Quantum cellular automata: computing with molecules

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The purpose of this lecture is to present in an accessible form the concept of molecular quantum cellular automata (QCA), a paradigm for nano-electronics, in which binary information is encoded in charge configuration of the quantum dots. The QCA devices promise nanometer-scale logic gates with ultra-high device densities operating at very high switching speed and room-temperatures, consuming extremely small amounts of electrical power and small heat release. Important, that the action of QCA devices is not restricted by the requirement of quantum coherence which is a difficult condition. Alternatively, the redox sites of a mixed-valence molecule can act as a molecular cell. The area of molecular QCA became a part of molecular magnetism being at the same time at the border between chemistry, physics and material sciences.

I will review the basic issues of the field and present the theoretical background in an accessible way for the charge polarized states in the four-site molecular QCA, based on the vibronic approach in mixed-valency. These include: 1) analysis of the electronic levels and adiabatic potentials of mixed-valence systems for which molecular implementations of QCA was proposed. The cell includes two electrons shared between four sites and correspondingly we employ the model which takes into account the relevant electron transfer processes as well as the Coulomb energies for different instant positions of localization; 2) the adiabatic potentials are evaluated for the low lying Coulomb levels in which the antipodal sites are occupied, the case just actual for utilization in molecular QCA. The conditions for the vibronic self-trapping in spin-singlet and spin-triplet states are revealed in terms of the actual transfer pathways and strength of the vibronic coupling; 3) then the strongly non-linear cell-cell response function is discussed in the framework of the vibronic approach; 4) along with the semiempirical study (based on the Hubbard-like Hamiltonians) we report the quantum-chemical analysis of the series of organic compounds as candidates to act as molecular cells in QCA: 1,4-dithia-compound with two S-atoms connected by saturated carbon bridge CH₂CH₂ and the
corresponding tetrameric structures of the crown ethers 1,4,7,10-tetrathio-cyclododecane as parent neutral molecule, cation and dication radicals playing role of a square-planar bi-hole cell. Quantum-chemical evaluations allowed us to estimate the key parameters of the two kinds of molecular cells.

Finally, I will describe a new concept within the general trend of molecular implementation of QCA. As distinguished from the previous ideas in the molecular QCA area, in which a molecule was supposed to act as a quantum cell, the proposal reported here employs a molecule as a logical gate. Within this concept a molecule can not only encode the binary information, but also proceed information. I will demonstrate molecular design of the logic gates, such as inverter, fanout, majority gate in one molecule. Quantum-chemical modeling of the porphyrins family shows that this goal can be reached through the computer design of molecular structures.

The details of the theoretical studies of molecular QCA can be found in following references: