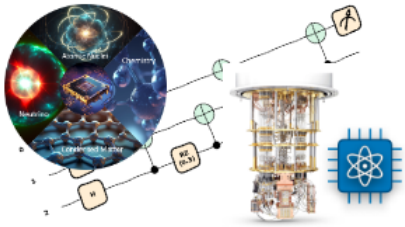

Contribution ID: **36** Type: **Contributed Talk (45min including questions)**

Quantum Algorithm for Real-Space Chemistry on Adaptive Molecular Grids

Tuesday, November 18, 2025 5:05 PM (45 minutes)

First-quantized, real-space formulations of quantum chemistry on quantum computers are appealing: qubit count scales logarithmically with spatial resolution, and the two-body Coulomb term achieve quadratic scaling, rather than usual quartic scaling in orbital-based approaches. However, existing schemes employ uniform discretizations whose resolution is imposed by the electron-nuclear cusps of the wave functions in high-density regions, thereby oversampling low-density regions and wasting computational resources. To address this, we repurpose the non-uniform, molecule-adaptive grids long used for DFT integration, which concentrate points where the electronic density is highest, to discretize the molecular Hamiltonian. Once encoded as a quantum operation, its ground state can be obtained with standard Quantum Phase Estimation. We further derive a transcorrelated, non-Hermitian yet isospectral Hamiltonian that removes Coulomb singularities and associated cusps in its eigenfunctions, whose ground-state energy is accessible through the recent generalized Quantum Eigenvalue Estimation protocol. Numerical validation on benchmark systems confirms this ab initio framework paves a promising route to ground-state chemistry on quantum hardware.

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