

Predicting Complex Materials Energetics with a Scalable Compact Nine-Qubit Quantum Machine-Learning Model

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Accurate machine-learning (ML) prediction of material energies typically relies on large models with thousands to hundreds of thousands of parameters and scales poorly with the system size. Here, we present a compact hybrid classical-quantum ML framework that predicts the energies of complex materials using fewer than ten qubits, regardless of system size. By compressing local atomic descriptors into a fixed-size feature spectrum, we enable amplitude encoding of chemically diverse systems into shallow quantum circuits. We implement quantum convolutional neural networks (QCNNs) and quantum deep neural networks (QDNNs) with fewer than 100 trainable parameters and achieve prediction errors below 0.05 eV/atom on chemically complex alloys ($\text{Co}_{25}\text{Ni}_{25}(\text{HfTiZr})_{50}$) and lithium-intercalated metal-organic frameworks. Our results demonstrate the feasibility of scalable quantum assisted materials modeling and introduce a resource-efficient route toward quantum machine learning for atomistic simulations.

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I. INTRODUCTION

Machine learning (ML) has become an emerging tool for accelerating materials discovery by enabling fast and accurate predictions of physical properties across a vast chemical space. It has been applied to predict the phase behavior of high-entropy alloys [1], surface adsorption energies [2], and reaction barriers [3–5]. Recent advances in ML-based interatomic potentials allow energy evaluations at speeds orders of magnitude faster than density-functional theory (DFT), while maintaining comparable accuracy [6–8]. This capability has facilitated property prediction and evaluation of complex energy materials; e.g., the microstructures of complex mixed-ion perovskite [9] and graphite intercalation compounds [10]. However, high-performing ML models often require tens or hundreds of thousands of parameters and large training sets, and their computational cost limits applicability to small or medium-scale systems [11–14].

Quantum machine learning (QML) has emerged as a promising avenue for extending ML capabilities, with

recent studies exploring its potential for generalization in data-limited settings and high-dimensional representations [15,16]. Quantum convolutional neural networks (QCNNs) [17] extract local features via two-qubit operations and reduce dimensionality via pooling, analogous to classical CNNs, while quantum deep neural networks (QDNNs) [18,19] offer powerful function approximation based on the universal approximation theorem [20]. While QML models have shown promise in chemistry and condensed-matter applications, scalability to large complex systems such as high-entropy alloys or battery electrodes, in which site occupancy or permutations are pivotal to material properties, remains a key challenge, as most prior approaches require at least one qubit per atom [21–23].

In this work, we introduce a scalable hybrid classical-quantum ML framework that predicts total energies of materials containing arbitrary numbers of atoms using only nine qubits. We achieve this by compressing atomistic bispectrum descriptors into a fixed-size feature spectrum, enabling quantum encoding independent of system size. We benchmark our framework using QCNN and QDNN architectures on two chemically and structurally complex systems: a high-entropy intermetallic alloy $[\text{Co}_{25}\text{Ni}_{25}(\text{Hf,TiZr})_{50}]$ [24] and a lithium-intercalated Pb-BTC metal-organic framework (MOF)—where BTC refers to 1,3,5-benzenetricarboxylic acid ligands—a promising anode material for high-capacity lithium-ion batteries

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[25]. These complex materials feature intricate inter-atomic interactions including metallic bonding and ionic, covalent, and van der Waals interactions, making them ideal for testing our hybrid QML framework for complex energy materials. Our compact quantum models, with fewer than 100 trainable parameters, yield root-mean-square prediction errors below 0.05 eV/atom. These results establish a practical and resource-efficient strategy for quantum assisted property prediction or evaluation of complex energy materials, including emerging multication or halide-based photovoltaic materials, high-capacity battery anodes, advanced solid-state electrolytes, and next-generation cathode materials. This approach provides a scalable pathway to accelerate materials discovery and optimization in critical energy applications.

II. METHODS

The flow chart presented in Fig. 1 illustrates the process of our hybrid QML framework for predicting atomistic properties of materials. The framework consists of four steps: (1) generating the atomic feature vectors, (2) condensing the atomic feature vectors into the feature spectrum, (3) embedding the feature spectrum, and (4) predicting with the QML model. Steps (1) and (2) are performed on the classical computer to generate the system

representation to be encoded, whereas steps (3) and (4) map system information to qubit bases in the quantum circuit and make predictions. In the following, we will elaborate each step within our hybrid QML framework.

