



OPEN Tripartite interaction representation algorithm for crystal graph neural networks

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Driven by emerging research paradigms, the application of artificial intelligence models presents innovative tools for designing materials and optimizing their performance. In the field of materials science, there is a current research emphasis on exploring techniques for characterizing material structures to achieve precise descriptions. This paper proposes a crystal graph convolution neural network model that incorporates a tripartite interaction approach. The model not only incorporates atomic information, bond lengths, and bond angles but also offers a method for updating atoms and bond lengths, facilitating accurate descriptions of crystal structures by capturing implicit structural information. Focusing on predicting the formation energy of crystalline compounds, our results demonstrate improved predictive accuracy compared to existing representation algorithms. The average error of the formation energy in the random dataset, demonstrating robust generalization, is merely 0.048 eV/atom, with an impressive R^2 value of 0.994. Additionally, this paper establishes a crystal graph neural network framework for predicting algorithm performance. By integrating automatic parallel algorithms and an automated process, we achieve a synthesis of these techniques, enhancing computational efficiency and streamlining algorithm usage.

The rapid evolution of artificial intelligence technology, coupled with the accumulation of extensive materials data, has sparked a significant transformation in the materials science research paradigm. This transformation is particularly evident in the field of new materials design, where machine learning methods now achieve levels comparable to density functional theory^{1,2}, while surpassing previous computational speeds by an order of magnitude³. Moreover, for cases with insufficient data or experimental results cases, machine learning methods also provide viable solutions^{4–6}. Nevertheless, a crucial challenge in employing machine learning methods for materials research lies in the accurate mapping of material structural information to descriptors. In simpler terms, it is necessary to represent crystal structures of varying sizes as feature vectors suitable for training machine learning models and practical applications^{7–10}. Researchers, in recent years, have seen extensive researches dedicated to addressing the challenge of constructing structural descriptors¹¹, resulting in various approaches, such as the structure matrix constructed using atomic features¹², multi-body tensor networks¹³, and feature reorganizations^{14,15}. However, these existing methods often depend on feature combinations aided by empirical techniques, requiring intricate and problem-specific operations, which limits their general applicabilities.

Currently, graph neural network (GNN) models¹⁶, which encode graph information into a rich representation space, are becoming increasingly popular among materials researchers. The unstructured nature of material structures and their interactions within multi-dimensional systems make GNNs well-suited to characterizing these structures. Originally designed for extracting descriptors from molecular graphs, GNNs are now being applied to graphical representations of crystal structures^{17,18}, resulting in improved prediction accuracy^{19–21}. The Crystal Graph Convolutional Neural Network (CGCNN) framework²² transforms crystal structures into corresponding graph grids, where each node represents an atom and edges represent bond lengths. This approach enables learning material properties from atomic interactions in crystals, using vectors for atoms and bonds to represent nodes and edges. The Representation Learning from Stoichiometry (Roost) model²³ is a physics-driven machine learning framework for predicting material properties in previously unknown crystal structures. It represents material components and stoichiometric ratios as dense weighted maps. The SchNet model²⁴ has demonstrated remarkable performance for molecules using only atomic numbers and atomic coordinates in a graph-based neural network model. The Message Passing Neural Networks (MPNN)²⁵ is a graph neural network framework abstracted from concrete graph neural network model. MACE²⁶ is a new equivariant message-passing

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neural network that improves the computational efficiency of the model by reducing the number of iterations required to reach convergence through a higher-order message-passing mechanism. MACE constructs local inter-atomic messages based on two-body features and then extends these features through tensor-product and symmetrization operations to implicitly encompass higher-order multi-body interactions.

In contrast to the conventional CGCNN model, the subsequently introduced MatErials Graph Network (MEGNet) model²⁷ offers universally high performance on a broad variety of target properties of molecules and crystals. It uses global state properties to construct a generalized framework for predicting state-property relationships, while also offering a quantitative approach to address the influence of structural periodicity on material properties. Materials 3-body Graph Network (M3GNet)²⁸ combines three-body interactions based on MEGNet, involving geometrical characterization of angles and dihedral angles of three atoms (not explicitly encoding multi-body interactions). The introduction of multiple angular information provides a comprehensive description of the atomic environment and shows high accuracy in the prediction of multiple material properties. In the Atomistic Line Graph Neural Networks (ALIGNN) framework²⁹, the initial graph encompasses atomic attributes, bonding attributes, and a set representation with global state attributes. The convolutional layer alternates between message passing on the graph and its bonding angle line graph to describe the crystal structure. This innovative approach incorporates edge vectors representing cosine values of bond angle relationships among three atoms, effectively utilizing angular information to enhance the accuracy of structure and molecular characteristics modeling. Although ALIGNN explicitly contains bond angle information, using the cosine value of the bond angle relationship between the three atoms, it does not explicitly encode higher-order many-body interactions. The Graph Neural Network Force Field (GNNFF) model¹⁹ can directly predict atomic forces by extracting features from the local atomic environment, achieving precise predictions of atomic forces and energy. Compared to ALIGNN, Atom-Distance-Angle Graph Neural Network (ADA-GNN)³⁰ proposes a crystal structure modeling based on dual scale neighbor partitioning mechanism, which optimizes the processing of bond-angle information by using different scales of cut-offs for edge neighborhoods and angle neighborhoods. The network processes node information and structural information separately, which improves the accuracy of prediction. It also considers the optimization of bond angle information without considering the multi-body interaction features.

