AVS Quantum Workshop
Room 301 & 302 - Session AQS-FrM

AVS Quantum Science Workshop

Moderators: Charles R. Eddy, Jr., Office of Naval Research Global - London, UK, **Rachael Myers-Ward**, U.S. Naval Research Laboratory

8:20am **AQS-FrM-1 AQS Workshop Opening Remarks**,

9:00am **AQS-FrM-3 Electronic Excitations of Defects in Semiconductors – First-Principles Simulations and Quantum Embedding**, ***André Schleife***, University of Illinois **INVITED**

Defects are present in semiconductors both intrinsically and through doping and critically determine the material properties. In particular, their electronic excitations underlie the optical response in many cases and transitions between electronic energy levels are promising for quantum information purposes. Hence, modeling these properties from first-principles is an important research direction of quantum mechanical computational materials science. Total energies and the electronic structure as well as the optical properties are described by density functional and many-body perturbation theory.

In this presentation I will outline the fundamentals of these techniques and illustrate applications to defects in MgO and Al2O3. Results for atomic geometries and optical properties will be compared to experiment for the oxygen vacancy in MgO and various defects in Al2O3. Subsequently, I will discuss recent attempts from the literature to incorporate quantum embedding techniques into solving the electronic structure problem and computing optical properties including excitonic effects.

9:40am **AQS-FrM-5 Break**,

10:00am **AQS-FrM-6 Running Quantum Circuits on a Neutral Atom Quantum Computer**, ***Mark Saffman***, University of Wisconsin-Madison and ColdQuanta **INVITED**

One of the daunting challenges in developing a computer with quantum advantage is the need to scale to a large number of qubits while maintaining the fidelity and isolation of pristine, few qubit demonstrations. Neutral atoms are one of the most promising approaches for meeting this challenge, in part due to the combination of excellent isolation from the environment and the capability to turn on strong two-qubit interactions by excitation to Rydberg states.

I will present results of running quantum algorithms for preparation of multi-qubit GHZ states, phase estimation with application to a basic quantum chemistry problem, and hybrid quantum/classical optimization. The circuits use a universal set of quantum gates based on microwave and optical control of Cs atom qubits. Two-qubit gates are implemented using Rydberg interactions.

These results on a neutral atom quantum processor are the “tip of the iceberg” relative to what we believe will be possible with further development of the neutral atom approach. Atomic qubits are identical, have excellent coherence properties, and are essentially cost free with no fabrication required. Realizing the full potential of programmable large scale atomic arrays requires solving some outstanding challenges including atom loss due to imperfect vacuum conditions, optical addressing with large space-bandwidth product, high power and low noise control lasers, and crosstalk-free measurements. I will discuss these challenges and point to fruitful directions for future progress.

10:40am **AQS-FrM-8 Unitary Coupled Cluster Ansatz as an Efficient Way to Perform Electronic Structure Calculations**, ***Jim Freericks***, Georgetown University **INVITED**

In this talk, I will review work recently completed on how to use the factorized form of the unitary coupled cluster ansatz as an efficient way to perform electronic structure calculations via the variational quantum eigensolver and its variants. I will describe the universal nature of the factorized form and how the variational principle improves accuracies more than expected from simple error bounds. I will discuss how this quantum computer ansatz compares with the conventional coupled-cluster ansatz and I will discuss how one can trade off measurements for circuit depth to perform calculations on molecules that use very low-depth circuits (with potential implementations on near-term hardware). I will also describe how one can improve the circuit depth for higher-rank factors by incorporating additional ancilla or by using linear combinations of unitaries. I will end with some prospects for the near term in how quantum chemistry calculations are likely to be performed.

11:20am **AQS-FrM-10 AQS Panel Discussion**,
Each AQS Workshop speaker will participate in this Q&A Session

12:00pm **AQS-FrM-12 AVS Quantum Workshop Closing Remarks**,

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