# Modeling and analysis of molecular technologies for the implementation of Field-Coupled Nanocomputing

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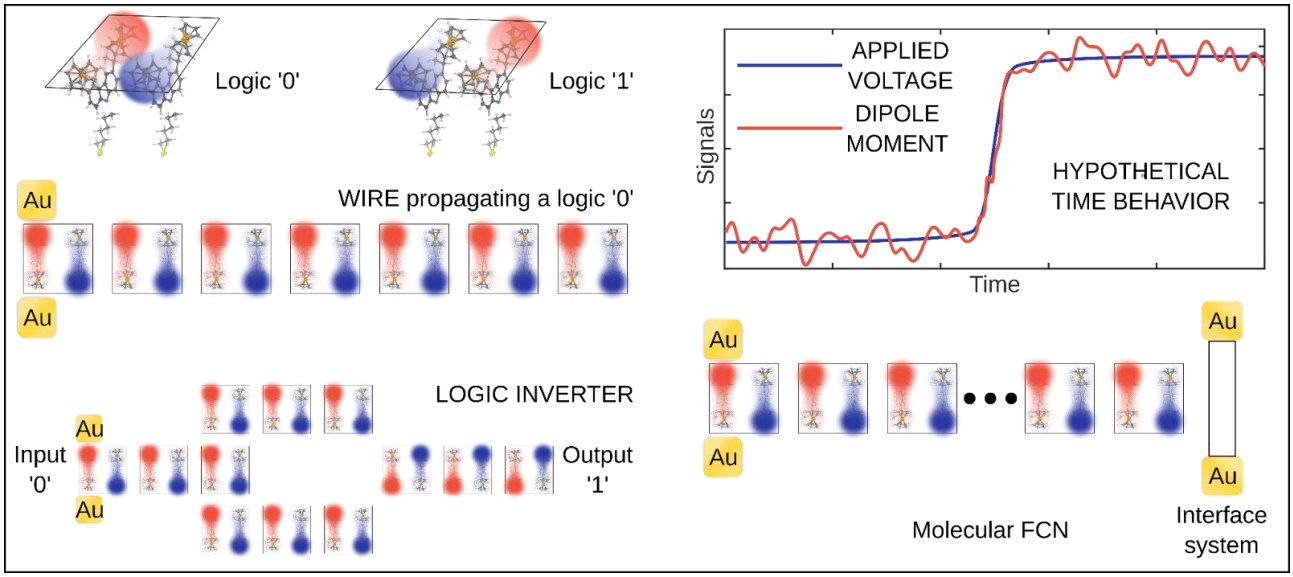
In recent years, researchers proposed different technologies to face the current demand for ultra-scaled electronic devices. Molecular Field-Coupled Nanocomputing (FCN) is a beyond-CMOS technology that encodes the logic information in the aggregated charge of redox centers of ad-hoc synthesized molecules [1]. Neighboring aligned molecules interact differently depending on their particular electrostatics [2]. Moreover, thanks to Coulomb's repulsion force, it is possible to propagate information or design logic gates. The main advantages of this technology are the high device density per unit area and the ultra-low power consumption since no currents are involved. Moreover, the Coulomb's interaction between neighboring molecules is strong enough for molecular FCN to operate at room temperature [3]. The molecular FCN implementation also offers the possibility to exploit self-assembly techniques. Nevertheless, the need for precise nanopatterned structures slows down the possibility of obtaining a working prototype. A recent result demonstrated the possibility of performing molecular FCN computation on a uniform self-assembled monolayer, though some challenges still must be addressed [4]. Another crucial aspect to consider is the need to measure the charge on a molecule to transduce it into an electrical quantity and enable the interface with conductive electronics.

More specifically, we concentrate on the computational assessment of the molecular FCN to extract useful indications before realizing a working prototype. In our group, we concentrate on mainly two aspects. On one side, we are developing a framework to perform architectural-level simulations of devices implemented in molecular FCN. On the other side, we perform *ab initio* simulations to improve the model description of a single molecule. Indeed, in molecular technologies, it is fundamental to define simple behavioral models that allow the simulations of complex circuits. It is also essential to include all the physical characteristics in the model to obtain precise predictions. One fundamental aspect on which we are currently working regards the dynamic molecule behavior, so we are simulating molecules in the time domain to precisely describe how molecules react to applied electric fields. Indeed, the molecules dynamics characterization will give us essential parameters for electronic devices. Still related to molecular modeling, we are also investigating the possibility of reading the charge distribution on these molecules by interfacing them with conductive systems. We are also currently working to adapt the paradigm to simplify the realization of a prototype and the output measurement, both at the circuital level and the prototypal level with charge measurements, eventually exploiting scanning probe microscopy techniques.

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