Molecular Wires and Logic Circuits Integration in a Single Molecule?

Christian Joachim

Molecular Nanosciences & Picotechnology Group
CEMES-CNRS
29, Rue J. Marvig BP 4347 31055 Toulouse Cedex France

ABSTRACT

Hybrid Molecular electronics do not offer good perspectives for miniaturization because (a) the interconnection length between 2 molecular devices must sufficient for Kirchhoff laws to be applicable and (b) the molecular self-assembly process will not position millions of molecules, with a correctable defect rate. We describe our progresses starting from our understanding of the tunnel transport phenomenon through a molecular wire. The differences between saturated, conjugated molecular wires and atomic wires will be exposed.

Keywords: molecular wires, logic circuits, integration, single molecule, hybrid molecular electronics

1 INTRODUCTION

Hybrid Molecular electronics (one molecule per device) do not offer good perspectives for miniaturization on the long term because (a) the interconnection length between 2 molecular devices must be at least a few 10 nm on the circuit for the Kirchhoff laws to be applicable and (b) because the molecular self-assembly process will not be able to position at a good place millions of molecules, one molecule per device, with a defect rate able to be well corrected by hardware or even software compensation techniques.

At the nanoscale, the full integration of a calculator inside a molecule will demand all the power of the quantum states superposition to run the quantum machine. To design a quantum computing nano-machine, the trend (1) is to design a super molecule integrating a spatial intramolecular electronic circuit by mastering the electronic super-exchange mechanism. The trend (2) is to structure the molecules in qubits leading to time circuits.

We describe our progresses towards trend (1) starting from our understanding of the tunnel transport phenomenon through a molecular wire. The differences between saturated, conjugated molecular wires and atomic wires will be exposed.

Circuit rules for "in series" and "in parallel" bonding of molecular wires groups to form a longer molecular wire or a molecular circuit are also discussed. They differ from the well known G. Kirchhoff electrical circuits laws which are normally applicable for the standard scale and mesoscopic Wheatstone bridges presented fig. 1a and 1b but not for the molecular Wheatstone bridge presented fig. 1c.

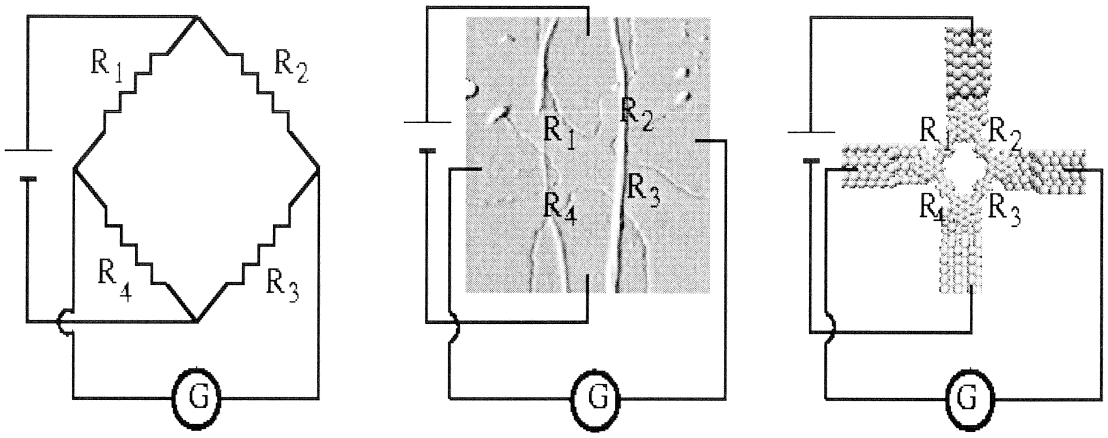

Figure 1: The different scale of a Wheatstone bridge: (a) standard, (b) mesoscopic with SWCNT and (c) made of a single molecule.

Using modified circuit laws to take into account intramolecular quantum behaviours and a special mono-molecular circuit simulator based on the N-ESQC extension of our 2 electrodes Elastic Scattering Quantum Chemistry Calculation (ESQC), simple OR and AND gates integrated inside a single molecule have been designed as presented in fig. 2 and 3.

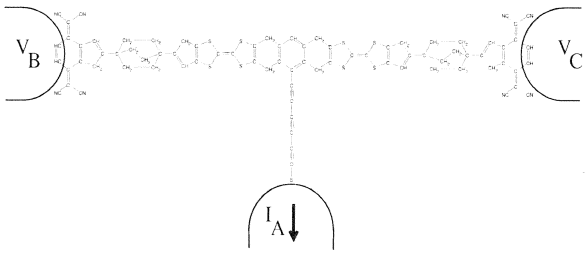

Figure 2: The molecular model of a mono-molecular OR gate.

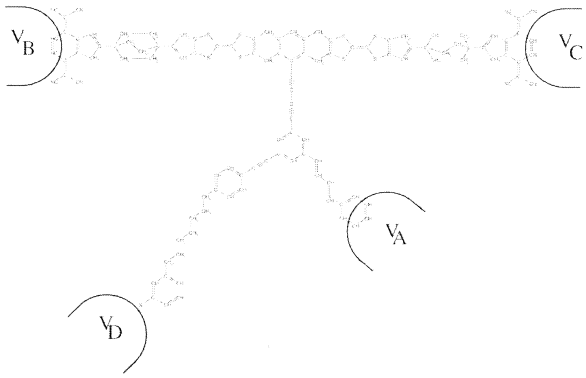

Figure 3: The molecular model of a mono-molecular AND gate.

All the multi-electrodes and multi-channels scattering properties of these 2 molecular logics have been calculated in detail together with their logic response. We will point out our difficulties to design larger intramolecular logic circuit in the spatial domain and advocate a mixed approach between technology (1) and (2).

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