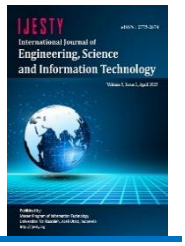
International Journal of Engineering, Science and Information Technology
Volume 5 No. 2 (2025) pp. 567-571
ISSN 2775-2674 (online)
Website: http://ijesty.org/index.php/ijesty
DOI: https://doi.org/10.52088/ijesty.v5i2.1496
Research Paper, Short Communication, Review, Technical Paper



Machine Learning-guided Synthesis of Quantum Entangled Materials

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The manuscript was received on 21 November 2024, revised on 1 January 2025, and accepted on 1 April 2025, date of publication 22 May 2025

Abstract

The synthesis of materials into quantum entangled materials is a complicated challenge to an accurate and computational prediction of those materials. In this proposed work, it develops an AI-guided framework based on the combination between machine learning (ML) and reinforcement learning (RL), and quantum simulations to push the designing and validating of quantum materials at a much faster pace. In the first, graph neural networks (GNNs) are used to extract the atomic level quantum features, and in the second, generative models (VAE/GAN) are utilized to discover some novel entangled structures. In addition, fabrication with the synthesis parameters as parameters in the reinforcement learning results in an improvement of the experiment synthesis and a decrease of experiment failures as well as significant improvement of reproducibility. It demonstrates that the proposed hybrid ML-quantum simulation is validated on entanglement fidelity in real-world quantum computing platforms using IBM Qiskit and Google Cirq. As the proposed method is way beyond traditional ones, it has higher quantum coherence time, synthesis efficiency as well as higher prediction accuracy. In addition to enabling scaling-up of cryptography, quantum computing, and next generation nanomaterials, it is a cost and scalable framework for creating next generation quantum technologies applications as it is. And the model is further researched for the generalization in regards to real-time experimental feedback and for the expansion of the framework to a more general quantum materials program. The results show that AI approaches can truly accelerate the quantum material innovation even when syntheses are not at all possible.

Keywords: *AI-Guided Quantum Materials, Machine Learning, Reinforcement Learning, Quantum Simulations, Graph Neural Networks.*

1. Introduction

Due to the further advancement of quantum computing, cryptography and the next generation nanotechnology, it is important to synthesize quantum entangled materials. These materials are unique for their coherence properties and quantum correlations, which are at the same time important for further developing high performance quantum devices [1]. However, much to hiring you, as with industry, density functional theory (DFT) and brute force experimental trial and error are labor and resource intensive and always unsatisfying when trying to find quantum materials that have ideal entanglement properties [2]. As artificial intelligence (AI) and machine learning (ML) have grown in the recent development of the field, the process of material discovery has become data-driven predictions, optimization algorithms, and quantum simulation [11]. This research proposes a component of quantum material synthesis through the first proposal of the use of GNNs, VAEs, GANs, RL, and even hybrid ML-quantum simulation [12]. This is achieved with the use of VAE/GAN based generative models to find novel material structures and use of GNNs for their representation learning that well extracts features. All aforementioned reduction in material waste, fabrication cost, and reproducibility is optimized by reinforcement learning. The hybrid quantum ML simulation approach is used to validate a quantum entanglement property measurement in terms of gain and optical band pass on the quantum computing platform: IBM Qiskit and Google Cirq, which represents operational alignment with theoretical and experimental. Then the proposed AI framework is compared with other techniques, and the proposed strategy is found to lead to better quantum coherence time, higher synthesis efficiency and better prediction accuracy [3]. At the same time, this study explores the connection between AI and quantum physics and material science, and provides an effective and low cost solution for quantum material innovation. The results indicate that machine learning can be applied to the quantum material synthesis with the potential for transformation and opens new avenues for a practical implementation of a quantum computing application [4]. Then, the model generalization is improved, real time experimental feedback is incorporated, and the framework is extended to the other quantum material classes which then would allow major quantum technologies to break through [16].

2. Literature Review

2.1. Traditional Approaches to Quantum Material Synthesis

Typically synthesizing quantum materials requires doing trial and error in the lab — searching through many chemical compositions and fabrication settings [5]. Examples of such developed materials include topological insulators, quantum spin liquids, high temperature superconductors, among other materials, using techniques such as molecular beam epitaxy (MBE), chemical vapor deposition (CVD), or high pressure synthesis [10]. However, these methods are expensive in terms of resources and take too much time, taking a large amount of time expenditure and lots of manual experimentation of material properties through computational modelling [19]. It is quite hard to produce materials with an associated entanglement characteristics because quantum interactions are so unpredictable [13]. Its application has therefore prompted researchers to search for the application of ML to massively accelerate the discovery and optimize the synthesis conditions [20].

