Biomolecular, Organic and Inorganic Processing *Fabrics*: Design and Synthesis of Processing Cells and Primitives

Sergey Edward Lyshevski

Department of Electrical and Microelectronics Engineering
Rochester Institute of Technology
Rochester, NY 14623, USA
E-mail: Sergey.Lyshevski@mail.rit.edu

ABSTRACT

This paper addresses the problem of three-dimensional interfacing, networking and aggregation of molecules within processing *fabrics*. Our ultimate objective is to study the feasibility of synthesis of molecular processing f*abrics* for envisioned sensing and processing systems. For molecular sensing and processing primitives, we examine synthesis solutions which may ensure technological feasibility and practicality. The spatially-distributed sensing and processing primitives should guarantee sensing and processing utilizing quantum phenomena. In particular, the quantum effect induced transductions should be used. In living organisms, biomolecular *fabrics* guarantee information processing, integrated quantum-mechanical ↔ electrochemomechanical functionality, integration, interface, etc. It is important to examine a broad spectrum of possible solutions in order to ensure processing by *microscopic* devices, develop consisted synthesis technologies, as well as *engineer* sensing and processing systems.

Keywords: molecule, processing, quantum mechanics, sensing, synthesis

1. INTRODUCTION

Tremendous progress was achieved by utilizing complementary metal-oxide-semiconductor technology to fabricate ICs designed using ultra-large-scale integration methodology. In microelectronics, fundamental and technological limits emerge [1, 2]. Currently, there are relatively modest evolutionary microelectronic and solid-state semiconductor devices advancements. To improve performance and capabilities of various computing and processing systems, computer organizations and architectures have being enabled. Unfortunately, there are trade-offs and limits on the expected advancements.

Though microelectronics may encounter prevailing limits, the current and expected solutions are sufficient to guarantee reasonable data processing capabilities needed. Even if alternative solutions will not emerge, there will be a very modest overall impact. Despite this fact, further developments toward molecular sensing and processing (computing) can be critical due to possible revolutionary changes at the device and system levels. These transformative developments may lead towards enabling sensing and super-high-performance processing. Furthermore, these advancements may enable understanding processing in living organisms. In fact, various processing tasks (information storage and retrieval, communication, coding, decoding and other) are exhibited at the molecular and cellular level (neurons). Therefore, new inroads may result in an enormous implication in neuroscience, biophysics, etc.

We are considering *microscopic* sensing and processing. The envisioned molecular platforms should be synthesized as molecular *fabrics*. The conventional *macroscopic – microscopic* interfacing may not guarantee functionality because interconnect significantly changes the overall behavior of *microscopic* devices. We attempt to typify biomolecular *fabrics* which exhibit extraordinary interfacing, communication, sensing and processing capabilities. While studying sensing and processing by *microscopic* systems, the device- and module-level processing abilities must be supported by synthesizing *fabrics*. Molecular and biomolecular communication, sensing and processing are fundamental and technological frontiers of this century. Performing a transformative research, we study the feasibility, consistency and practicality of sensing and processing by molecules, aggregating them into *fabrics*.

2. PROPOSED SOLUTION

High-performance processing (computing), as a forefront challenging theme, has being emerged. New electronic and optical communication and processing devices were proposed, studied and verified [1]. However, the *macroscopic*-pertinent fundamental and technological limits cannot be overcome, or, solutions are yet unknown. Departing from a conventional *macroscopic* premise, we study an alternative *microscopic* paradigm.

Various molecular devices were proposed. Numerous experimental studies were performed with the attempt to examine, test and characterize these molecular devices [1-7]. Unfortunately, due to the *macroscopic – microscopic* interfacing, the results are found to be inconclusive. Testing, evaluation and characterization of *microscopic* systems can be performed if unperturbed and undisturbed functionality is achieved. Though some devices promise to exhibit phenomena which ensure overall functionality, these devices must be synthesized and tested.

Sensing and processing can be accomplished by means of electron transport, conformational changes and other quantum-mechanical and electrochemomechanical transductions. The device functionality, which is predefined by the device physics, should be supported by synthesis solutions and interfacing feasibility. We propose to synthesize molecular devices and *fabrics* using the following solution:

1. Use the polypeptide backbone as a structural skeleton with side groups, which exhibit interactive quantum-mechanical and electrochemomechanical transductions, ensuring *state* transition relevant to sensing and processing;
2. Aggregate the side groups of neighboring primitives forming neuronal hypercells (^{N}hypercells).