A. Feature-vector generation

The initial step in our hybrid QML framework involves converting the atomistic configurations, specifically the atomic types and coordinates denoted as $\{Z_i, \mathbf{r}_i\}$, into a set of feature vectors $\{Z_i, \mathbf{G}_i^{(j)}\}$ that is invariant under translation, rotation, and interchange of identical atoms. Here, $\mathbf{G}_i^{(j)}$ represents the feature vector of atom i . These vectors are capable of representing the chemical environment of each atom. In our study, we utilize the bispectrum components. Bartók *et al.* [26] have demonstrated that bispectrum components can be represented as an infinite overcomplete array with tunable sensitivity. In principle, the quantum nearsightedness principle ensures that the local atomic density around atom i can be written as

$$\rho_i = \delta(R) + \sum_{R_{ij} < R_c} f_c(R_{ij}) w_j \delta(R - R_{ij}), \quad (1)$$

where the weighting factors w_j enable element-wise distinctions. By projecting this atomic density onto a four-dimensional unit sphere via a triple correlation

$$(\emptyset, \theta, \theta_0) = (\tan^{-1}(\frac{y}{x}), \cos^{-1}(z/|\mathbf{r}|), |\mathbf{r}|/r_0), \quad (2)$$

the bispectrum matrix can then be constructed and expanded as

$$B_{j_1 j_2 j} = \sum_{m'_1, m_1 = -j_1}^{j_1} \sum_{m'_2, m_2 = -j_2}^{j_2} \sum_{m, m' = -j}^j (u'_{m'm})^* \times C_{j_1 m_1 j_2 m_2}^{jm} \times C_{j_1 m'_1 j_2 m'_2}^{jm'} u'_{m'_1 m'_1} u'_{m'_2 m'_2}, \quad (3)$$

where $C_{j_1 m_1 j_2 m_2}^{jm}$ denotes the ordinary Clebsch-Gordan coefficients and $u'_{m'm} = \langle U'_{m'm} | \rho \rangle$ is the inner product of the atomic density with the Wigner matrices [27]. In practice, truncated elements of $B_{j_1 j_2 j}$ are chosen, with all indices $j_1 j_2 j$ not exceeding the desired $J_{\max}$.

B. Feature condensation and embedding

The total number of descriptors describing the atomistic system is $J \times N$, where J is the length of each atomic feature vector and N is the total number of atoms in the system; however, $J \times N$ is in general a large variable number that cannot be handled by a limited number of input qubits within quantum circuits. In this work, we propose using the following approach to condense feature vectors.

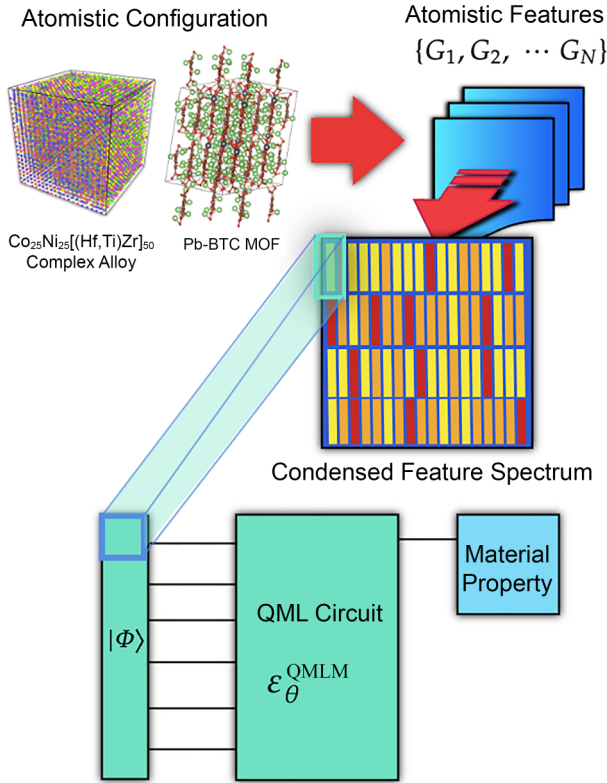


FIG. 1. The schematics of the hybrid classical-QML prediction framework of our atomistic simulations.