While the existing crystal graph neural network models have demonstrated impressive results, they are currently limited to two-body interactions within the graph neural network convolution function. For most models, higher-order multi-body interactions are not explicitly encoded, and edge vectors in the crystal structure remain static, which is crucial for characterizing global information. The methodology for facilitating message passing between nodes and edge vectors requires further in-depth exploration. In this paper, we propose a novel neural network characterization algorithm for crystal graphs, that incorporates tripartite interactions. This approach explicitly encodes details of atoms, bond lengths, and more detailed features about bond angles, while introducing feature updates for edge vectors within the convolutional layer to capture implicit structural information. These enhancements aim to provide a more accurate method for characterizing crystal structures, aligning with the evolving research paradigm in materials science.

Tripartite interaction representation algorithm for crystal graph neural networks

In a graph neural network, the crystal structure is modeled as a crystal graph that encodes atomic information and bonds interactions between atoms. Subsequently, a graph convolutional neural network is constructed to extract the characteristic information of the crystal structure. The crystal graph describes the geometrical structure of the material, and the physical information is expected to be derived through the computation of the graph convolutional layer. Therefore, enhancing the capture of crystal structure information within the convolutional layer is crucial for accurate characterization. The current graph convolutional layer calculation method (as in CGCNN) is represented by Eq. (1):

$$\nu_i^{(t+1)} = \nu_i^{(t)} + \sum_{j,k} \sigma \left(z_{(i,j)k}^{(t)} W_1^{(t)} + b_1^{(t)} \right) \odot g \left(z_{(i,j)k}^{(t)} W_2^{(t)} + b_2^{(t)} \right) \quad (1)$$

where, W_1 and W_2 are training weights, b_1 and b_2 are biases, k represents the edge connecting two atoms, σ is a scalar gating mechanism used to learn parameters of inter-atomic interactions, g functions as the activation function for introducing non-linear coupling between layers, ν is the feature vector of the node, and z is the superposition of the atomic feature vectors and feature vectors of neighboring nodes, as well as feature vectors of connecting edges, computed using the expression $z_{(i,j)k}^{(t)} = \nu_i^{(t)} \oplus \nu_j^{(t)} \oplus u_{(i,j)}$. Here, $\odot$ represents element-wise matrix multiplication, and $\oplus$ represents direct vector addition. These operations are employed to learn the parameters of inter-atomic interactions. Additionally, batch normalization is applied to the convolutional layer to reduce the risk of model overfitting and to optimize computational efficiency.

While this method effectively characterizes atomic information and bond lengths, it lacks explicit characterization of the crucial bond angle information, which significantly influences the shape of the structure. Additionally, the current approach only updates node vectors during convolutional layer computation and does not address edge updates and expansion. To address these limitations, this paper introduces a novel graph structure description method that includes nodes, edges, and three-body roles. This method explicitly incorporates atoms, bond lengths, and bond angles, resulting in a comprehensive representation of the crystal structure. It accurately portrays chemical correlations involving three-body relationships (bond angles) and inter-atomic bonds (bond lengths) formed by neighboring atoms. An overview of the convolutional layer description is shown in Fig. 1.

After incorporating explicit characterisations of bond angles, the node vectors are updated using Eq. (2).