This solution mimics, to some extent, *biomolecular fabrics*. However, this does not imply that we mimic or approach *natural* information processing, data processing or sensing. We *engineer* molecular sensing and processing primitives which inherently possess 3D topology.

The synthesis and technological practicality can be achieved by using 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 was documented for biomolecules and proteins, there is a need to depart from the attempt to blindly prototype *biomolecular fabrics* due to immense unsolved fundamental and synthesis problems. For example, one may not be able to:

- Synthesize and aggregate biomolecules ensuring technological feasibility, practicality or rationale;
- Utilize *natural* biomolecular and protein functionality which is based upon virtually unknown transductions, mechanisms, etc.

Our objective is to design *engineered* processing primitives and ^{N}hypercells which could be distinct (structure, functionality, phenomena utilized, etc.) as compared to biomotifs. 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 consistency.

To *engineer* molecular primitives, we utilize side groups which must ensure and exhibit:

- Overall device functionality, capabilities and characteristics (conformational changes, controlled electron transport, switching characteristics, energy exchange and other transductions depending on devices under consideration);
- Assembling, interfacing, networking and interconnecting features.

As depicted in Figure 1, a primitive is *engineered* utilizing:

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

The $(–N–C–C–)_n$ chains provide a structural skeleton (structure), while side groups S_{ijk} must guarantee the overall functionality within the specified device physics. Each S_{ijk} may integrate multi-terminal, and, multi-functional devices *engineered* from organic or inorganic molecules. The 3D-topology aggregation, interfacing and interconnect of primitives (P_{ijk}) is accomplished by S_{ijk}.

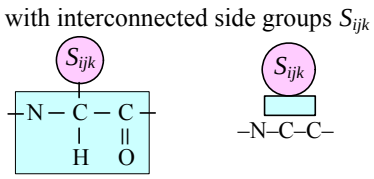


Figure 1. 3D-topology P_{ijk} formed by the polypeptide backbone and a side group S_{ijk}

A 3D-cube-topology ^{N}hypercell, which consists of primitives P_{ijk}, is schematically represented in Figure 2. ^{N}Hypercells can be clustered to form macrocells, thereby forming PPs.

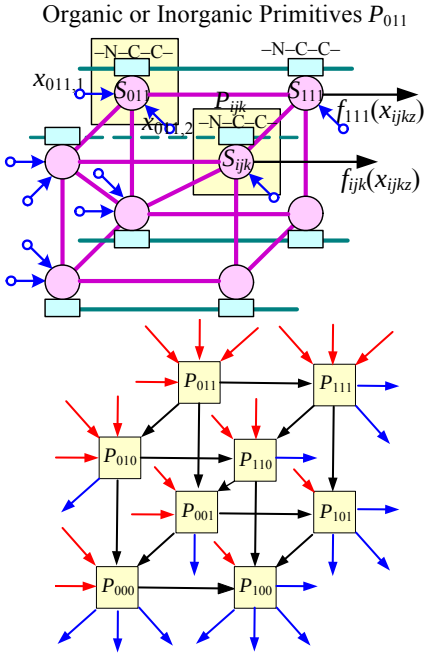


Figure 2. 3D-topology ^{N}hypercell comprised from P_{ijk}

3. PROPOSED SOLUTION: EXAMPLES

Example 3. 1.

Polypeptides and cystein monomers (amino acids with sylfhydril side groups CH_2-SH) are reported in Figure 3. As an ^{N}hypercell is synthesize, specific electrochemomechanical transductions must be ensured and utilized to accomplish processing.

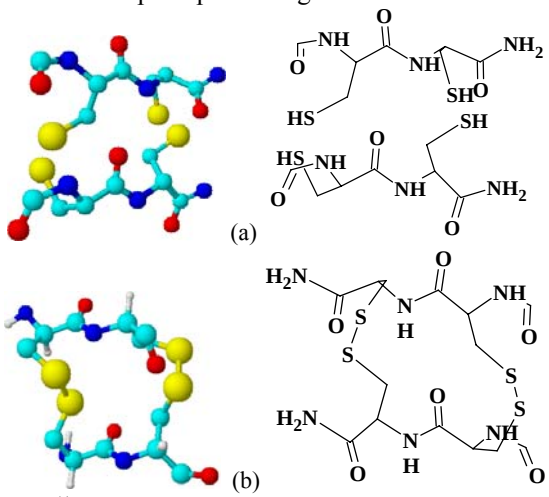


Figure 3. ^{N}Hypercell and processing transductions:
(a) Polypeptides and cystein monomers;
(b) Forming covalent bonds (disulfide bridges) upon mild oxidation.