We compress a series of atomic feature vectors along the dimensions of the atom type and the atom index into an atomic feature spectrum

$$\tilde{\mathbf{h}}_j^K = \sum_{i=1}^N \mathbf{G}_j^{(i)} \delta_{Z_K, Z_i}, \quad (4)$$

where $\tilde{\mathbf{h}}_j^K$ is the condensed-feature-map component of the j th descriptor of the K th atom type. By utilizing this dimension-reduction approach, the $J \times N$ dimensions of the atomic features are then reduced to $J \times M$, where M specifies the total number of atom types in the system. The encoding of $\tilde{\mathbf{h}}_j$ into qubit states can be performed via amplitude embedding and thus the initialized quantum state can be written as

$$|\Phi\rangle = \sum_{l=1}^M \sum_{j=1}^J \frac{\tilde{\mathbf{h}}_j^l}{\alpha} |\psi_l\rangle, \quad (5)$$

where $|\psi_l\rangle$'s ($l=0, 1, \dots, J \times M - 1$) are the standard n -qubit bases $\{|0\rangle, |1\rangle\}^{\otimes n}$ and the normalization factor $\alpha = \sqrt{\sum_{l=1}^M \sum_{j=1}^J (\tilde{\mathbf{h}}_j^l)^2}$. It must be noted that the amplitude-embedding step is nontrainable and in the worst-case scenario, where the input vector is unstructured and fully dense, the gate complexity for exact amplitude encoding scales as $\mathcal{O}(2^n)$, which equals $\mathcal{O}(J \times M)$ in our case. While this represents a non-negligible overhead, it is incurred only during input loading and remains decoupled from the trainable part of the quantum circuit. Moreover, this fixed cost is acceptable given that the variational models (QDNN and QCNN) operate with low circuit depth and few trainable parameters, preserving the overall resource efficiency of the QML pipeline.

In this study, both the $\text{Co}_{25}\text{Ni}_{25}[(\text{Hf}, \text{Ti})\text{Zr}]_{50}$ complex alloy and the Li-intercalated Pb-BTC MOFs contain five atomic species. For bispectrum components, $J_{\max} = 4$ has been selected, leading to a total number of 55 feature-vector components for each atom. Consequently, the dimension of the condensed feature maps using bispectrum components is $J \times M = 275$. Hence, the number of qubits required for the input quantum state is $\lceil \log_2(275) \rceil = 9$. We can then utilize only nine qubits to encode the system information of complex materials of arbitrary sizes. It is worth emphasizing that a nine-qubit register can represent feature vectors of up to 512 dimensions. Our current feature-compression scheme leaves ample room to incorporate additional atomic descriptors, chemical fingerprints, or environment-dependent features when modeling even more complex materials, without increasing the number of qubits. This feature-space headroom ensures that our approach remains flexible and future proof, accommodating growing descriptor sets derived from richer structural databases or more chemically diverse systems.

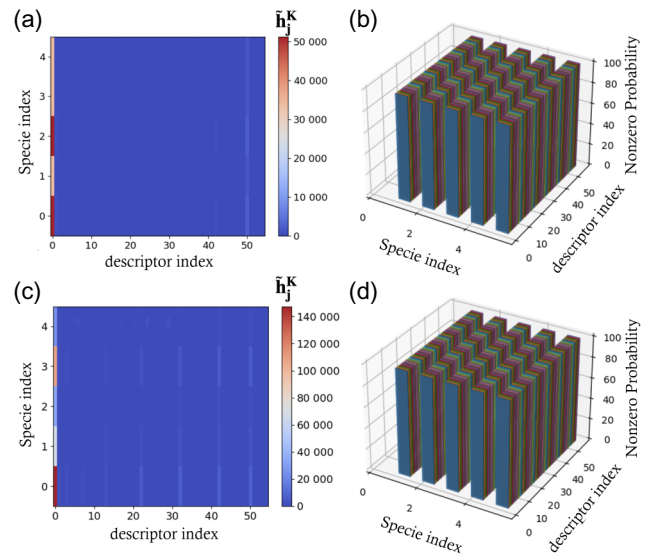


FIG. 2. The (a),(c) condensed feature maps and (b),(d) nonzero-pixel probability distributions for (a),(b) the $\text{Co}_{25}\text{Ni}_{25}[(\text{Hf}, \text{Ti})\text{Zr}]_{50}$ complex alloy and (c),(d) the Li-intercalated Pb-BTC MOFs.

