Spin effects in molecular quantum cellular automata

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The systems we focus on are the square planar mixed-valence (MV) clusters regarded as molecular cells in quantum cellular automata (QCA), which act as current-free alternative to the traditional CMOP electronics.

In almost all studies dealing with QCA only charge degrees of freedom have been analyzed. Recently we have demonstrated [1] that by polarizing one of the cells acting as a ”driver-cell” one would be able not only to polarize the neighboring (‘‘working”) cell but also under some conditions to switch the ground state from the spin-singlet to the spin-triplet. The proposed electronic model of the cell includes the three parameters, which are the two transfer parameters t_n and t_d describing the one-electron transfer processes occurring along the sides and along the diagonals of the molecular square and the Coulomb energy gap U between the diagonal-type and the side-type charge configurations. The considered most topical case is that of strong Coulomb interaction when $U >> t_n$, t_d . By evaluating the effect of the neighboring driver cell on the ground spin-state of the working cell we have demonstrated that in the range of parameters $0 < t_d/U < 1/4$ strong enough electrostatic field of the driver cell can induce spin-switching from S = 0 to S = 1.

Another class of molecules we discuss includes the MV molecular squares in which electronic pair is delocalized over four paramagnetic centers (“spin cores”). The detailed analysis of the cell based on the transition-metal tetramer of the type of $d^2{-}d^2{-}d^1{-}d^1$ [2] shows that depending on the relative strength of the double exchange and the Heisenberg−Dirac−Van Vleck exchange the ground state can be either localized spin-triplet or delocalized spin-singlet. Due to different sensitivities of these states to the electrostatic field of the driver cell, the latter is shown to produce switching between different spin-states.

Therefore, by combining the ideas related to seemingly completely different areas of the QCA-based molecular electronics and the molecular spintronics, one can, in principle, create multifunctional device with such two beneficial functions as the cell–cell response and the spin switching.

The work was performed with funding from the Ministry of Science and Higher Education of the Russian Federation (Grant No. 075-15-2020-779).

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