System level bistability of molecular Field-Coupled Nanocomputing

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Abstract:

Chemists and physicists have investigated and demonstrated through simulations the possibility of exploiting redox centers to aggregate charge in precise regions of oxidized molecules. This property allows the information encoding and enables the information transfer, via electrostatic interaction, through ordered sequences of molecules. This evidence makes the implementation of molecular Field-Coupled Nanocomputing (FCN) possible[1]. The natural nanometric size of molecules and the absence of charge transport highlight molecular FCN as a possible technology for the future low power digital electronics. Our work consists in providing a methodology for the analysis, the design and the fabrication of molecular FCN devices, moving the focus from the single molecule, which has been already deeply discussed in the literature, to the molecular system. We develop an efficient model for studying systems of molecules organized as logic units, reducing the computational cost of ab initio simulations at the system level and keeping the chemical and physical properties of the assembled molecules.

More specifically in this work, we characterize the single molecule through DFT analyses and we use the results to analyze the capability of a molecular FCN wire to propagate digital information (Fig 1A). A self-consistent algorithm[2] based on the aggregated charge[3,4] (evaluated from the electrostatic potential surfaces) is used to model the electrostatic behavior of the molecules. It provides quantitative results about the information propagation and the energy associated with the electrostatic interaction among molecules (Fig 1B). We demonstrate the bistability of the molecular cell when inserted in a molecular system: it retains the digital information when the polarization of an input molecule is varied (Fig 1C). The bistability is enhanced by increasing the number of molecules in the wire and shortening the intermolecular distance (i.e. by strengthening the electrostatic interaction).

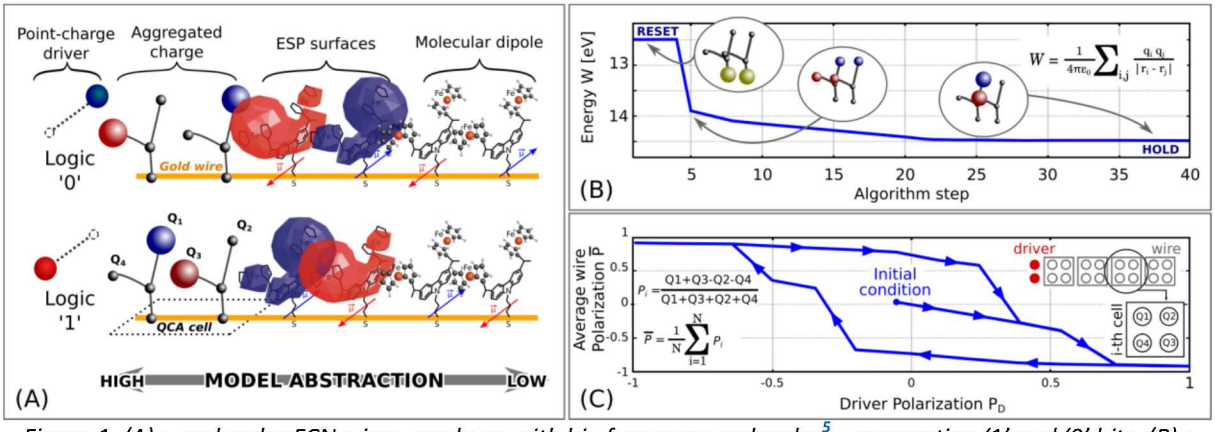

Figure 1. (A) : molecular FCN wires, made up with bis-ferrocene molecules[5], propagating '1' and '0' bits. (B) : Electrostatic Energy trend among molecules in a wire when polarizing (from RESET to HOLD state). (C) : average polarization of cells in an FCN wire composed of 8 molecules with 1.0 nm intermolecular distance.

References:

[1] C.S. Lent et al., 10.1021/ja026856g, JACS, **2003**. [2] R. Wang et al., 10.1109/NMDC.2016.7777166, IEEE-NMDC, Toulouse, **2016**. [3] A. Pulimeno et al., 978-3-662-43722-3_13, Springer ISBN 978-3662437223, **2014**. [4] Y. Ardesi et al., 10.3390/jlpea8030024, JLPEA, **2018**. [5] V. Arima et al., 10.1039/C1NR10988J, Nanoscale, **2012**.