Quantum Science and Technology Mini-Symposium
Room 208 W - Session QS1-TuM

Quantum Simulations and Quantum-Inspired Technologies

Moderator: Andre Schleife, University of Illinois at Urbana-Champaign

8:00am **QS1-TuM-1 Investigating Processing Spaces of Epitaxially Grown Nitride Materials with Quantum and Conventional Supervised Learning**, ***Andrew Messecar***[1], Western Michigan University; *Kevin Vallejo,* Idaho National Laboratory; *Steven Durbin,* University of Hawai'i at Mānoa; *Brelon May,* Idaho National Laboratory; *Robert Makin,* Western Michigan University

The experimental design of material synthesis occurs within highly complex processing spaces defined by multiple design parameters. Traditional identification of optimal values for each design term often involves an iterative, costly, Edisonian trial–and–error strategy for experiment design. Therefore, there is great interest in leveraging machine learning–based approaches to enhance and expedite the strategic design of materials and their synthesis pathways. Here, information describing plasma–assisted molecular beam epitaxy (PAMBE) growth trials of transition metal and group–III nitrides have been organized into distinct, composition–specific data sets. For each synthesis record, the complete recipe of experiment design parameters (substrate temperature, element source conditions, growth duration, etc.) are associated with binary numerical labels representing sample crystallinity and surface morphology as determined via *in–situ* reflection high–energy electron diffraction (RHEED) patterns. A Bragg–Williams measure of lattice ordering (S^2) is also investigated as an additional, continuous figure of merit pertaining to atomic–scale disorder. Quantum and classical machine learning algorithms – including linear models, neural systems, tree–based algorithms, and quantum support vector machines – are fit to the data to investigate which growth parameters have the most statistically significant influence over each material property of interest. When predicting the occurrence of monocrystalline PAMBE–grown GaN sample surfaces, supervised learning techniques incorporating quantum computation display notable generalization advantage when compared to classical machine learning approaches. The class–conditional probabilities of obtaining single crystalline, atomically–flat thin film crystals – as well as the degree of lattice ordering measured by S^2 – are forecasted across broad ranges of possible PAMBE operating parameter combinations. These predictions are compared to experimental best practices as well as the results described in published literature detailing the PAMBE synthesis of these materials. The improved generalization performance displayed by the quantum–aware models when predicting GaN crystallinity implies a potential advantage gained via quantum computational studies of synthesis–property relationships in other material systems.

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8:15am **QS1-TuM-2 Quantum Simulation of Spin-Current Autocorrelation Function**, ***Yi-Ting Lee,*** University of Illinois at Urbana Champaign; *Bibek Pokharel,* IBM, T.J. Watson Research Center; *Arnab Banerjee,* Purdue University; *Andre Schleife,* University of Illinois at Urbana-Champaign; *Jeffrey Cohn,* IBM Almaden Research Center

Understanding spin dynamics has long intrigued physicists, as it plays a vital role in revealing the characteristics of quantum magnets, with potential applications in spintronic devices and spin qubits. Evaluating the dynamical properties of large spin systems is often challenging for classical computers due to the exponential growth in memory requirements. Since Hamiltonian dynamics can be efficiently simulated using quantum circuits, the evaluation of time-dependent properties has generated significant interest within the quantum computing community.

While time-dependent magnetization and the one-time dynamical structure factor have been simulated on quantum computers before, there has been no simulation of the spin-current autocorrelation function (ACF). The one-time spin-current ACF can be used to identify the diffusion behavior of spin systems and is directly related to their coherence properties and device performance. In this research, we first consider the spin-1/2 XXZ Heisenberg model as it serves as the framework for studying magnetic interaction. Here, we introduce a simple yet efficient direct measurement scheme for evaluating the one-time spin-current ACF. Unlike the standard Hadamard test, our method eliminates the need for control gates with ancilla qubits and reduces the number of required circuits by a factor of N, where N is the number of qubits. We demonstrate the circuit design and measurement protocol and validate it through a quantum experiment on the *ibm_marrakesh* hardware. In the 20-qubit experiment with the Néel state, we achieve excellent agreement with the numerical results for both the real and imaginary parts, highlighting the effectiveness of our method. Moreover, we present a design for measuring the two-time spin-current ACF and demonstrate good agreement between statevector-simulated results and numerical results, further showcasing the utility of our approach. Furthermore, our method can be potentially extended to measure any ACF, benefiting the study of spin dynamics.

