# Embedding-Based Quantum Simulations for Multi-Scale Modeling of Chemical Systems

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***Abstract*—Embedding-based quantum simulations have emerged as a promising paradigm for bridging quantum and classical scales in complex chemical systems. As molecular processes span multiple spatial and temporal regimes—from localized electron correlation to mesoscale reactivity—traditional quantum chemistry and classical potentials often fail to describe these interactions with sufficient accuracy and scalability. This study explores hybrid embedding frameworks that integrate quantum subspace models, density functional embedding, and quantum many-body solvers within hierarchical multi-scale workflows. By partitioning chemically active regions and treating them with quantum processors while embedding them within larger classical environments, the approach improves accuracy in reaction barrier estimation, excited-state dynamics, and strongly correlated interactions. We evaluate state-of-the-art quantum embedding techniques, discuss advances in quantum resource allocation and error mitigation, and demonstrate how embedding can reduce computational depth while preserving chemically essential features. The study highlights key opportunities for developing next-generation quantum-enhanced multi-scale simulation pipelines capable of accelerating catalyst design, energy storage materials, and biochemical modeling.**

Chemical systems operate across a wide hierarchy of spatial and temporal scales, making accurate simulation fundamentally challenging. Localized electronic phenomena—such as bond breaking, electron correlation, and charge transfer—occur at the quantum scale, whereas macroscopic behavior emerges from molecular assemblies interacting over larger domains. Conventional computational chemistry methods, such as density functional theory (DFT) and classical molecular dynamics (MD), provide valuable insights but struggle to capture all interactions simultaneously. In particular, strongly correlated electronic structures and large active spaces push classical algorithms toward computational intractability [1];[2]. Recent advances in quantum computing offer new pathways for addressing these limitations by enabling more accurate treatment of many-body interactions at polynomial scaling.

Embedding-based quantum simulations represent one of the most promising strategies in this context. Instead of attempting to treat an entire chemical system on a quantum processor—which is currently impractical due to qubit and coherence constraints—embedding methods partition the system into regions of differing computational complexity. The chemically active region, where strong correlation

*Digital Object Identifier 10.62802/fb48dj33*

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


Published by the ABA Yayıncılık