# EXPLORE MOLECULAR EXCITED STATES ON NEAR-TERM DEVICES

**Yongbin Kim and Anna I. Krylov**

*Department of Chemistry, University of Southern California*

The electronic structure theory is a field where one can easily find classically intractable tasks due to limited resource scaling. The advent of quantum devices is expected to facilitate quantum chemical research through quantum supremacy [1]. Research efforts have focused on designing efficient quantum algorithms, and several developments have shown successful ground-state studies for small molecules using near-term devices [2]. Apart from the ground-state studies, significant effort has been made to develop the framework for molecular excitation energies, such as Variational quantum deflation (VQD) [3], Subspace-search VQE (SS-VQE) [4], and quantum Equation-of-Motion (qEOM and EOM-VQE) [5,6]. Inspired by the quantum version of the equation-of-motion with the unitary coupled-cluster (UCC) theory, we introduce qEOM-UCC/Davidson algorithm to compute excitation energies. We carry out numerical simulations on $H_2$/6-31G, $H_4$/STO-3G, LiH/STO-3G, and $H_2O$/STO-3G to validate the performance of qEOM-UCC/Davidson. In order to construct a quantum circuit (ansatz), *Gray code* decomposition [7] is employed for numerical simulations. qEOM-UCC/Davidson allows one to work within a particular subspace of the entire Hilbert space depending upon desired symmetries. In addition, we demonstrate the extension of our qEOM-UCC/Davidson within the framework of VQE, giving rise to a similar performance to its non-variational version.

**References**

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