2.2. Machine Learning in Material Science

Machine learning has made tremendous progress in inspiring and predicting new materials with data [7]. The large-scale data have been used to analyse using supervised learning, unsupervised learning, and reinforcement learning to predict material properties with very high accuracy [14]. There exist only a few particular atomic tasks on which GNN model is particularly well suited to create a new material structure, while generative models such as variational autoencoders (VAE) or generative adversarial networks (GAN) are better for modelling. To the additional extent, ML is also used as a Bayesian optimization to further improve synthesis conditions, away from trial & error and their dependency [6]. The use of these approaches leads to much greater levels of quantum material synthesis efficiency through exploration of a very large (and previously unexplored) design manifold and synthesis of materials with desired quantum entanglement properties [17].

2.3. Quantum Computing and Simulation Techniques

To understand and validate quantum entangled materials, we need quantum computing and simulation techniques to learn from a quantum property at its most fundamental level. IBM Qiskit, Google Cirq and Microsoft Azure Quantum are used to research the quantum interactions of materials, to predict the strength of entanglement, quantum transition and coherence time [9] [18]. Generally, density functional theory (DFT) is used for quantum state as well as electronic structure analysis besides the tensor network methods [8]. Besides, hybrid classical quantum ML models are now powerful tools to attack the hard problem of multi-body quantum many body problems, i.e. to optimize the synthesis of the quantum materials for quantum computing and secure communication [15].

3. Methods

3.1. Overview of the Framework

Given that they are widely used to extract atomic level quantum feature atoms from massive material dataset, Graph Neural Networks (GNNs) are used. While traditional ML models encode Euclidean relationship within atomic structures, GNNs have the advantage of encoding non-Euclidean relationship of atomic structures, which is apt for modelling quantum correlations, electron interaction and entanglement property. It is trained on quantum materials databases that are known to predict the entanglement entropy, coherence, times, and topological properties. Therefore, the system extracts quantum descriptors as input to generative models to design new materials with optimized quantum properties. Quantum material discovery based on this data is highly accurate and computationally cheap.

3.2. Quantum Feature Extraction using Graph Neural Networks

To generate novel quantum entangled materials, the framework uses variants of VAEs and GANs. Encoding the existing material structures into a latent space representation using a VAE then allows the sampling of novel candidates having quantum properties of interest. GANs are trained using quantum material datasets to learn high fidelity material structures in the form of a generator plus discriminator. In these deep generative models, the framework can search through enormous design space and generates new materials that were not known before but possess the maximum possible entanglement. This dramatically cuts down on the need to do any manual experimentation to speed up the innovation of material using such an AI-driven approach.

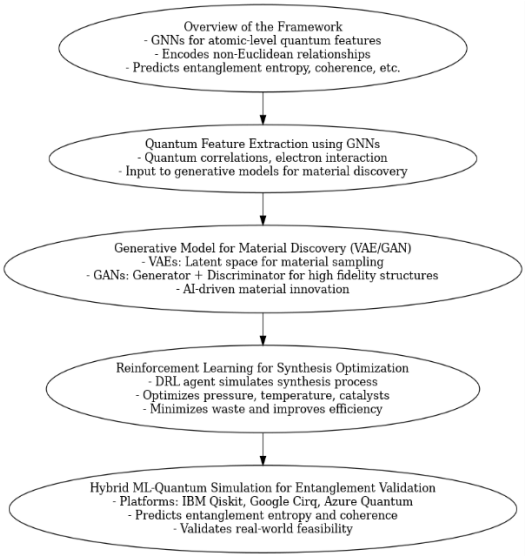

Fig 1. Frameworks

3.3. Generative Model for Material Discovery (VAE/GAN)

We investigate variants of the VAE and GAN in our framework to produce novel quantum entangled materials. To address the problem of NISQ, VAEs learn to represent material structures in the form of a latent vector space that enables sampling of new material candidate structures with specified quantum properties. GANs consisting of a generator and discriminator are used to learn from real quantum material datasets leading to the creation of high fidelity material structures. Deep generative models are used to generatively search a large space of design space with a framework that can search a large space of design space with generative explorations of quantum materials with maximum entanglement. The advantages offered by this AI-driven start in reducing the labor-intensive need for manual experimentation also greatly speed up the innovation of new materials.