Example 3. 2.

Polypeptides and cystein monomers are documented in Figure 4. We engineer ^{N}hypercells from organosulfur utilizing the specificity of the thiol group (R−SH) and its weak S−H bond. For the ^{N}hypercell, the S−H bond dissociation energy is ~80 kcal/mol, and, its weakness allows oxidative coupling reaction. When thiol reacts with mild oxidative agents, as hydrogen peroxide (H_2O_2), the product is disulfide, as shown in Figure 4. The oxidation reaction is

$$2\ RS{-}H + H_2O \rightarrow RS{-}SR + 2\ H_2O$$

Using this distinct ability of thiols, bond formation and dissociation may be accomplished ensuring overall functionality. In particular, conformation changes and charge distribution variations are guaranteed by bond formation and braking.

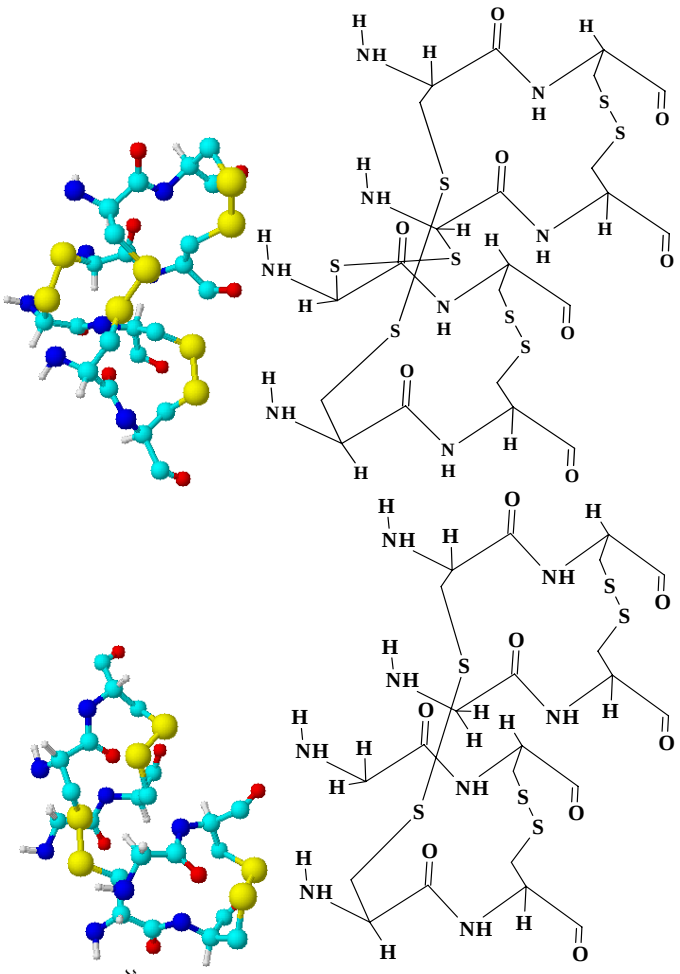
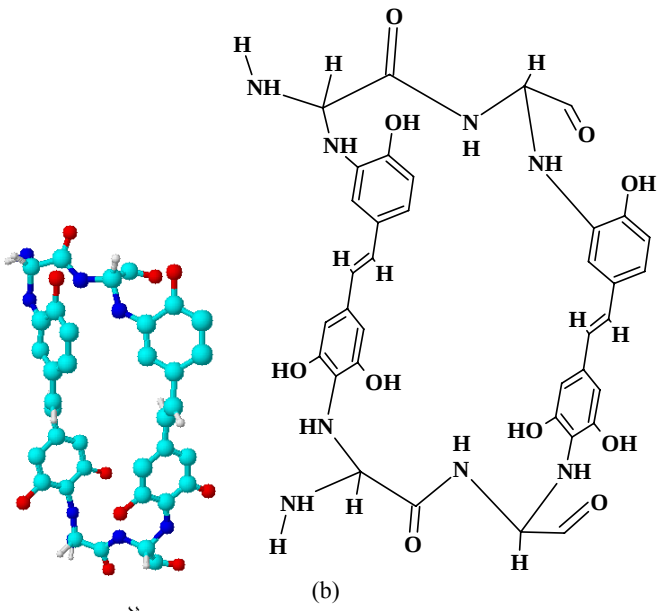


Figure 4. ^{N}Hypercells *engineered* by means of polypeptides and cystein monomers: One S-S disulfide atomic bond is broken changing the conformation

\ *Example* 3. 3.