Sample condensed feature maps of the $\text{Co}_{25}\text{Ni}_{25}[(\text{Hf}, \text{Ti})\text{Zr}]_{50}$ complex alloy and of the Li-intercalated Pb-BTC MOFs are displayed in Figs. 2(a) and 2(c), respectively. It is important to note that zeros in the condensed feature maps could lead to a high proportion of zero components when encoding into the input quantum state [Eq. (5)]. This, in turn, can cause a notable loss in variance in atomistic structures and severely restrict the exploration of the Hilbert space during both training and prediction processes. The probability of zero pixels in the condensed feature maps of all the training data is conducted [Figs. 2(b) and 2(d)], revealing the complete absence of zero pixels in these maps. We emphasize that the absence of zero pixels in the $J \times M$ condensed feature maps does not imply a dense quantum state. When embedded into the $2^9 = 512$ dimensional Hilbert space of a nine-qubit system, only 275 amplitudes are populated, with the remaining 237 amplitudes (approximately 46.3%) being zero by construction. This moderate sparsity level opens opportunities to reduce the gate complexity using approximate state-preparation schemes to reduce the preparation cost, depending on the allowed fidelity error. These methods are actively being developed and could be employed to further optimize performance on near-term quantum devices.

Moreover, there exists an alternative scheme with less-reduced compression, where atomic features have been encoded as histograms instead of being aggregated over atom types. In this histogram-based approach (detailed in Sec. 3 of the Supplemental Material [28]), the value range of each bispectrum component has been discretized into multiple bins, producing a $J \times K$ (where K refers to the

number of bins; see Sec. 3 of the Supplemental Material [28]) two-dimensional histogram map for each structure. These maps have then been flattened and amplitude encoded into quantum states. However, this method leads to a significant fraction of zero-valued bins (see Figs. S3 and S4 in the Supplemental Material [28]), introducing sparsity into the encoded input states. As a result, the predictive performance of both QDNN and QCNN models deteriorates noticeably (see Fig. S5 in the Supplemental Material [28]), likely due to the reduced distinguishability among quantum states representing structurally different samples.

C. QML architectures

We have constructed our QML circuits based on two quantum machine learning model (QMLM), namely, QCNN and QDNN. The QCNN model, depicted in Fig. 3(a), largely adheres to the architecture outlined in the literature [17], with the exception that a task-specific Hamiltonian representing the total energy of a material system is tailored to our specific objective. Regarding the QDNN model shown in Fig. 3(b), we have designed our quantum neural-network layer (QNNL) based on the references provided in the literature [29]. We have demonstrated that instead of constructing a QDNN with multiple deep layers of QNNLs, a single layer of QNNL (comprising an encoder layer, a transformation layer, and an output layer in sequence) along with a task-specific Hamiltonian as in our QCNN model, is adequate to achieve reasonable accuracy. It is important to highlight that both quantum circuits are designed with the specific goal of

steering clear of the barren-plateau landscape [30–32]. Our QCNN model, built upon the existing architecture, naturally avoids the occurrence of barren plateaus due to renormalization-group flow [33]. Similarly, our QDNN model is constructed with a layer-wise design emphasizing a relatively shallow depth [30,31]. Furthermore, in both QMLM, the task-oriented Hamiltonian is selected to adopt a concise local Pauli-Z operator form acting on the first qubit rather than being presented as a sum of global measurements [30]:

$$\mathcal{H} = \sigma_z^{(1)}. \quad (6)$$

This observable, adopted from Ref. [21], is imposed to extract energy predictions from the final quantum state to map the expectation value of the final quantum state onto a scalar quantity corresponding to the target property—in our case, the DFT-calculated total energy. The number of trainable parameters in the QDNN circuit decreases to 63, while in the QCNN circuit, the number of trainable parameters remains at 99 due to weight sharing. It is also noteworthy that in the context of the task-oriented Hamiltonian mentioned here, there is no assumption made about the form of energy partitioning [26,34]. In many classical ML frameworks of atomistic simulations of scalable system sizes, breaking down the total energy of a specific configuration into individual atomic energy estimates is a prevalent method for developing scalable interatomic potentials. With the introduction of the current QMLM in this paper and the task-specific Hamiltonian directly representing the total energy of a given system, we eliminate the traditional process of assigning individual energetic contributions to relevant atomic partitions. We note that in the current implementation, our QML framework focuses on total energy prediction and does not yet incorporate atomic force estimation. Predicting atomic forces within variational quantum circuits would require explicit force labels in the loss function and the computation of second derivatives of parametrized quantum gates with respect to both the circuit parameters and the atomic coordinates. Such calculations significantly increase the computational overhead and are known to introduce numerical instability, often resulting in poor accuracy for force components even when the energy predictions remain reasonable [22]. These limitations are intrinsic to current variational quantum models and constitute an active area of our future research direction.

