Quantum Science and Technology Mini-Symposium
Room 123 - Session QS2-MoM

Quantum Simulations: Materials, Power Distribution, Computing, and Machine Learning Applications

Moderators: Andre Schleife, University of Illinois at Urbana-Champaign, **Sisira Kanhirathingal**, Rigetti Computing

10:30am **QS2-MoM-10 Power System Dynamic Simulation with Generalized Quantum Carleman Linearization***, J. Chen,* ***Yan Li,*** The Pennsylvania State University **INVITED**

The dynamics of power systems are described by a set of nonlinear differential-algebraic equations (DAEs). Over the past few decades, the expansion of the power system scale has led to a notable increase in the dimension of DAEs, posing a substantial challenge for conventional numerical integration methods to simulate power system dynamics. Herein, we introduce a novel generalized quantum Carleman linearization method to tackle dynamic simulation of large-scale power systems, substantially mitigating computational complexity compared to conventional methods. In light of the characteristics of nonlinear power system DAEs, they are transformed into 4th order inhomogeneous polynomial DAEs through a diffeomorphic transformation. By iteratively employing high-dimensional hyperplanes for approximating nonlinear algebraic equations, the classical ordinary differential equation solver, Carleman linearization, can be extended to solving the high-order DAEs of power systems. Consequently, the proposed method can yield a quantum state proportional to the solution of the DAEs in time O(log (n)), exponentially smaller than the linear complexity of Euler's method. Numerical results demonstrate that the proposed method can successfully obtain the trajectory of dynamic simulation of power systems with small errors under various scenarios.

11:00am **QS2-MoM-12 Quantum Computer Simulation of Near-Surface Oxygen Vacancies in α-Al_2O_3 (0001)***, Vijaya Begum-Hudde, Y. Lee,* University of Illinois at Urbana-Champaign*; B. Jones,* IBM*; A. Schleife,* University of Illinois at Urbana-Champaign

Aluminum oxide is a technologically-relevant material as it is employed in a wide range of applications such as catalysis, quantum devices, aviation, and ship industry, among others. Corrosion is a naturally-occurring process in this material, and due to its detrimental effect on the optimal performance, initiation and propagation of corrosion is an area of active research. The near-surface vacancy in the most stable phase, α-Al_2O_3, plays an important role in corrosion, and an improved understanding of the electronic structure is necessary to describe these processes.

We employ first-principles calculations and quantum simulations for an in-depth study of the near-surface O vacancies in α-Al_2O_3 (0001). The geometry of the relaxed Al-terminated pristine (0001) surface obtained with the hybrid exchange-correlation functional (HSE06) are consistent with X-ray diffraction results. Upon introducing an O vacancy, a shallow in-gap electronic defect state. Its band-decomposed charge density and that of the second unoccupied state reveal a strong charge localization near the O vacancy and the adjacent surface Al atom. We study these vacancy states with quantum-defect embedding theory (QDET) calculations to unravel their ground- and excited-state properties. We define an active space consisting of strongly localized states near the defect and treat the remainder as environment. An effective Hamiltonian is solved for the active space which includes the effective screening from the environment within the random phase approximation to obtain the eigenvalues with full configuration interaction (FCI).

Furthermore, we solve the effective Hamiltonian on a quantum computer by employing a model consisting of an active space of one occupied and one unoccupied band from the QDET calculation. On a four-qubit circuit with a Unitary coupled-cluster (UCC-3) ansatz, we calculate the ground-state energy for the active space with the variational quantum eigensolver (VQE). On the noiseless simulator, we achieve excellent agreement with the reference FCI values. Upon introducing noise with a noise model from hardware, the simulator renders an error of 0.19±0.03 eV. We use zero-noise extrapolation with global folding for error mitigation, and successfully reduce the error to 0.01±0.04 eV. Also, a subspace-search VQE implementation to calculate the excited-state eigenvalues for the minimum model results in very good agreement with the first and second excited FCI values.

Funding by the IBM-Illinois Discovery Accelerator Institute is gratefully acknowledged.

11:15am **QS2-MoM-13 Quantum Inception Score: A Quality Measure of Quantum Generative Models***, Akira Sone,* University of Massachusetts Boston

This presentation is based on our recent work [arXiv:2311.12163]. One of the most significant areas in quantum machine learning is quantum generative models. These models are a leading strategy for unsupervised learning, which focuses on uncovering hidden patterns in unlabeled data sets and classifying them. The primary goal of generative models is to train a generator to produce data with high accuracy and substantial diversity from a large amount of unlabeled data, reflecting their quality. Here, we focus on the quantum generative models where both the generators and classifiers are fully quantum. We introduce a novel quality measure called the quantum inception score, linking the classical capacity of the quantum channel playing a role as a quantum classifier. We demonstrate that the entanglement output generated by the quantum generator could contribute to further quality enhancement due to the potential superadditivity of the classical capacity. Also, we demonstrate that the quality degradation due to the quantum decoherence can be captured by using the quantum fluctuation theorems. We also show the application of the quantum inception score in the quantum phase classification in the one-dimensional spin-1/2 chain system. Our results underscore the importance of exploring quantum foundations and communication approaches in studying quantum machine learning protocols.

This work is supported by NSF under Grant No. MPS-2328774.

11:30am **QS2-MoM-14 Deep-learning-based Randomness Assessment of Quantum Random Number Generators***, Hamid Tebyanian,* University of York, UK

Abstract—This paper explores a novel randomness evaluation method for data produced by quantum random number generators (QRNGs), leveraging quantum mechanics to ensure the data's randomness. We employ neural networks and machine learning techniques to analyze the operational principles of QRNGs, enabling the test suites to assess the generators based on their predictability scores. Our findings demonstrate that our model's ability to predict outcomes surpasses that of comparable approaches. Additionally, we discuss the optimal timing for conducting these tests—specifically, analyzing the raw output from QRNGs before processing through an extractor yields the best performance.

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