On the Search of Novel Molecules Demonstrating Quantum Cellular Automata Properties. A Theoretical Approach

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The molecular quantum-dot cellular automata (QCA) approach is a new computing paradigm in which binary information is encoded by the charge configuration of redox-active molecules. QCA computing can be achieved by arranging these molecules (individual cells) on a substrate and exploiting intermolecular Coulombic coupling. Importantly, no current flow between molecules is required. The simplest molecular QCA cell is a symmetric mixed-valence complex in which the binary states are represented by the location of a mobile electron at one metal center or the other. It has been shown, however, that four-metal molecular QCAs cell are more advantageous because such molecules would be more versatile building blocks for constructing logic units than two-metal cells. Consequently, some attempts to design ‘square’ molecules with two stable charge configurations suitable for representing binary information have been performed.

We have ourselves theoretically examined a series of real or hypothetical “four-dot” and “two-dot” organometallic compounds to address important questions for QCA. Some recent results will be discussed.

Biography

Professor Jean-François Halet is Research Director at the National Center for Scientific Research (Centre National de la Recherche Scientifique, CNRS) in France. His research centers on the understanding of the chemical bond in transition metal inorganic chemistry. He uses a variety of quantum chemical computational tools including Density Functional methods to tackle problems of electron-counting, structure, physical properties and reactivity of both molecular and solid state systems. He is the author of 262 books, chapters of books, papers and reviews and currently a member of the editorial boards of Polyhedron and Journal of Cluster Science.