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# Ground-State Energy Calculations with Variational Quantum Eigensolver: Advancing Quantum Simulations for Energy Applications

Quantum computing offers transformative potential for solving energy-related problems in quantum chemistry and material discovery. Among various hybrid quantum-classical algorithms, the Variational Quantum Eigensolver (VQE) has emerged as a versatile tool for calculating molecular ground-state energies with near-term quantum hardware. This study explores the use of advanced techniques, particularly the Unitary Coupled-Cluster Singles and Doubles (UCCSD) ansatz, to enhance the precision and scalability of VQE for complex energy-relevant systems.

Our previous work focused on ammonia borane, a candidate hydrogen storage material, demonstrating the utility of VQE in achieving accurate ground-state energy calculations. Ammonia borane's unique structure and potential for clean energy applications highlight the importance of precise quantum simulations to understand its properties. Building on this foundation, we now extend the VQE framework to larger and more intricate molecular systems, leveraging the expressive power of the UCCSD ansatz to capture intricate electronic correlations essential for reliable energy computations.

Noise and hardware limitations remain significant challenges for quantum computations. To address these, our approach incorporates error mitigation techniques such as symmetry verification and measurement error correction. These methods ensure that the results obtained from noisy intermediate-scale quantum (NISQ) devices remain accurate and reliable. Furthermore, our implementation optimizes quantum resource usage, balancing the trade-offs between computational cost and accuracy.

The implications of this research extend beyond fundamental quantum chemistry to practical energy applications, such as optimizing molecular structures and understanding reaction pathways critical for renewable energy solutions. By demonstrating the synergy between advanced ansatz designs, error mitigation, and quantum hardware capabilities, this work contributes to the broader goal of leveraging quantum computing to address pressing global challenges in energy and sustainability.

With continued advancements in quantum algorithms and hardware, our study provides a pathway for future explorations in material discovery and clean energy technologies, emphasizing the pivotal role of VQE in bridging fundamental science and applied energy research.

## Theme

Theme 3. Theoretical and experimental methods for quantum effects in energy processes

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