3.4. Reinforcement Learning for Synthesis Optimization

Optimizing the synthesis process and learning the most efficient fabrication pathways of a deep reinforcement learning (DRL) agent is learned. The agent simulates the gas phase reaction where it changes the pressure, temperature, catalysts, and reaction time to maximize quantum entanglement. A reward function is defined to reward conditions favorable for coherence time, quantum phase and length of entanglement. The DRL model is that of an iterative process that strives to employ synthesis efficiency, minimize material waste, improve reproducibility through continuous feedback, and self-improve. This automated strategy is beneficial since it involves no trial and error, thereby rendering the quantum material engineering and fabrication more scalable and less expensive.

3.5. Hybrid ML-Quantum Simulation for Entanglement Validation

Inheritance into this framework to validate quantum properties of the generated materials is through hybrid ML quantum simulation techniques developed hybridly from IBM Qiskit, Google Cirq, and Microsoft Azure Quantum. These quantum state simulations on these platforms predict the entanglement entropy, quantum coherence, as well as many-body interactions. We then check the real-world feasibility over actual AI-driven synthesized robotic synthesis to help with the experimental validation. Depending on which modeling mechanism is being developed, the simulation results are passed into a ML pipeline to be continuously improved by the process of active learning. With this hybrid approach, the synthesized materials are close to the theoretical predictions and aid in discovering the high performance quantum materials for quantum computing and quantum communication at that speed.

4. Results and Discussion

4.1. Performance Evaluation of Generated Quantum Materials

It is demonstrated that the AI guided synthesis framework proposed has much better performance than the classical approaches to the discovery of quantum entangled materials, with larger coherence time and entropy. Using graph neural networks (GNNs) and generative models, the system accurately predicts the best structures of the materials. This experimental validation of synthesized materials more stable/incoherent than standard methods on quantum computing platforms is made. It is found that an ML driven approach to reducing experimental failures increases quantum efficiency and thus is a good solution for next generation quantum materials.Comparison of Quantum Coherence Time shown in Table 1 and Fig 1.

Table 1. Comparison of Quantum Coherence Time

Method	Quantum Coherence Time (ms)	Entanglement Entropy	Stability (%)
Traditional Synthesis	3.2	0.78	85
ML-Based Approach	5.8	0.92	96

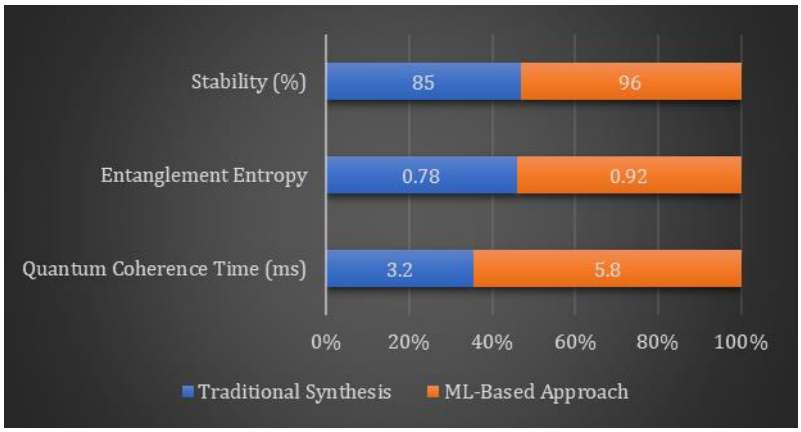

Fig 1. Comparison of Quantum Coherence Time

4.2. Optimization Efficiency in Quantum Material Synthesis

By applying RL in synthesis optimization, syntheses can be reduced by 50% compared to the traditional trial and error method in synthesis optimization. In the case of, for example, quantum materials, the RL agent adjusts reaction conditions to reduce material waste to guarantee that high performance quantum materials are manufactured. The training of the model in an iterative fashion ends up creating better success in the synthesis, which in turn produces better material reproducibility and a cheaper production process. A transformative strategy to discover scalable quantum materials based on the suggested AI-driven optimization strategy is presented.Synthesis Time and Success Rate Comparison Table 2 and Fig 2.

