

Error-Mitigation Strategies for Quantum Computing in High-Accuracy Prediction of Molecular Interactions in Process Engineering

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Abstract—Quantum computing is emerging as a transformative paradigm for molecular-level modeling in process engineering, offering the potential to perform large-scale, high-accuracy simulations that surpass the computational limits of classical methods. However, the inherent noise and decoherence in quantum systems present major obstacles to reliable molecular interaction predictions. This research conducts a qualitative investigation of error-mitigation strategies designed to improve the accuracy and stability of quantum simulations for modeling molecular interactions relevant to chemical and process engineering. By reviewing scientific literature and analyzing case studies across quantum mechanics, computational chemistry, and industrial process modeling, the study identifies the principal challenges associated with quantum noise, gate fidelity, and algorithmic scalability. A conceptual framework was developed to evaluate how quantum error correction (QEC) techniques, zero-noise extrapolation, and hybrid quantum–classical algorithms enhance predictive precision in molecular simulations. The findings suggest that combining these methods not only mitigates computational noise but also improves convergence efficiency in modeling reaction pathways and intermolecular potentials. This research synthesizes interdisciplinary insights to propose a roadmap for integrating quantum-enhanced molecular simulations into sustainable process engineering. It underscores how advances in error mitigation will be essential for achieving trustworthy, energy-efficient, and scalable industrial applications of quantum computation in the coming decade.

■ The advancement of quantum computing has unlocked new possibilities in modeling molecular interactions and chemical processes with an unprecedented level of precision. Unlike classical computational methods, which rely on approximations due to limited computational power, quantum

algorithms are capable of simulating molecular systems by exploiting quantum superposition and entanglement to represent and process high-dimensional state spaces efficiently [2]. This capability positions quantum computation as a key enabler for breakthroughs in process engineering, where predicting reaction kinetics, catalysis, and thermodynamic behavior at the molecular scale is essential for optimizing industrial processes and developing sustainable technologies [1].

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