D. Model training

The training procedure of the QMLM is depicted schematically in Fig. 4. The QCNN and QDNN models are denoted as $\varepsilon_{\theta}^{\text{QMLM}}(\cdot)$, where θ encompasses continuous trainable parameters within each Pauli gate in conjunction with the data pool $\mathcal{D}$. The data pool $\mathcal{D}$ comprises a set

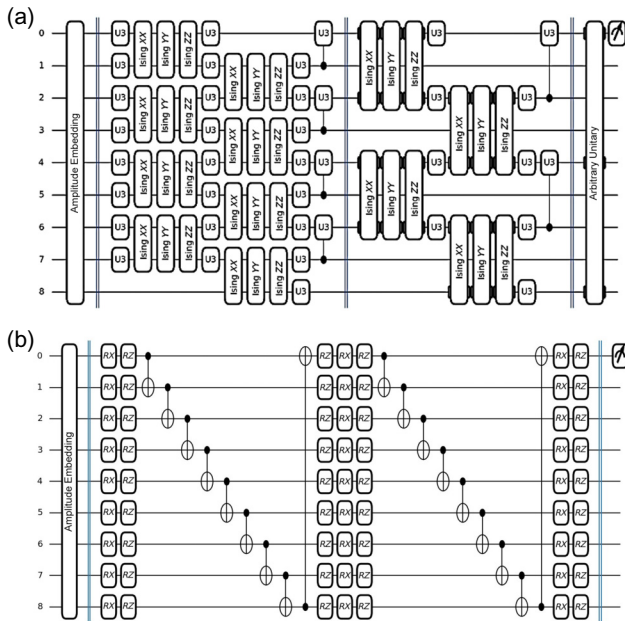


FIG. 3. The structure of the QMLM employed in the present study: (a) QCNN model; (b) QDNN model.

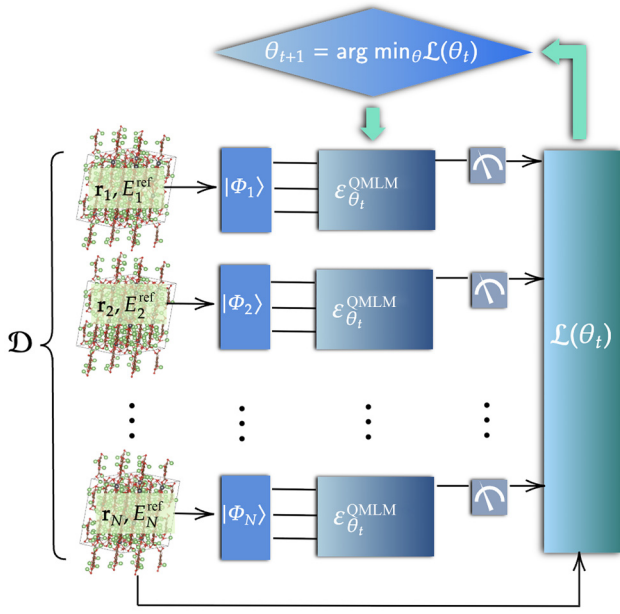


FIG. 4. The schematics of the training procedure of the QMLM.

of training images ($\mathbf{R}_m, E_m^{\text{ref}}$), where $\mathbf{R}_m$ denotes a specific configuration of a material system (i.e., the data entry) and E_m^{ref} represents the corresponding label, typically pertaining to material properties such as total energy or band gaps. During the training process, we have randomly selected K training images and the configuration of each state $\mathbf{R}_m$ in $\mathcal{D}$ is transformed into the respective quantum state Φ_m within QMLM using amplitude embedding. The QMLM parameter set θ is trained in an iterative manner. For training step t with parameter set θ_t , the loss function $\mathcal{L}(\theta_t)$ can be expressed as

$$\mathcal{L}(\theta_t) = \sqrt{\frac{1}{K} \sum_{m=1}^K \left\{ \text{Tr} \left[\mathcal{H}(\epsilon_{\theta_t}^{\text{QMLM}} \rho_m) \right] - E_m^{\text{ref}} \right\}^2}, \quad (7)$$

