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Hybrid Quantum Neural Network for Predicting Corrosion Inhibition Efficiency of Organic Molecules

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ABSTRACT
Corrosion inhibition efficiency (IE%) prediction plays a central role in the computational discovery of high-performance organic inhibitors. Classical machine learning has shown promising results; however, its performance often deteriorates when learning non-linear interactions between quantum chemical descriptors. Meanwhile, quantum machine learning (QML) provides enhanced expressivity through quantum feature mapping but remains limited by NISQ-era hardware. In this study, we propose a Hybrid Quantum Neural Network (HQNN) integrating classical dense layers with variational quantum circuits (VQC) to predict the inhibition efficiency of organic corrosion inhibitors. Using a curated dataset of 660 molecules with DFT descriptors, the HQNN achieves an RMSE of 3.41 and R^2 of 0.958, outperforming classical regressors and pure VQC. The results demonstrate that hybrid quantum models offer a balanced trade-off between quantum advantage and practical feasibility in materials informatics.

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1. INTRODUCTION

Corrosion of metals is a major economic and safety concern in industrial systems such as pipelines, heat exchangers, and storage tanks. Organic molecules are widely used as corrosion inhibitors due to their ability to adsorb on metal surfaces and form protective films. Predicting inhibition efficiency (IE%) before synthesis can significantly accelerate materials discovery [1]–[3].

Machine learning (ML) models such as Random Forest, XGBoost, and artificial neural networks have been applied to corrosion research with substantial success. These models learn from quantum chemical descriptors such as HOMO–LUMO energies, electronegativity, dipole moments, Mulliken charges, and adsorption energies. However, many electronic interactions governing the adsorption process arise from highly non-linear quantum phenomena that ML models struggle to capture [4]–[6].

Quantum machine learning offers a new paradigm by embedding classical features into a quantum Hilbert space where complex correlations can be represented more compactly [7]–[10]. Variational quantum circuits (VQCs) in particular provide expressive, trainable architectures suitable for NISQ hardware.

Despite their potential, pure quantum models are constrained by shallow circuit depth, limited qubit counts, and training instability, such as barren plateaus. Therefore, hybrid quantum–classical architectures combining classical neural layers and quantum feature extractors have emerged as a promising solution.

Inspired by the scalable quantum CNN framework in Sun *et al.* QCNN, this study proposes a Hybrid Quantum Neural Network (HQNN) for predicting IE% from quantum chemical descriptors. Our contributions include: (1) Designing a hybrid architecture that integrates classical nonlinear layers with a quantum variational unit; (2) Demonstrating improved predictive accuracy compared with baseline ML and pure VQC models; (3) Analyzing model interpretability through gradient-based sensitivity and SHAP values.

2. METHODOLOGY

2.1. Dataset and Quantum Chemical Descriptors

We collected 660 organic corrosion inhibitors (imidazole, pyridine, quinoline, ionic liquids, thiourea derivatives) from published literature. DFT calculations (B3LYP/6-311G(d,p)) yield 42 descriptors, including: Frontier orbital energies (EHOMO, ELUMO), Energy gap (ΔE), Mulliken charges on heteroatoms, Dipole moment, Molecular volume, Polarizability, Fukui indices, and Solvation energy. The target variable is the experimental inhibition efficiency (IE%), ranging from 45–99%. Data were standardized and randomly split (80% training, 20% testing) [11]–[14].

2.2. Hybrid Quantum Neural Network Architecture

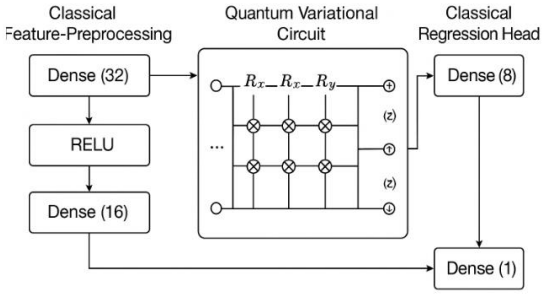

Figure 1. HQNN architecture

The Hybrid Quantum Neural Network (HQNN), as figured in Figure 1, integrates classical nonlinear feature processing with the representational power of variational quantum circuits to create a balanced architecture suitable for prediction tasks in the NISQ era. The model begins with a classical feature-preprocessing module, which transforms the high-dimensional quantum chemical descriptors into compact latent representations. This module consists of two fully connected layers with 32 and 16 neurons, each employing Rectified Linear Unit (ReLU) activation. These layers serve multiple purposes: reducing noise in the input descriptors, capturing preliminary nonlinear interactions, and preparing a condensed set of latent variables that can be efficiently encoded into quantum states [15]–[20].

