Nanoscale Single-electron Switching Arrays for Self-evolving Neiromorphic Networks

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1. Introduction

The goal of this project was to start a multi-disciplinary study of molecular single-electron devices ("latching switches") and of possible use of 2D arrays of such switches for hardware implementation of adaptive ("plastic") neuromorphic networks. Preliminary estimates show that such networks may combine extremely high density (beyond 10^{12} functions per cm^2) and high speed (intercell communication latency below 100 ns) at acceptable power dissipation (below 100 W/cm^2). This gives every hope that eventually such networks will be able, after initial training, not only provide complex information processing including fast image recognition, but possibly reproduce the natural evolution of their biological prototype at time scale 4 to 5 orders of magnitude shorter.

The objective of the first stage of the project was to address two key issues of this remarkable opportunity:

(i) development of single-molecule, single-electron devices capable of chemically-directed self-assembly, and

(ii) development of neuromorphic network architectures enabling effective training without external access to an individual synapse.

The goal of this document is to give a brief overview of our progress in these two directions.

2. Single-molecule devices

Despite the spectacular recent progress in experimental demonstration of single-molecule electron devices [1] (including single-electron transistors), the methods of their fabrication still do not allow simultaneous self-assembly of billions of such devices, necessary for the implementation of VLSI circuits. The goal of our first effort in this direction was to develop such methods for relatively simple molecules that should function as single-electron transistors.

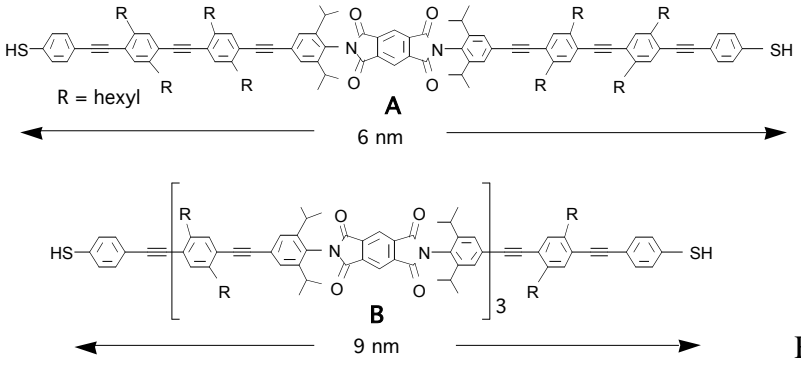


Fig. 1

Figure 1 shows the two molecules that have been synthesized for this purpose. The components of the molecules, oligo(phenyleneethynylene) molecular wires (including the thiol

groups for contacts to gold), and diimide groups have been selected because of their proven properties as molecular conductors [1] and electron acceptors [2]. The compounds have been synthesized in protected form as the diacetyl derivatives by a series of palladium-catalyzed ethynyl-iodoarene coupling reactions [1]. All intermediates and the final products were purified by chromatography on silica gel and identified by ^{1}H NMR and IR spectroscopy. For shorter intermediates, mass spectra were obtained as well. We have found that chains of type **B**, which contain several pyromellitimide groups, are chemically and thermally considerably more stable than chains of similar length that contain only a single pyromellitimide group, but longer phenyleneethynylene portions.

In order to test transport properties of these molecules, we have developed special gold nanowire structures, fabricated on SiO_2-covered silicon wafers by direct e-beam writing. Figure 2 shows an SEM picture of a sample where two gold nanowires, 15 nm thin and approximately 100 nm wide, are separated by ~4-nm gap. (So far, gaps between 7 and 9 nm are more typical for our samples). The deposition of molecules on nanostructures was performed from diluted solutions of the molecular compounds in tetrahydrofurane (THF). The electrical measurements are performed on an automated setup based on ultra-sensitive Keithley 6430 SourceMeter which allows measurements of very low currents (down to a few fA).

