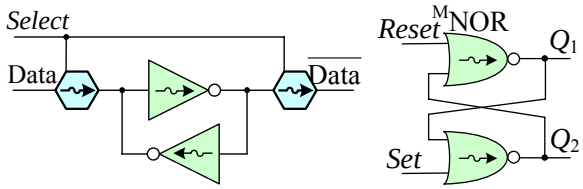

Figure 4. Molecular memory: SRAM cell and 2×2 array of SRAM cells implemented as ^{N}hypercell

ACKNOWLEDGEMENTS

The second author sincerely acknowledges a support from the US Department of Energy under the contracts DE-FG02-06 *Three-Dimensional Biomolecular Computing Architectures.*

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6. CONCLUSIONS

Fundamental, applied, experimental and technological features of molecular processing were studied. We proposed an innovative and elegant concept. Typifying the *natural* polypeptides and side groups, we utilized the *natural* or *synthetic* polypeptides and side groups ensuring functionality and synthesis features. Examples are reported with the foreseen technology assessments. We proposed an alternative solution to solve a three-fold problem for envisioned ^{M}PPs by: (a) Devising and researching device physics of ^{M}devices; (b) Developing a technology-sound solution; (c) Devising functional and sound ^{M}primitives, ^{M}devices and ^{N}hypercells which comprise of ^{M}PPs. We progressed towards 3D ^{M}PPs which promise to ensure neuromorphological reconfigurable data processing. To some extent, we applied the *natural* processing solutions to *engineered* one. Correspondingly, we focused on the transformative science and engineering. The proposed concept promises massive vector processing utilizing robust and reconfigurable neuromorphological organizations, high-radix processing, molecular hardware, etc.

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