where $\mathcal{H}$ represents the task-oriented Hamiltonian, $\rho_m = \rho_m(\mathbf{R}_m)$ represents the density operator of the corresponding input state, and E_m^{ref} denotes the energy label of the m th training image in $\mathcal{D}$. Hence, Eq. (7) calculates the root-mean-square errors (RMSEs) between the QMLM predictions and the image labels in the training pool $\mathcal{D}$. The QMLM parameter is subsequently updated by minimizing $\mathcal{L}(\theta_t)$, namely, $\theta_{t+1} = \text{argmin}_{\theta} \mathcal{L}(\theta_t)$. Since the task-specific Hamiltonian $\mathcal{H} = \sigma_z^{(1)}$ acts only on the first qubit, the loss function is strictly local in nature, ensuring that the measured observable has a support that is independent of the system size and avoids the gradient delocalization (barren-plateau effects) associated with global cost functions [31,35]. As a result, the gradient of the loss function

is influenced only by a small backward light cone encompassing an $\mathcal{O}(1)$ -depth region of the circuit regardless of the total number of qubits.

In this work, the total energy derived from DFT calculations is utilized as the label for the QMLM training. The training data sets for this system have been established through extensive DFT calculations using the Vienna *ab initio* simulation package (VASP) [36–38] along with an all-electron projected-augmented-wave (PAW) pseudopotential [39,40]. A cutoff energy of 400 eV and a $3 \times 3 \times 3$ Monkhorst-Pack k -point mesh [41] have been employed. Additionally, van der Waals interactions have been accounted for by applying the Grimme dispersion correction (DFT-D3) [42]. The quantum simulations have been conducted using PennyLane [43]. The generation of feature vectors from atomistic configurations to atomistic descriptors has been accomplished by employing the LAMMPS package [44]. Optimization of the variational parameters has been carried out with the Adam optimizer from JAX [45].

For the training data sets, 400 sets have been randomly chosen from the data pool $\mathcal{D}$, while an additional 100 sets have been randomly selected for independent testing purposes. For the high-entropy alloy system, the data pool consists of B2-type structures generated through imposed strain ranging from -10% to $+10\%$, as well as structures with a variety of atomic site permutations, covering both geometrical and chemical variations. In the case of the Li-intercalated Pb-BTC MOF system, the data set comprises structures with varying degrees of Li intercalation (namely, capacity), leading to structural rearrangement due to the interplay of ionic interactions, van der Waals forces, and framework flexibility. As depicted in Fig. 4, the training processes can be parallelized [46] after utilizing the feature-compression approach. Furthermore, the principal-component analysis (PCA) to down-size input features can also be employed. Optimized parameters θ can be found in Tables S1–S4 for the QCNN model, and Tables S5 and S6 for the QDNN model, in the Supplemental Material [28].

III. RESULTS AND DISCUSSION

The training results are depicted in Fig. 5. The overall RMSEs of trained QMLMs range at approximately 0.05 eV/atom (1.15 kcal/mol) for the $\text{Co}_{25}\text{Ni}_{25}[(\text{Hf,Ti})\text{Zr}]_{50}$ alloy and 0.04 eV/atom (1 kcal/mol) for the Li-intercalated Pb-BTC MOF. This level of accuracy aligns with earlier studies that integrated the quantum energy-estimation (QEE) approach [47] into variational quantum eigensolver (VQE) algorithms. During the training processes, we have found that regularization (e.g., weight decay or parameter norm penalties) does not significantly affect the training or test accuracy, suggesting that under the current dataset size and model architecture, the QDNN does not suffer from overfitting. Nonetheless, regularizations may become

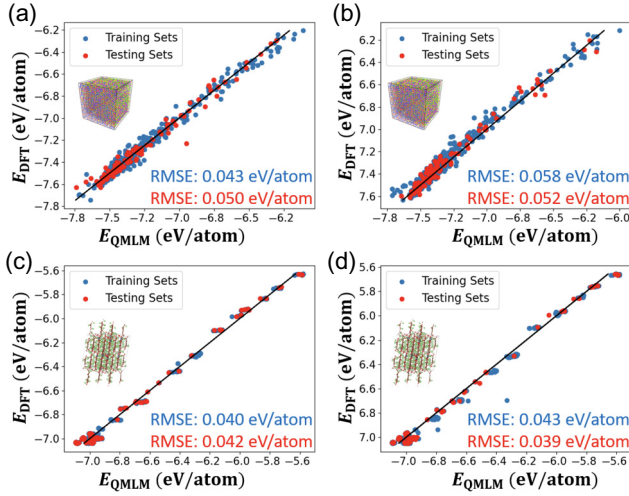


FIG. 5. Energy-parity plots for (a),(b) the $\text{Co}_{25}\text{Ni}_{25}[(\text{Hf}, \text{Ti})\text{Zr}]_{50}$ alloy and (c),(d) the Pb-BTC MOFs. (a),(c) Predictions from QCNN models. (b),(d) Results from QDNN models.

