Pacific Northwest
NATIONAL LABORATORY

PNNL-38450

QUCODE

End-to-End Qubit Co-Design

September 2025

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U.S. DEPARTMENT of ENERGY

Prepared for the U.S. Department of Energy
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1.0 Introduction

Designing a quantum computer is a complex task that requires world-class expertise in material science, quantum chemistry, and computer science. Today, the different aspects of such an enterprise are often pursued in isolation: Material scientists pursue novel molecular structures and dopants to build qubits with high decoherence times, often without taking into account the environment that such qubits would operate in, which affects noise levels and ease of construction. On the other end of the spectrum, computer scientists develop algorithms that are simulated on idealized hardware, disregarding effects from physical systems that may impact the performance of the algorithm.

1.1 Considerations for qubit design

An important consideration in designing materials for building qubits is the decoherence of the qubit's spin states due to interactions of the qubit with other qubits or with its environment. Scientists distinguish between two characteristic times, the relaxation time T_1 and the dephasing time T_2, where $T_2 \leq 2T_1$. In the following we limit our considerations for effects that limit qubit capabilities to those affecting T_2.

A quantum computer can be thought of in terms of the layers shown in Figure 1. A goal of an end-to-end design approach is to understand the interfaces between the different layers, so that on can design an optimal hardware system for a desired application and vice versa create algorithms and applications that take optimal advantage of provided hardware.

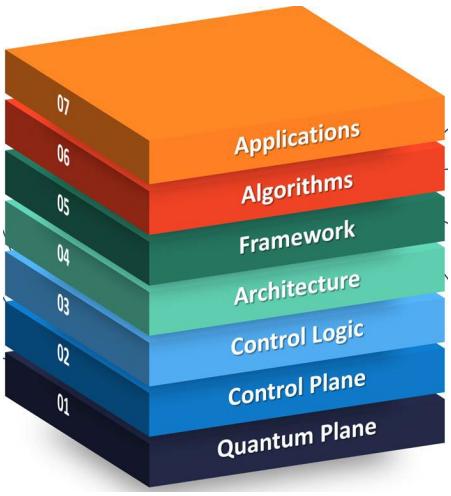

Figure 1 Conceptual Layers of a Quantum Computing System

In the following, we summarize knowledge gaps and opportunities for an increased footprint in the research of quantum computing systems.

2.0 Design Considerations

Research related to the conceptual layers presented in Figure 1 is often conducted in isolation. Here we focus on knowledge gaps that are related to the interfaces between the layers, specifically between the quantum plane, architecture, and applications.

2.1 Materials

Since the performance of a quantum computing application depends significantly on the interaction of the qubit with a host material, both must be chosen carefully to optimize T_2.

2.1.1 Qubit Candidates

PNNL has deep expertise in a class of materials that could be suitable candidates for qubit design, Polyoxometalates (POMs) [1]. These could be used to form molecular qubits that can be synthesized in PNNL lab spaces and arranged to form a quantum device using in-house capabilities such as ion soft landing (e.g., [2]). With these capabilities, fine control of materials can be applied to design for specific properties. Baldinelli et al. developed design rules to engineer the spin structure of a molecular qubit [4], specifically to control the Zero Field Splitting (ZFS). This property is correlated with the decoherence time T_2, and an investigation into similar design rules for POMs is a promising research direction.

2.1.2 Host Materials

In a physical material, qubits interact with their environment, so designing a good host matrix, requires solving To design a good host matrix, one has to compute the time evolution of the spin Hamiltonian $H = H_S + H_B + H_{(S-B)}$, where H_S is the electron spin, H_B is the bosonic bath, $H_{(S-B)}$ is the interaction term. Kanai et al. have developed an algorithm to scan over 12,000 host materials [4], using cluster correlation expansion. They found good agreement between their predictions and experiments. Their approach to scanning material should be extended to materials relevant for designing POMs and POM assemblies. Additionally, some assumptions in their work simplifies calculations, but presents significant experimental challenges, such as operating in an environment with a magnetic field of B = 5 T.

2.1.3 Contributing factors to spin decoherence

A main contributor to spin decoherence in physical materials is via spin—phonon coupling. The research in this area [5-8] is currently hard to integrate into quantum simulators. We have done some preliminary studies of how to integrate a molecular dynamics software package (LAMMPS), with a quantum simulator (qiskit), to combine quantum-mechanical computations with a realistic phonon spectrum. This would allow incorporating a realistic noise model into those calculations and to respond to physical changes of the system during computations.

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