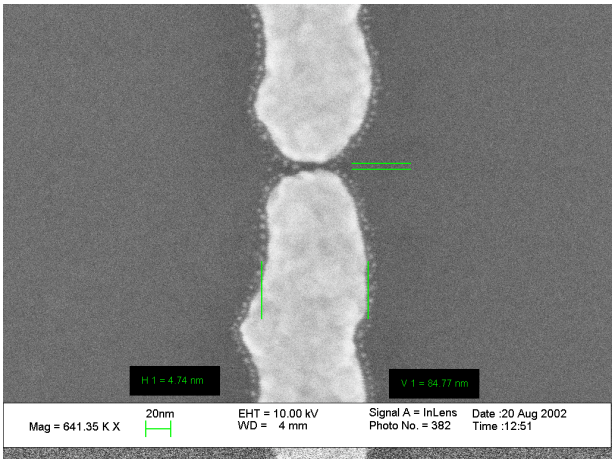


Fig. 2

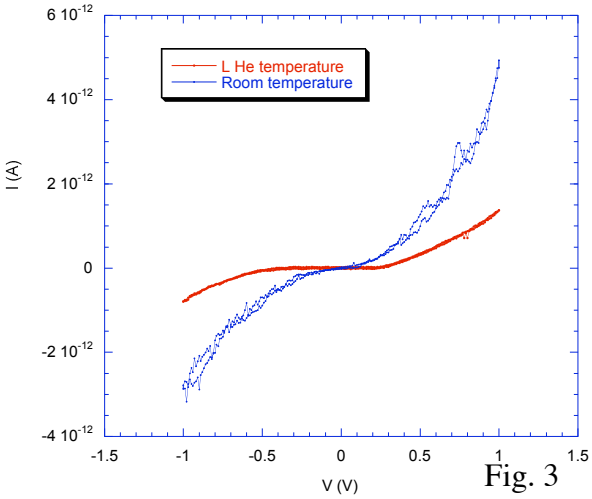


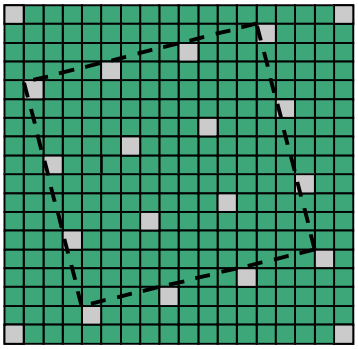
Fig. 3

We have succeeded to measure dc *I-V* curves of molecules after some depositions (see, e.g., Fig. 3), but at this stage the results are not quite reproducible. We are currently working on refining our nanowire cleaning and molecule deposition techniques, as well as on device gating (using conducting substrate as a back gate).

3. Architecture of neuromorphic networks with nanoscale components

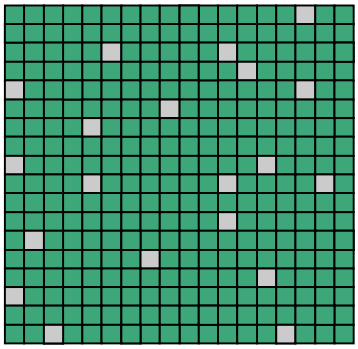
We have suggested a simple single-electron latching switch that may be implemented, in particular, using single-molecule devices [3, 4], and an architecture (dubbed *CrossNet*) for neuromorphic networks based on dense, rectangular 2D arrays of such switches connected by parallel systems on nanowires [5]. Figure 4 shows two basic versions of this architecture, for the case of non-Hebbian networks. The circuits are built on of a large field of synaptic plaquettes (green squares), each with 8 latching switches (Fig. 5a). (Hebbian networks use 32 switches per plaquette.) Each switch plays the role of a BiWAS (binary-weight, analog-signal) adaptive synapse that may connect or disconnect axonic wires (red arrows) and synaptic wires (blue

arrows), depending on the local activity of the network. The wires run to, respectively, outputs and inputs of somatic cells (gray squares in Fig. 4) that are essentially nonlinear differential amplifiers (Fig. 5b). Cell connectivity M in CrossNets is just the ratio of the number of synaptic and somatic plaquettes; since prospective applications will require $M >> 1$, the latter plaquettes may be relatively large and implemented using advanced (e.g., 45-nm-technology-node) CMOS circuits.