important when scaling to larger models or when training with smaller data sets. Furthermore, PCA tests reducing the dimensionality of the input features do not significantly degrade the model performance (as can be checked with the demo code provided on GitHub), implying that key chemical information is already well captured by the current bispectrum-based descriptors and embedding. Therefore, the scalability of our framework stems not from an increase in qubit count but from the intelligent structuring of input features, enabling generalization across complex materials within a fixed quantum register.

Although certain recently proposed QNN schemes can yield very low RMSE values [21–23], these models typically rely on assigning at least one qubit per atom, leading to substantial circuit width and depth. Such designs quickly become impractical for large or compositionally complex materials due to exponential hardware demands. By contrast, our approach maintains a fixed circuit width of nine qubits and uses only 63–99 trainable parameters, independent of the system size or number of atoms. This compactness enables energy predictions for chemically diverse and configurationally complex systems in which the microstructure—defined by permutations in atomic site occupancy—plays a critical role beyond macroscopic chemical compositions in determining functional properties, while remaining feasible on near-term quantum devices with limited qubit counts and coherence times. In this study, our QML models have achieved meaningful predictive accuracy despite being trained on modest data-set sizes, reflecting the efficiency of our feature-condensation scheme. Furthermore, our model framework is agnostic to the nature of the training labels; given appropriate data sets, the same architecture could be extended to predict other energy-relevant quantities such

as adsorption energies, reaction barriers, and electronic band gaps—properties critical for the design of catalysts, electrodes, and porous frameworks in sustainable energy technologies. Thus, the compactness, scalability, and generalizability of our QML models provide a promising foundation for quantum enhanced materials discovery in energy science.

To characterize the information accessibility and generalizability of our QML framework more quantitatively, we have examined the effective dimension [48] of our models. Given a statistical model M_θ , where $M_\theta = \varepsilon_\theta^{\text{QMLM}}$ in our case, its effective dimension is defined as

$$d_n(M_\theta) = 2 \frac{\log \left(\frac{1}{V_\theta} \int_\theta \sqrt{\det(\mathcal{I} + \frac{n}{2\pi \log(n)} \mathcal{F}(\theta))} d\theta \right)}{\log \left(\frac{n}{2\pi \log(n)} \right)}, \quad (8)$$

where V_θ is the volume occupied by the θ 's in the parameter space $\mathbb{R}^d$ and $n \in \mathbb{N}$ is the number of training data for M_θ . The Fisher information matrix $\mathcal{F} \in \mathbb{R}^{d \times d}$ (where d is the number of trainable parameters) has components

$$\mathcal{F}_{ij}(\theta) = \frac{1}{|\mathcal{X}|} \sum_{x \in \mathcal{X}} \sum_{\ell} \frac{1}{p_\ell(x; \theta)} \frac{\partial}{\partial \theta_i} p_\ell(x; \theta) \frac{\partial}{\partial \theta_j} p_\ell(x; \theta), \quad (9)$$

where $\mathcal{X}$ denotes a finite subset of samples drawn from the data pool $\mathcal{D}$. The inner summation corresponds to the per-input classical Fisher information, which follows the formulation in Ref. [49]. The probability $p_\ell(x; \theta)$ of obtaining a specific bit string ℓ is defined as

$$p_\ell(x; \theta) = \langle \psi(x, \theta) | \Pi_\ell | \psi(x, \theta) \rangle, \quad (10)$$

where $\Pi_\ell = |\ell\rangle\langle\ell|$ are projectors onto computational basis states ($\ell \in \{0, 1\}^n$). Here, $|\psi(x, \theta)\rangle$ denotes the quantum state produced by the variational quantum circuit $\varepsilon_\theta^{\text{QMLM}}$ on $|\Phi\rangle$ given input x and parameters θ . It should be noted that $\varepsilon_\theta^{\text{QMLM}}$ [see also Eq. (7)] is not associated with any specific target operator. We employ full computational-basis measurements to probe how large a volume the manifold of quantum states $|\psi(x, \theta)\rangle$ spans in Hilbert space. This allows us to assess the expressive capacity of the quantum model rather than to analyze a particular observable (further details are provided in Sec. 4 of the Supplemental Material [28]). In short, the effective dimension assesses the capability of ML models by quantifying the extent of the model space that they cover. Research suggests that a higher effective dimension is associated with better generalizability and trainability [21, 48, 50].