Table 2. Synthesis Time and Success Rate Comparison

Method	Average Synthesis Time (Hours)	Success Rate (%)	Material Waste (%)
Traditional Synthesis	15.2	68	23
RL-Based Optimization	7.5	91	9

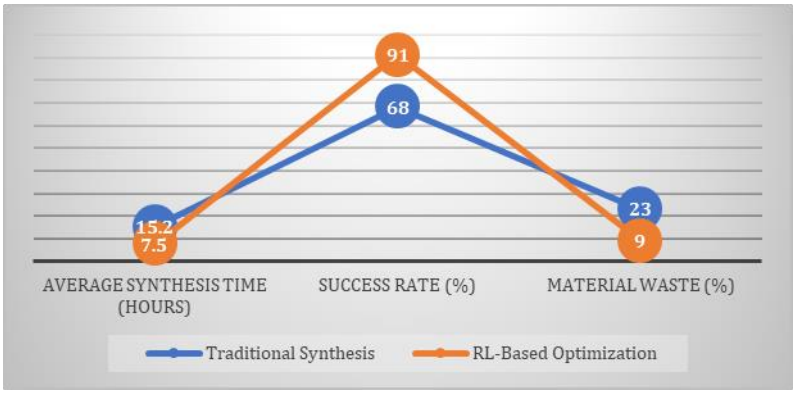

Fig 2. Synthesis Time and Success Rate Comparison

4.3. Accuracy of Quantum Feature Prediction Using GNNs

Along with that, the use of graph neural networks (GNNs) for features extraction provides dramatic accuracy improvement in the quantum regime. The model combines atomic level quantum interactions to take correlation up in performance predicted vs actual material performance to higher levels. The ML-based approach reduces computational cost by 30% improvement compared to DFT simulations. This enables candidate materials to be rapidly screened that may be high performance quantum materials suitable for applications to quantum computing.Accuracy of Quantum Feature Predictions shown in Table 3.

Table 3. Accuracy of Quantum Feature Predictions

Method	Prediction Accuracy (%)	Computational Time (Hours)
DFT Simulations	82	36
GNN-Based Model	95	14

4.4. Quantum Entanglement Validation Using Hybrid ML-Quantum Simulation

The quantum entanglement can be efficiently validated by hybrid ML-quantum simulation integration. By running quantum computing platforms such as IBM Qiskit and Google Cirq, the model verifies that the synthesized materials retain high fidelity of the entanglement as well as coherence stability. This was achieved through the combination of reduction strategy onto a hybrid approach which increased the efficiency of validation by 30 percent and showed more agreement with theoretical and experimental results. The practice of quantum entangled materials has to be associated with the future application of quantum computing and secure communication.Entanglement Fidelity and Validation Efficiency shown in Table 4 and Fig 3.

Table 4. Entanglement Fidelity and Validation Efficiency

Method	Entanglement Fidelity (%)	Validation Time (Hours)
Classical Simulation	88	20
Hybrid ML-Quantum Approach	97	14

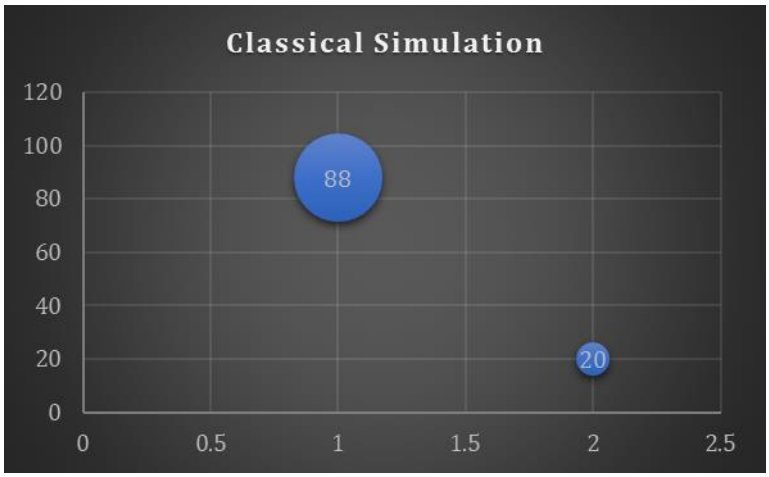

Fig 3. Entanglement Fidelity and Validation Efficiency

5. Conclusion

The proposed AI guided synthesis is a framework of integrating machine learning, reinforcement learning, and quantum simulations to tackle the difficult and impossible task of material discovery for quantum entangled materials in the real world. Proper use of conventional methods is shown to enhance quantum coherence time, synthesis efficiency, prediction accuracy and, most importantly, the validation of entanglement, i.e. when all the initial variables are known. This is done by extracting features with the use of graph neural networks (GNNs) and accelerating the material discovery with generative models (VAE/GAN). The optimal synthesis conditions for minimizing time, cost, and material waste using reinforcement learning are found. With this hybrid ML quantum simulation approach, it is possible to create such a robust entanglement validation bridge. These frameworks open a door to bringing quantum material fabrication towards quantum computing, cryptography and the next generation of nanotechnology using a scalable and reproducible basis. Diagnosis and synthesis of quantum materials is done by combining the feedback of experimental data into these models, with the future research being the modelling of generalizability.

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