Quantum-Enhanced Computational Catalysis: Optimizing Reaction

Pathway Simulations with Advanced Tensor Decomposition Techniques

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***Abstract*—Quantum-enhanced computational catalysis offers a transformative framework for modeling complex reaction pathways with unprecedented accuracy and scalability. As catalytic processes often involve strongly correlated electrons, multidimensional potential energy surfaces, and dynamic coupling between nuclear and electronic degrees of freedom, classical simulation methods face steep computational barriers. This study explores a hybrid quantum–classical workflow that integrates quantum algorithms for electronic structure with advanced tensor decomposition techniques to compress, analyze, and optimize high-dimensional reaction data. By leveraging tensor-network representations—such as matrix product states, tensor-train formats, and hierarchical Tucker decompositions—the approach systematically reduces computational cost while maintaining chemically relevant accuracy. The research demonstrates how tensor-optimized quantum simulations can accelerate transition-state discovery, enhance reaction pathway resolution, and improve predictions of catalytic efficiency across heterogeneous, homogeneous, and photocatalytic systems. The synergy between quantum solvers and tensor decomposition establishes a powerful platform for next-generation catalytic modeling and materials discovery.**

Catalysis lies at the heart of modern chemical science, enabling sustainable energy production, environmental remediation, pharmaceutical synthesis, and materials development [4]. Despite its wide-ranging importance, accurately modeling catalytic reaction pathways remains one of the most challenging problems in computational chemistry. Reaction coordinates are often governed by strongly correlated electronic states, multi-step transition mechanisms, and high-dimensional potential energy surfaces that are difficult to capture using classical computational frameworks [6]. As system size increases, traditional methods such as density functional theory or coupled-cluster approaches struggle with exponential scaling, limiting their ability to explore complex catalytic landscapes.

Recent advances in quantum computing offer new opportunities to overcome these limitations. Quantum algorithms designed for electronic structure and reaction dynamics can directly address many-body interactions with improved scaling, enabling simulation of catalytic processes that have remained inaccessible to classical methods [3]. However, near-term quantum hardware is constrained by limited qubit counts, noise, and coherence times, necessitating complementary strategies to maximize efficiency and reduce resource requirements.

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