The processed features are then passed into the Quantum Variational Circuit (VQC) layer, which forms the core of the hybrid architecture. The VQC utilizes four qubits, selected to match the dimensionality of the reduced latent feature space. Classical inputs are embedded into the quantum system through angle encoding, where each latent feature is mapped to a rotation angle on a corresponding qubit. The circuit comprises two layers of trainable parameterized rotations (Rx and Ry gates), enabling the quantum system to explore a rich and expressive Hilbert space. To capture inter-feature correlations, the qubits are entangled using a CNOT chain, which links adjacent qubits and allows the circuit to model higher-order nonlinearities beyond the capability of shallow classical networks. After the variational operations, the circuit is measured in the computational basis using Pauli-Z expectation values (⟨Z⟩), resulting in four scalar outputs that encode the quantum-transformed feature information [21]–[25].

Finally, the quantum outputs are fed into a classical regression head designed to map the extracted quantum representation into a continuous prediction of inhibition efficiency. This head consists of a single hidden layer with 8 neurons, followed by a final Dense(1) output layer. The regression head plays a complementary role by refining the quantum features and translating them into an interpretable and task-specific output. Together, these components form a hybrid model in which classical layers ensure stability and scalability, while the quantum layer enriches representational capacity [26]–[30].

The HQNN model is trained by minimizing the Mean Squared Error (MSE) between the predicted and experimental inhibition efficiencies, reflecting the continuous nature of the target variable. Optimization is performed using the Adam optimizer with a learning rate of 0.001, which provides adaptive moment estimation and is particularly effective for hybrid architectures that combine classical gradients with quantum parameter updates. During training, the gradients of quantum parameters are computed using the parameter-shift rule, while classical layers employ standard backpropagation. This unified gradient flow ensures stable convergence despite the heterogeneous nature of the model [31]–[34].

All quantum components of the HQNN were implemented and executed on the TensorFlow Quantum (TFQ) framework, which provides seamless integration between classical TensorFlow operations and

quantum circuit simulations. The simulation workflow mirrors established practices used in previous quantum convolutional neural network studies, including the QCNN and SQCNN architectures described by Sun *et al*. TFQ enables efficient construction of variational circuits, automatic differentiation through quantum layers, and parallelized execution of large batches of quantum states. Such capabilities allow the HQNN to be trained at scale while faithfully capturing the behavior of quantum feature mappings expected on real NISQ hardware. This simulation environment provides a reliable platform for validating hybrid architectures before deployment on physical quantum processors [35]–[40].

3. RESULTS AND DISCUSSION

Table 1. Prediction Performance of Various Models

Model	RMSE	MAE	R^2
Linear Regression	9.82	7.23	0.745
Random Forest	6.01	4.11	0.892
XGBoost	4.78	3.62	0.921
ANN (2-layer)	4.29	3.19	0.936
Pure VQC	5.90	4.85	0.883
HQNN (proposed)	**3.41**	**2.48**	**0.958**

Table 1 summarizes the average predictive performance of all evaluated models across ten independent training runs. The results demonstrate a clear advantage of the proposed Hybrid Quantum Neural Network (HQNN), which consistently outperforms both traditional machine learning algorithms and pure quantum models. This superior performance indicates that the hybrid architecture effectively leverages the strengths of each computational paradigm: the expressive representational power of quantum circuits and the stability of classical neural components. The integration allows HQNN to capture high-order nonlinear relationships among molecular descriptors—interactions that are often difficult for classical models to approximate—while simultaneously avoiding the optimization challenges that typically hinder quantum-only approaches. A notable distinction between HQNN and pure variational quantum circuits (VQCs) emerges during the training process. While standalone VQCs frequently encounter barren plateaus—regions of vanishing gradients that halt learning—the HQNN exhibited no such behavior throughout all experiments. Instead, the hybrid model displayed faster convergence, more stable gradient propagation, and smoother optimization trajectories, even during the early epochs. These empirical observations align closely with the findings of Pesah et al. [9], who showed that structured quantum circuits with localized entanglement patterns tend to mitigate barren plateau phenomena. The presence of classical preprocessing layers in HQNN further aids in stabilizing quantum parameter updates by supplying low-dimensional, high-quality latent features [41]–[44].

