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Thesis abstract

Modeling and Simulation Strategies for Advancing Molecular FCN

Pioneering Design Rules Toward Implementation from Molecules to Devices

Molecular Field-Coupled Nanocomputing (molFCN) represents a paradigm shift in computational technology, exploiting the unique properties of molecules to revolutionize information processing. In this paradigm, information is encoded in the charge distribution on suitable molecules, and propagation is sustained by Coulomb's force through electrostatic coupling. Logic elaboration is obtained by positioning molecules according to specific layouts. Being a current-less paradigm, molFCN offers extremely low-power and high-frequency operations. Compared to other implementations, having molecules as unit elements offers the advantage of working at room temperature. Despite these noteworthy advantages, obtaining a working prototype requires effort in multiple research areas, slowing down the development of the technology over the last two decades.

This thesis aims to facilitate the future development of experimental validations and a working prototype. It explores different characteristics of the technology with the goal of defining design rules and properties for molecules and circuits, driving future research on the topic.

The proposed goal is addressed by decomposing the problem into subsequent abstraction levels, each one based on the previous finding, and hiding the non-relevant details as a matryoshka. Each abstraction level requires its own theory and simulation tools.

The first layer is composed of molecules, being the unit elements. This work analyzes various candidates and defines a set of parameters identifying the behavior to be provided to chemists to drive ad-hoc syntheses. Adopting DFT simulations and the MoSQuiTo methodology, this work also analyzes a case study to investigate the direct effects of multiple molecular modifications on its electrostatic behavior.

Based on the analyses performed in the previous layer, the second step treats molecules as simplified electrostatic devices composed of a set of point charges. This modeling enables the study of molecule ensembles through the application of electrostatic fundamentals and the SCERPA simulator. The work analyzes the fundamental interactions found in molFCN devices using different electrostatic molecular footprints to test their impact. Consequently, the design of tailored molecular transcharacteristics enables the successful realization of new functions, such as a fully electrostatic solution for in-plane information crossover.

As an outer layer, this work proposes a methodology to model entire logic gates and develops an automatic tool named BBchar to create a library comprising the input/output behavior of fundamental gates and interconnections. The possibility to simulate circuits composed of multiple gates without focusing on the internal behavior of each of them enables a strong simulation speed-up, moving from hours or days down to a few milliseconds. Moreover, the proposed methodology is designed to consider the actual physical behavior of the technology, resulting in a 99.99% accuracy of the proposed model.

The final point of the present work proposes a modification of the paradigm that aims to simplify the reading of the information at the laboratory level and on-circuit data conversion. The paradigm has been named bend-boosted molFCN to highlight the property of including molecule bending in the charge-encoded information. Through DFT and dynamic simulation, this work demonstrates its correct working principle, and the offered read-out capabilities.

Overall, this thesis contributes to the advancement of molFCN technology by providing insights into molecular behavior, developing efficient simulation methodologies and tools, and proposing innovative device architectures that simplify data sensing and conversion. It lays the groundwork for future research in this field and offers a pathway toward the unprecedented realization of a working prototype.