Inclined Distributed Crossbar ("*InBar*") architecture

Fig. 4a



Randomized Distributed Crossbar ("*RandBar*") architecture

Fig. 4b

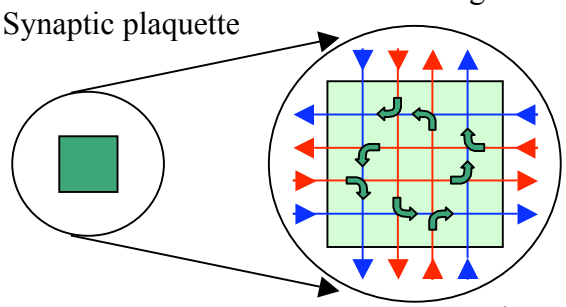


Fig. 5a

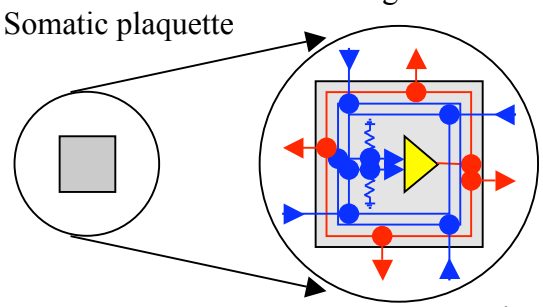


Fig. 5b

We have carried out extensive simulations of CrossNet properties using our new Beowulf-style 162-processor computer cluster *Njal* (purchased within the framework of DoD's DURINT program). As a result, the basic statistical properties of these networks have been already understood quite well. This has allowed us to proceed to the development of CrossNet training procedures. The main challenge here is the absence of external access to individual synapse, making it impossible to use such well developed neural network training techniques as backpropagation.

We have suggested training procedures for two modes of CrossNet operation:

(i) as a Hopfield network (essentially, an associative memory), and

(ii) as continually running network trained in runtime.

So far, only the first of these procedures has been confirmed by numerical simulations, with very good results. The work on the second, practically much more important, option is in progress.

4. Education and Outreach

So far, the project has involved 5 graduate students (Y. Gao, X. Liu, Q. Zao, I. Muckra, and O. Turel), a full-time undergraduate student (N. Simonian), an undergraduate minority summer student (N. Saint-Fleur) and a summer high school student intern (T. Feldman). We feel that the work in such a multi-disciplinary team allows these students to overcome inter-departmental barriers in their education.

References

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[2] W. B. Davis,; M. A. Ratner, and M. R. Wasielewski, "Dependence of electron transfer dynamics in wire-like bridge molecules on donor-bridge energetics and electronic interactions", Chem. Phys. **281,** 333 (2002).

[3] S. Fölling, Ö. Türel, and K. Likharev, "Single-Electron Latching Switches as Nanoscale Synapses". In*: Proc. of the Int. Joint Conference on Neural Networks* (Int. Neural Network Society, Mount Royal, NY, 2001), p. 216.

[4] S. Fölling, Ö. Türel, and K. Likharev, "Self-Evolving Neuromorphic Networks with Single-Electron Switching Latches as Synaptic Nodes". In*: Proc. of the 15th Eur. Conf. On Circuit Theory and Design*, vol. 1 (Helsinki Univ. of Technology, Espoo, Finland, 2001), p. I-177.

[5] Ö. Türel, and K. Likharev, "CrossNets: Possible Neuromorphic Networks Based on Nanoscale Components". Accepted for publication in Int. J. of Circuit Theory and Applications **31**, No. 1 (2003); preprint available at http://rsfq1.physics.sunysb.edu/~likharev/nano/Preprint070102.pdf.

[6] Further information about this project may be obtained at the following Web sites:

- general description: http://rsfq1.physics.sunysb.edu/~likharev/nano/SELINA.htm,
- dynamics of Hopfield-mode image recognition by Hebbian InBar (short movies):
  http://hana.physics.sunysb.edu/neural/Hopfield_Single_Image/text.gif,
  http://hana.physics.sunysb.edu/neural/Hopfield_Single_Image/cameraman.gif,
  http://hana.physics.sunysb.edu/neural/Hopfield_Single_Image/testpat1.gif,
- Njal supercomputer cluster: http://njal.physics.sunysb.edu/,

or directly from Prof. K. Likharev (klikharev@notes.cc.sunysb.edu, phone 631-632-8159).