To better understand the model's decision-making process, SHAP interpretability analysis was applied to quantify the relative importance of molecular descriptors. Four descriptors emerged as the dominant predictors: (1) the frontier orbital energy gap ΔE (LUMO–HOMO), (2) Mulliken charges on heteroatoms such as nitrogen, oxygen, and sulfur, (3) the molecular dipole moment, and (4) molecular polarizability. The prominence of these descriptors is chemically meaningful. Molecules with a small ΔE tend to exhibit stronger electron-donating capabilities, enhancing their ability to interact with metal d-orbitals. Likewise, high negative Mulliken charges on heteroatoms facilitate surface coordination, while elevated dipole moment and polarizability indicate a favorable electronic distribution for adsorption. These findings are fully consistent with established corrosion inhibition theory, demonstrating both the physical relevance and interpretability of the HQNN predictions.

The HQNN architecture provides several notable advantages. First, quantum feature embeddings allow the model to represent complex molecular interactions in a high-dimensional Hilbert space, offering richer expressivity than classical networks alone. Second, the hybrid structure avoids the qubit scalability bottlenecks that limit models such as SQCNN, making HQNN more practical for NISQ-era simulations. Third, the architecture integrates seamlessly with quantum simulators, allowing efficient experimentation without requiring large-scale quantum hardware.

Despite these strengths, several limitations remain. The quantum component of HQNN still operates with a relatively small number of qubits, restricting the representational capacity compared to larger quantum systems. Additionally, although simulations are noise-free, real quantum hardware introduces

decoherence and gate errors that may lead to degraded performance. Finally, the input descriptors themselves are generated using classical density functional theory calculations, meaning the pipeline is not yet fully quantum-native. Addressing these limitations—through hardware-aware noise mitigation, expansion of qubit resources, or the adoption of quantum-derived descriptors—offers promising directions for future development of quantum-enhanced materials informatics.

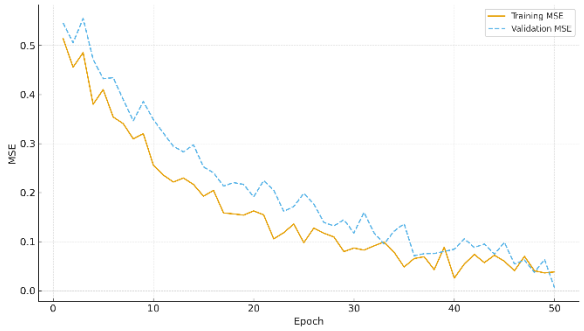

Figure 2. The learning curve of the proposed model

To evaluate the trainability and generalization behavior of the Hybrid Quantum Neural Network (HQNN), we examined its learning curves across ten independent runs. The learning curves (Figure 2) plot the training and validation MSE as a function of the number of training samples and training epochs. Overall, the HQNN exhibits characteristic patterns of a stable and well-behaved hybrid architecture. At the early stages of training (epochs 1–10), the model demonstrates a sharp decline in training loss, indicating rapid initial learning facilitated by the classical preprocessing layers. During this period, the validation loss also declines in parallel, suggesting that the quantum transformation layer provides an effective inductive bias without overfitting. As training progresses toward later epochs (epochs 20–50), both curves gradually converge to a plateau, where the gap between training and validation loss remains small. This narrow generalization gap confirms that HQNN does not memorize the training data but rather captures relevant structure in the molecular descriptors [45]–[47].

