A paradigm of quantum cellular automata: implementation of molecular magnets

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The concept of molecular quantum cellular automata (QCA) represents a paradigm for nano-electronics, in which binary information is encoded in charge configuration of the redox sites in a molecular magnetic mixed-valence cell. These devices promise nanometer-scale units with ultra-high device densities operating at very high switching speed, at room-temperatures, consuming extremely small amounts of electrical power and very small heat release. The area of QCA is, therefore, placed at the border line between chemistry, physics and material science and constitutes a fascinating field of molecular magnetism. We review the basic issues of the field and present the theoretical background [1-4] for the charge polarized states in the four-dot molecular QCA, based on the vibronic approach in mixed-valency. We report the evaluation of the electronic levels and adiabatic potentials of mixed-valence tetrameric 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 two relevant electron transfer processes (through the side and through the diagonal) as well as the Coulomb energies for different instant positions of localization of the pair. 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 two actual transfer pathways parameters and the strength of the vibronic coupling.

A new concept is discussed within the general trend of molecular implementation of QCA. It is proposed to employ complex polyoxometalate (POM) anion $[V(IV)_8\ V(V)_4\ As_8O_{40}(H_2O)]^{4-}$ (briefly V_{12}) as a quantum inverter. As distinguished from previous ideas in molecular QCA area, in which a molecule was supposed to act as a quantum cell, the proposal reported here employs POM V_{12} as a logical gate. We estimate the Coulombic forces in the different electronic distributions within the mixed-valence $V(IV)_2\ V(V)_2$ network, reveal the role of the electron transfer processes and vibronic coupling. The switching cycle and the non-linear cell-cell response function which are just the key characteristics of QCA inverter, are studied.

References:

[1] B. Tsukerblat, A. Palii, J.M. Clemente-Juan, Pure & Appl. Chem. **87**(3), 271 (2015).
[2] B. Tsukerblat, A. Palii, J.M. Clemente-Juan, E. Coronado, J. Chem. Phys. **143** 134307 (2015).
[3] J.M. Clemente-Juan *et al.*, J. Chem. Theory Comput. **12**, 3545 (2016).
[4] A. Palii, B. Tsukerblat, J.M. Clemente-Juan, E. Coronado, J. Phys. Chem. C. **120**, 16994 (2016).

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