

Advancing Molecular-Field Coupled Nanocomputing Actualization: Unifying Device Fabrication, Molecular Modelling, and Integration Strategies

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Abstract

Since the introduction of CMOS technology, digital electronics has experienced extraordinary growth, establishing itself as the dominant paradigm of computation for decades. Yet, as devices continue to shrink and performance demands intensify, CMOS is approaching its fundamental physical and economic limits. This has prompted the exploration of alternative technologies capable of ensuring scalability, energy efficiency, and high speed. Among these emerging approaches, Molecular Field-Coupled Nanocomputing (MolFCN) stands out as a promising candidate, offering the possibility of charge-less information propagation through the electrostatic interactions between polarized molecules. By leveraging the intrinsic nanoscale dimensions, room-temperature stability, and charge localization capabilities of molecular systems, MolFCN holds the potential to enable ultra-dense and energy-efficient logic architectures.

Despite this promise, MolFCN remains at a theoretical stage, with no experimental prototype demonstrated to date. This thesis addresses the fundamental challenges that currently prevent the transition of MolFCN from theoretical models to practical implementation, and proposes a systematic framework encompassing molecular design, device engineering, fabrication strategies, and read-out solutions.

A first challenge lies in the design of realistic device architectures that can host molecular cells and provide the input fields essential for MolFCN operation. Idealized structures often fail to capture the complexity of real substrates and field distributions. To overcome this, the thesis introduces the MoSQuiTo framework, which combines finite-element simulations of device fields with molecular- and circuit-level models. Through progressive refinement, three possible device architectures are proposed and analyzed, providing a device-aware environment in which the molecular responses can be faithfully embedded. Consequently, the fabrication of suitable devices for MolFCN is preliminary addressed. Bridging the gap between conceptual device designs and physical prototypes requires the use of established nanofabrication processes. The thesis presents preliminary steps toward this goal, including substrate preparation and dielectric trench fabrication via

atomic layer deposition and electron beam lithography. These efforts highlight both the feasibility and the technological bottlenecks in moving toward experimental realization.

The central challenge concerns the identification and validation of suitable molecular candidates. Molecules must not only exhibit stable charge localization and tunable dipolar responses under applied fields, but also be synthetically accessible and sustainable. To address this, the thesis develops a methodology that goes beyond conventional electronic structure approaches, integrating conformational sampling, perturbation-based charge clustering, and time-dependent simulations to evaluate candidate molecules under realistic conditions. The framework enables the extraction of semi-static input–output characteristics of the candidate molecule and their integration into circuit-level simulations, thus providing a direct bridge between quantum-chemical properties and information propagation.

Finally, the thesis addresses the problem of interfacing and read-out, which is essential for validating MolFCN operation and integrating it with conventional technologies. Two possible strategies are investigated: single-molecule junctions, which allow direct electrical access to the dipole states of individual molecules, and suspended semiconductive graphene nanoribbons, which offer a platform for collective read-out of molecular arrays. Both approaches are analyzed as potential routes to hybrid integration with CMOS, thereby opening paths toward system-level applicability.

In summary, this thesis presents a comprehensive framework to advance MolFCN from a theoretical paradigm toward experimental feasibility. By systematically combining molecular design, device simulation, fabrication strategies, and read-out concepts, it demonstrates that the evaluation of candidate molecules can be standardized, device architectures can be realistically modeled, and initial fabrication and read-out routes can be established. Although a complete prototype has yet to be realized, the results presented here represent a significant step forward, providing both theoretical and technological foundations for the implementation of MolFCN in future nanoelectronic systems.