Embedding-Based Quantum Simulation of Complex Energy Systems

for Smart Grid and Sustainable Engineering Applications

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***Abstract*—The increasing complexity of modern energy systems—driven by distributed renewable generation, dynamic grid behavior, and multi-scale interactions—necessitates computational models capable of capturing nonlinearities, stochastic variability, and high-dimensional optimization landscapes. Embedding-based quantum simulations offer a promising path forward by integrating quantum solvers into classical energy modeling frameworks, enabling more accurate analysis of localized subsystems while maintaining tractable large-scale system evaluations. This study investigates quantum embedding techniques applied to power flow analysis, renewable integration, grid stability assessment, and energy storage optimization. By partitioning complex energy networks into quantum-treated active regions embedded within classical architectures, the approach enhances the fidelity of system-level simulations while reducing computational overhead. The research highlights the potential of hybrid quantum–classical workflows to accelerate decision-making in smart grid design, improve forecasting under uncertainty, and support the development of sustainable engineering solutions. The results outline a roadmap for deploying quantum-embedded simulations in future energy infrastructures.**

Sustainable energy systems are becoming increasingly intricate as society transitions toward decentralized power generation, widespread electrification, and real-time grid monitoring. Smart grids must efficiently coordinate renewable energy sources, storage devices, power electronics, electric vehicles, and demand-response mechanisms, all while ensuring resilience, reliability, and economic feasibility [1]. Modeling such systems requires capturing interactions that span multiple scales—ranging from the quantum mechanical behavior of advanced materials in batteries and photovoltaics to the macroscopic dynamics of power flows across transmission networks [6].

Traditional energy modeling frameworks face challenges in resolving these complexities. Classical simulations often struggle with nonlinear power flow equations, stochastic fluctuations in renewable generation, high-dimensional optimization problems, and multi-scale coupling between components [4]. As grid architectures evolve into more distributed and adaptive systems, computational demands continue to escalate, highlighting the need for alternative modeling strategies that can handle greater complexity with improved accuracy.

Embedding-based quantum simulation presents a powerful approach to these challenges. Rather than

Digital Object Identifier 10.62802/qfxw5493

Date of publication 21 11 2025; date of current version 21 11 2025