Resveratrol (3,5,4'-trihydroxystilbene) is a polyphenolic phytoalexin which exists in *cis* or *trans* forms. The stable *trans* resveratrol can undergo isomerisation to the *cis*-form when exposed to ultraviolet irradiation. Resveratrol can be used in ^{N}hypercells as side group, as reported in Figure 5. Its ability to change conformation upon photoisomerization enables the thermal conformational isomerism because the thermal changes can be due to photon absorptions. Hence, the reported results are applicable because conformational changes are induced by the irradiation applied.



(b)

Figure 5. ^{N}Hypercell with polypeptides and resveratrol monomers

4. Functionality of Molecular Processing Primitives

Various quantum, electrostatic, electromagnetic, optical, mechanical and chemical phenomena and effects can be utilized to perform various sensing and processing tasks. The side groups must be *engineered* guaranteeing the specified evolutions, transductions and transitions [8]. For example, 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 overall applicability of spatial topology assembly (geometry and conformation) must be ensured through a coherent backbone–S_{ijk} aggregation [9].

5. Conclusions

Fundamental, applied, experimental and technological features of molecular sensing and processing were studied. We proposed an innovative and elegant concept. Typifying the *natural* polypeptides and side groups, we propose to utilize the *natural* or *synthetic* polypeptides and side groups ensuring functionality and synthesis features. Examples are reported with the foreseen technology assessments. An alternative solution is proposed to solve a three-fold problem for envisioned *microscopic* sensing and processing systems by:

1. Devising and researching device physics;
2. Developing a practical technology-relevant solutions;
3. Devising functional sensing and processing primitives and ^{N}hypercells.

We progressed towards new solutions which promise to ensure neuromorphic reconfigurable data processing. To some extent, we typify the *natural* processing solutions by utilizing quantum-mechanical/electrochemomechanical transductions and transitions, employing molecular *fabrics*, etc. Correspondingly, we focused on the transformative science and engineering developments. However, the proposed concept, in general, cannot be manifested to be biomimetic-centered because it is highly unlikely that the proposed sensing and processing primitives and ^{N}hypercells guarantee functional similarity or operational equivalence to biomolecules and *natural* biomolecular aggregates. That is, *natural* biomolecular solutions, functionality and other basic features are entirely distinct. However, we typify topology and possible biophysics of *biomolecular fabrics*. A significant departure from conventional concepts is achieved providing a viable alternative inroads.

References

1. *International Technology Roadmap for Semiconductors*, 2009 Edition, Semiconductor Industry Association, Austin, Texas, USA, 2009. http://public.itrs.net/
2. J. E. Brewer, V. V. Zhirnov and J. A. Hutchby, "Memory technology for the post CMOS era", *IEEE Circuits and Devices Magazine*, vol. 21, issue 2, pp. 13-20, 2005.
3. J. Chen, T. Lee, J. Su, W. Wang, M. A. Reed, A. M. Rawlett, M. Kozaki, Y. Yao, R. C. Jagessar, S. M. Dirk, D. W. Price, J. M. Tour, D. S. Grubisha and D. W. Bennett, *Molecular Electronic Devices*, *Handbook Molecular Nanoelectronics*, Eds. M. A. Reed and L. Lee, American Science Publishers, 2003.
4. J. C. Ellenbogen and J. C. Love, "Architectures for molecular electronic computers: Logic structures and an adder designed from molecular electronic diodes," *Proc. IEEE*, vol. 88, no. 3, pp. 386-426, 2000.
5. Handbook on *Nano and Molecular Electronics*, Ed. S. E. Lyshevski, CRC Press, Boca Raton, FL, 2007.
6. J. R. Heath and M. A. Ratner, "Molecular electronics," *Physics Today*, no. 1, pp. 43-49, 2003.
7. J. M. Tour and D. K. James, *Molecular Electronic Computing Architectures*, *Handbook of Nanoscience, Engineering and Technology*, Eds. W. A. Goddard, D. W. Brenner, S. E. Lyshevski and G. J. Iafrate, pp. 4.1-4.28, CRC Press, Boca Raton, FL, 2003.
8. S. E. Lyshevski, *Molecular Electronics, Circuits, and Processing Platforms*, CRC Press, Boca Raton, FL, 2007.
9. *Natural Product Synthesis*, Ed. J. Mulzer, Springer-Verlag, Berlin, 2005.