In Table I, we compare the normalized effective dimensions (d_{400}) of the QCNN and QDNN models for two material systems. The values are averaged over ten independent training trials, each initialized with random parameters

TABLE I. Normalized effective dimensions d_{400} with different materials and QNN models.

	QCNN	QDNN
$\text{Co}_{25}\text{Ni}_{25}[(\text{Hf},\text{Ti})\text{Zr}]_{50}$	0.64	0.78
Pb-BTC MOFs	0.64	0.75

and trained on 400 randomly sampled data sets from $\mathcal{D}$. Notably, the QDNN model exhibits consistently higher effective dimensions (0.75–0.78) compared to the QCNN model (0.64–0.64), suggesting that the QDNN model utilizes its parameter space more effectively despite having fewer trainable parameters. This higher effective dimension may enable richer feature extraction. However, the improved representation capacity of the QDNN model does not directly translate to superior predictive performance. To investigate this discrepancy between expressivity and performance, we have analyzed the eigenvalue spectra of the Fisher information matrix F_{ij} [48]. The eigenvalue distributions of both the QCNN and QDNN models can be found in Figs. S6 and S7 in the Supplemental Material [28]. The Fisher-spectrum analysis shows that while the QDNN model exhibits a higher normalized effective dimension—indicative of greater expressivity per parameter—it also shows an eigenvalue distribution that is more sharply concentrated near zero compared to the QCNN model. This concentration suggests reduced gradient diversity and increased optimization difficulty, consistent with a steeper or flatter loss landscape that impairs convergence. In contrast, the Fisher spectrum of the QCNN model is more evenly distributed, promoting smoother gradient flow and better generalizability, as reflected in its superior test performance. These findings reinforce the complementary roles of the effective dimension (capacity) and the Fisher spectrum (trainability), and underscore the importance of balancing model capacity with optimization tractability when designing variational quantum ML models.

Comparing with classical ML models, the hybrid QML model proposed in the present study yields unique advantages for property prediction and evaluation of advanced complex energy materials. For example, a classical ML model evaluating the microstructure of $\text{MA}_y\text{FA}_{1-y}\text{Pb}(\text{Br}_x\text{I}_{1-x})_3$ requires thousands of trainable parameters and extensive DFT-based training images [9]. In the present study, the input feature dimension is 275, derived from bispectrum components grouped by atomic species. A classical ML model such as the simple linear regression or shallow neural network trained on the same input vector would necessarily involve at least 275 trainable weights (in the first layer alone), not accounting for additional parameters from bias terms or hidden layers. In contrast, the compact hybrid QML model presented here uses fewer than 100 trainable parameters and only

hundreds of DFT training images while still achieving reasonable predictive accuracy. Hence, this resource-efficient framework offers a practical and scalable route to accelerate the exploration and optimization of a broad range of energy-relevant materials, including complex photovoltaic absorbers, high-capacity battery anode materials, advanced solid-state electrolytes, and next-generation battery cathodes.

IV. CONCLUSIONS

In summary, we have introduced a hybrid QML framework for energy prediction in complex material systems. Our approach employs an atomic feature-compression scheme that condenses high-dimensional atomic feature vectors (derived from bispectrum components) into a compact feature spectrum, enabling the encoding of an atomistic system of arbitrary number of atoms into a quantum input state using fewer than ten qubits. By leveraging QML models based on QCNNs and QDNNs, we have achieved competitive energy-prediction accuracy with fewer than 100 trainable parameters for two complex material systems: the $\text{Co}_{25}\text{Ni}_{25}[(\text{Hf},\text{Ti})\text{Zr}]_{50}$ alloy and the Li-intercalated Pb-BTC MOFs. These results not only demonstrate that atomistic simulations can be extended into the QML regime but also highlight the potential of our hybrid QML framework as a compact and efficient alternative for property prediction in complex materials.

The sample codes for QML training and energy prediction are available in Ref. [51] for the Pb-MOF system. The $\text{Co}_{25}\text{Ni}_{25}(\text{HfTiZr})_{50}$ data set is available from the authors upon reasonable request.

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DATA AVAILABILITY

The data that support the findings of this paper are not publicly available. The data are available from the authors upon reasonable request.

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