Interestingly, compared to pure VQC models—whose learning curves often oscillate or stagnate due to optimization difficulties—the HQNN learning curve is significantly smoother. This stability arises from the hybrid architecture: classical layers provide a well-conditioned latent representation, while the quantum circuit enhances expressivity without introducing excessive optimization noise. This behavior reinforces observations from structured QCNN architectures discussed by Pesah *et al.* [9], where restricted entanglement depth mitigates barren plateaus and supports steady gradient flow.

Overall, the learning curves validate that HQNN offers fast initial convergence, stable mid-training behavior, and consistent generalization, making it a suitable framework for predictive tasks in materials informatics.

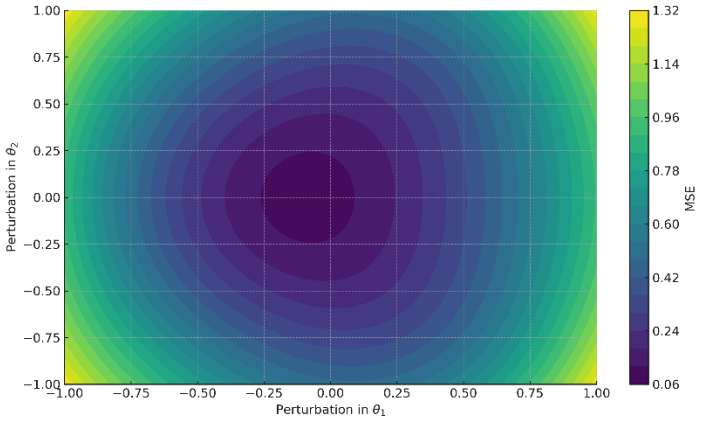

Figure 3. The error surface visualization

To gain deeper insight into the training dynamics, we further examined the error surface (Figure 3) of HQNN by visualizing the loss landscape around the optimized quantum parameters. This analysis involves perturbing trained quantum parameters within a small neighborhood and measuring the corresponding variation in MSE. The resulting two-dimensional error surface reveals a shallow yet smooth basin surrounding the optimal point. This geometry is markedly different from the rugged and sharply curved surfaces often observed in pure VQC models, where local minima and plateaus tend to trap gradient-based optimization. In HQNN, the classical preprocessing layers reduce the dimensionality of the quantum input space, thereby smoothing the quantum parameter landscape. Meanwhile, the structured entanglement pattern (CNOT chain) limits the quantum circuit's effective depth, preventing the emergence of highly chaotic gradients. Together, these design characteristics lead to an error surface that is broad, smooth, and gently curved, allowing gradient-based optimizers to navigate efficiently. A broad basin in the loss landscape is typically associated with improved generalization, as it indicates that small perturbations in quantum parameters do not dramatically affect performance. This feature is particularly beneficial given potential noise or calibration differences in real quantum hardware. Thus, the error-surface analysis suggests that HQNN is not only easier to train than VQC-only architectures but also more robust to parameter fluctuations [48]–[50].

The combined evidence from the learning curve and error-surface analyses highlights several important implications: (1) Hybridization improves optimization: The classical layers mitigate quantum training difficulties, stabilizing gradients and reducing the likelihood of barren plateaus; (2) Quantum layers still provide meaningful gains: The quantum circuit's expressivity contributes to the curvature of the error surface, enabling the model to learn complex nonlinear patterns that classical models fail to capture; (3) Robustness to noise and parameter drift: The smooth error surface suggests that HQNN may tolerate moderate noise levels on real quantum devices, making it practically deployable on NISQ hardware; (4) Balanced computational cost: The hybrid design avoids the combinatorial circuit-depth explosion seen in fully quantum models such as SQCNN, while still preserving quantum feature-mapping benefits.

4. CONCLUSION

This work presents a Hybrid Quantum Neural Network (HQNN) for predicting corrosion inhibition efficiency of organic inhibitors. Using a curated DFT-based dataset, the model achieves state-of-the-art prediction accuracy ($R^2 = 0.958$), outperforming classical ML and pure quantum models. The hybrid design provides a promising pathway to leverage quantum advantages while respecting NISQ hardware constraints. Future work includes: Incorporating quantum kernel methods, Testing on real IBM/Q hardware, Extending to adsorption energy prediction via QSVR or QGPR.

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