Bis-ferrocene molecules for QCA : a write-in method

# Bis-ferrocene molecules for QCA : a write-in method

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Quantum-dot Cellular Automata (QCA) is a new paradigm for digital computing that, theoretically, allows very high operating frequency and significant power consumption reduction [1]. According to the Lent theory [2], a possible implementation of a QCA cell could be physically obtained with a molecular system with two or more redox-centers, where the charge configuration encodes the binary information and the electrostatic repulsion provides the device-device interaction. Ideal molecular systems have been studied [3, 4], while we present a method to use a bis-ferrocene molecule (Fig. 1) [5] synthesized ad hoc to implement a QCA device with two redox-centers (represented by the ferrocenes): they are separated by a central carbazole bridge, that provides the isolation between the two dots. Though not conductive, this molecule can be influenced by an external electric field in order to change its internal state (HOMO), encoding thus the "0", "1" and NULL logic value. From an ab initio analysis, the HOMO of this molecule in its ground state is de-localized along the molecule and mainly on the carbazole (Fig. 1A). Applying an electric field along the x axis, we force a "1" or "0" state (Fig. 1B and 1C, respectively) obtained by the HOMO localization around one of the two ferrocenes. An electric field applied along the y axis has the effect of localizing the HOMO on the carbazole, forcing the molecule into a NULL state. We found that an electric field in the same direction but with opposite sign localizes the HOMO around the two ferrocenes, enhancing the molecule sensitivity to assume one of the two logical states in presence of a driver (a neighbour identical molecule). These results are important for what concerns the clock issues [6]. The applied electric field is of the order of 1 V/nm and could be easily obtained with a nanogap of about few nanometres: we are investigating the possibility to use this nanostructure in combination with conductive molecules for the read-out of the QCA cell state.

References

(1) C. S. Lent, P. D. Tougaw, and W. Porod, *IEEE PhysComp '94*, **1994**, pp- 5-13.
(2) C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, *Nanotechnology*, **1993**, *Vol. 4*, pp. 49–57.
(3) B. Isaksen, C. S. Lent and M. Lieberman, *J. Am. Chem. Soc.* **2003**, *Vol. 125*, pp. 1056–1063.
(4) C. S. Lent and B. Isaksen, *Electron Devices, IEEE Transactions on, **2003**, Vol. 50*, pp. 1890–1896.
(5) L. Zoli, *PhD Dissertation*, Università di Bologna, **2010**.
(6) V. Vankamamidi, M. Ottavi, and F. Lombardi, *IEEE-NANO 2006*, **2006**, *Vol. 1*, pp 343–346.

Figures

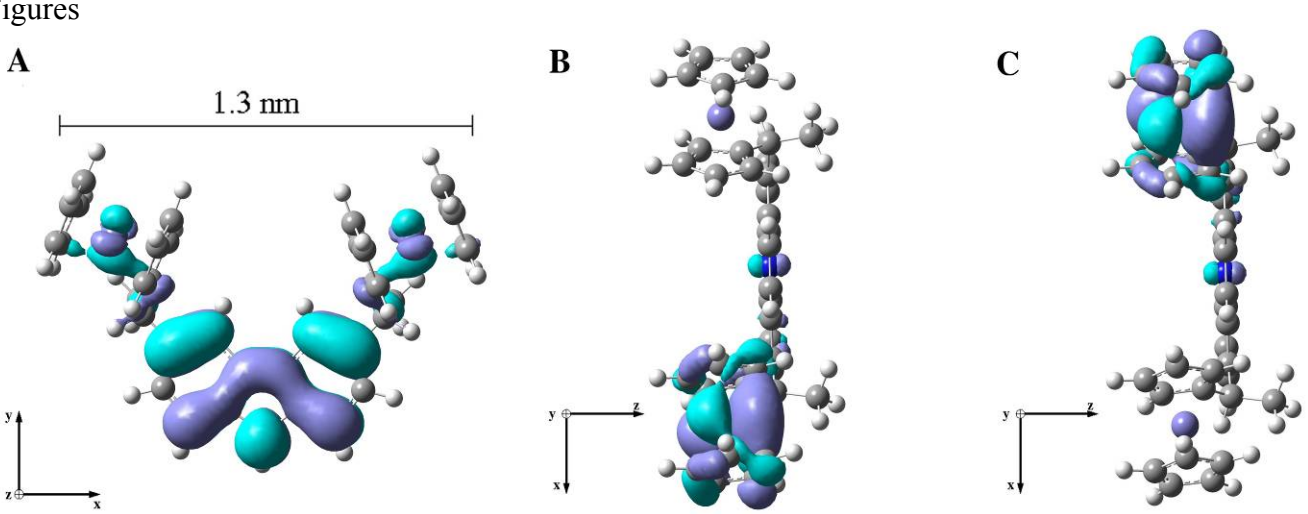


Figure 1. Bis-ferrocene QCA molecule: ground state HOMO (A); HOMOs of logical state "1" (B) and "0" (C).