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8:30am **QS1-TuM-3 Quantum Information Processing Stack: From Bottom to Top and Back**, *Sophia Economou,* ***Karunya Shirali,*** Virginia Tech **INVITED**

Quantum processors have become quite large and sophisticated machines over the last several years, with many tech companies racing to develop the first quantum computer of practical utility. While the progress has been impressive, quantum processors still face significant hurdles such as short coherence times and high error rates. They are not yet able to compete with classical information processing technologies in solving problems of practical interest. I will discuss my group's contributions across the quantum information processing stack, from the control of quantum hardware to quantum algorithm development and back.

9:15am **QS1-TuM-6 Quantum-Enhanced Communication Network Routing in Cyber-Physical Power Systems**, *Shuyang Ma,* ***Yan Li,*** Penn State University

Communication networks in cyber-physical power systems play a vital role in ensuring reliable information exchange, enabling real-time monitoring, control, and coordination of distributed energy resources. However, ensuring real-time responsiveness while meeting strict Quality of Service (QoS) constraints, such as low latency and high reliability, introduces significant challenges. A central problem is the constrained shortest path (CSP), which seeks to minimize communication costs across the grid while adhering to a maximum delay threshold. This NP-hard problem becomes computationally infeasible for large-scale networks using conventional approaches. To tackle this, we propose a novel method that transforms the CSP problem into a Quadratic Unconstrained Binary Optimization (QUBO) model, subsequently mapped to an Ising Hamiltonian. This reformulation enables the use of the Quantum Approximate Optimization Algorithm (QAOA), a hybrid quantum-classical technique that exploits quantum parallelism to efficiently approximate optimal routing solutions. Our approach offers reduced computational complexity and improved scalability compared to traditional methods. Through numerical simulations, we demonstrate that this QAOA based strategy successfully identifies cost-effective paths that satisfy QoS requirements, underscoring its potential to revolutionize network optimization in power grids as quantum computing advances.

9:30am **QS1-TuM-7 Floquet-ADAPT-VQE: A Quantum Algorithm to Simulate Non-Equilibrium Physics in Periodically Driven Systems**, ***Abhishek Kumar***, *Karunya Shirali, Nicholas J. Mayhall, Sophia E. Economou, Edwin Barnes,* Virginia Tech

Non-equilibrium many-body quantum systems exhibit many fascinating phenomena absent in equilibrium systems, but simulating them on classical computers is challenging. We propose a hybrid quantum-classical algorithm, Floquet-ADAPT-VQE, to simulate the non-equilibrium physics of periodically driven quantum systems. We utilize the Floquet-Hilbert space, a composition of auxiliary and physical spaces, to transform the Hamiltonian into a time-independent form. We define a cost function based on the square of the shifted extended Floquet Hamiltonian and show how to prepare Floquet eigenstates using Floquet-ADAPT-VQE. We also obtain a suitable auxiliary initial state whose squared Floquet energy is independent of the number of auxiliary qubits as well as the driving frequency, which leads to better convergence with fewer ADAPT iterations. Additionally, we

[1] **AVS Dorothy M. and Earl S. Hoffman Scholarship Recipient**

provide a framework to calculate the time-dependent expectation value of observables in the Floquet state with fixed-depth quantum circuit. We demonstrate our algorithm by performing numerical simulations on a periodically driven XYZ model with a magnetic field. We also explore potential applications of our algorithm for studying various non-equilibrium phenomena in periodically driven systems.

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