THE UNIVERSITY OF CHICAGO | THE COMMITTEE ON COMPUTATIONAL AND APPLIED MATHEMATICS

Dissertation Defense:

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"Computational methods for materials science with applications in next-generation computing architectures"

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ABSTRACT

Computing performance is constrained by the properties of the materials used to store, transmit, and manipulate information. For decades, improvements in silicon semiconductor technologies enabled rapid growth in computing capability through device scaling. However, as device dimensions approach atomic length scales, quantum tunneling, leakage currents, variability, and thermal dissipation increasingly limit computing performance and energy efficiency. These physical limits motivate the development of alternative computing paradigms, such as low-power multiferroic spintronics and quantum computing, whose realizations depend on discovering and engineering materials with specific functional properties. Computational materials science using classical computing is a powerful tool for identifying and characterizing such materials over a combinatorially large space, but efficient computational screening and characterization methods must be accurate, scalable, and effective with limited or noisy data. This thesis develops physics-informed computational algorithms that enable high-throughput computational screening and experiment-coupled characterization of materials for next-generation computing hardware. First, I introduce an automated and scalable implementation of Berry flux diagonalization to compute spontaneous polarization in insulating materials. This method enables robust high-throughput computational screening of candidate ferroelectric materials for applications in multiferroic spintronics. Second, I develop and validate a data-efficient numerical inference framework to reconstruct nuclear spin environments surrounding spin-defects from sparse, noisy data, enabling rapid experimental characterization of spin-defects for use as qubits. Finally, I demonstrate how this framework can guide high-throughput experimental design and establish sensing limits for spin-defect characterization. Together, these contributions provide a set of computational tools that integrate simulation, inference, and experiment to accelerate materials discovery for emerging computing architectures.