Molecular Excitation Energies Simulated
on a Superconducting Quantum Computer

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Exact quantum chemical treatment of electronically excited states exhibits exponential scaling with system size on classical computers. Quantum computing offers a formally more favorable scaling; however, current noisy intermediate-scale quantum (NISQ) devices impose stringent constraints on circuit depth. Practical demonstrations therefore require carefully optimized hybrid quantum–classical workflows that minimize hardware resource demands.

Here, we present a hybrid protocol for computing molecular excitation energies that integrates the ΔADAPT algorithm with optimized circuit preparation, quantum detector tomography, dynamical decoupling, informationally complete measurements, and tensor-network-based QPU postprocessing. Using IBM superconducting quantum hardware, we compute the lowest singlet–singlet ($S_0 \rightarrow S_1$) and singlet–triplet ($S_0 \rightarrow T_1$) excitation energies for representative fluorophores.

The computed results reproduce the correct singlet–triplet ordering and show good agreement with experimental measurements and high-level classical reference calculations. These findings demonstrate that, when combined with advanced error mitigation and postprocessing strategies, current quantum devices can capture essential excited-state energetics relevant to molecular systems used in photodynamic therapy and photocatalysis.