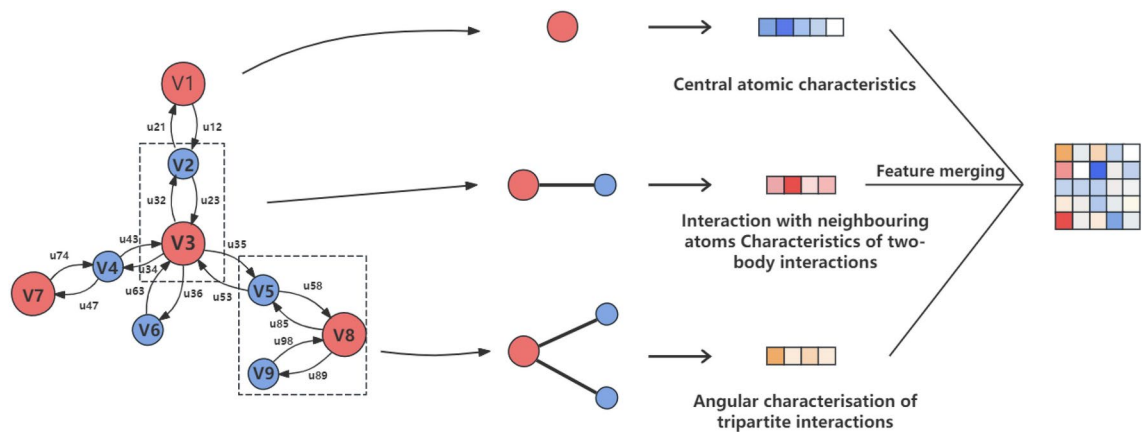


Fig. 1. Description of graph convolutional layer for feature calculation. A visual demonstration of our explicit encoding of tripartite interactions enriches the characterization information.

$$\begin{aligned} \nu_{(i,j)_k}^{(t+1)} = & \nu_{(i,j)_k}^{(t)} + \sum_{j,k} \sigma(z_{(i,j)_k}^{(t)} W_1^{(t)} + b_1^{(t)}) \odot g(z_{(i,j)_k}^{(t)} W_2^{(t)} + b_2^{(t)}) \\ & + \sum_{j,l,k,k'} \sigma(z_{(i,j,l)_{k,k'}}^{(t)} W_1'^{(t)} + b_1'^{(t)}) \odot g(z_{(i,j,l)_{k,k'}}^{(t)} W_2'^{(t)} + b_2'^{(t)}) \end{aligned} \quad (2)$$

A comparison between Eqs. (1) and (2) highlights that the latter explicitly describes the vector relationships among three atoms and two edges. In Eq. (2), i, j , and l represent atoms. The second term captures interaction information between the central atom and its immediate neighbors, while the third term accounts for bond angle information resulting from the interactions of the central atom with its two immediate neighbors and the three-body relationship formed by connecting edges. The relationships between node vectors and edge vectors connecting atoms i, j and l are consolidated to form as Eq. (3).

$$z_{(i,j,l)_{k,l'}}^{(t)} = \nu_i^{(t)} \oplus \nu_j^{(t)} \oplus \nu_l^{(t)} \oplus u_{(i,j)_k}^{(t)} \oplus u_{(i,l)_{l'}}^{(t)} \quad (3)$$

Where, v represents the feature vector of the node, and u denotes the feature vector of the edge. To provide a more comprehensive description of the local environment of the crystal, we introduce edge vector updates as Eq. (4).

$$u_{(i,j)_k}^{(t+1)} = u_{(i,j)_k}^{(t)} + \sigma(z_{(i,j)_k}^{(t)} W_1^{(t)} + b_1^{(t)}) \odot g(z_{(i,j)_k}^{(t)} W_2^{(t)} + b_2^{(t)}) + \sum_{l, k'} \sigma(z_{(i,j)_l k, k'}^{(t)} W_1'^{(t)} + b_1'^{(t)}) \odot g(z_{(i,j)_l k, k'}^{(t)} W_2'^{(t)} + b_2'^{(t)}) \quad (4)$$

In Eq. (4), the second term captures the effect of the two atomic node vectors connected to the edge vectors, and the expression for $z'_{(i,j,l)}{}_{k,k'}$ in the third term is consistent with Eq. (3).

The representation algorithm proposed in this paper for the crystal graph neural network with tripartite interactions aims to capture the interactions between atoms in a crystal structure more comprehensively. In traditional two-body interaction crystal graph neural networks, angle information may not be fully captured and could be overlooked during node or key updates. The proposed approach explicitly incorporates tripartite interactions, allowing for a more thorough and accurate representation of bond angle information. This in turn provides a more precise description of the local atomic environment by connecting each node to its neighboring nodes, updating the edge vectors and enhancing the overall representation.

Framework design and implementation

To facilitate the utilization of the proposed tripartite interaction neural network characterization algorithm, this paper introduces a new crystal graph convolutional neural network framework named “Tripartite interaction representation algorithm-enhanced Crystal Graph Neural Networks” (TiraCGCNN). The framework comprises two key components, as illustrated in Fig. 2, the structure graph representation network and the material property prediction network. The structure graph representation network is responsible for characterizing the material structure. It takes atom feature vectors and edge feature vectors as inputs, employs a fully connected layer(L1) for updating atomic graphs, and extends the graph’s scope through multiple convolutional layers. It then constructs graph vectors used as inputs to the material property prediction network after a pooling layer. The material property prediction network reads the graph vectors generated by the structural graph representation network,

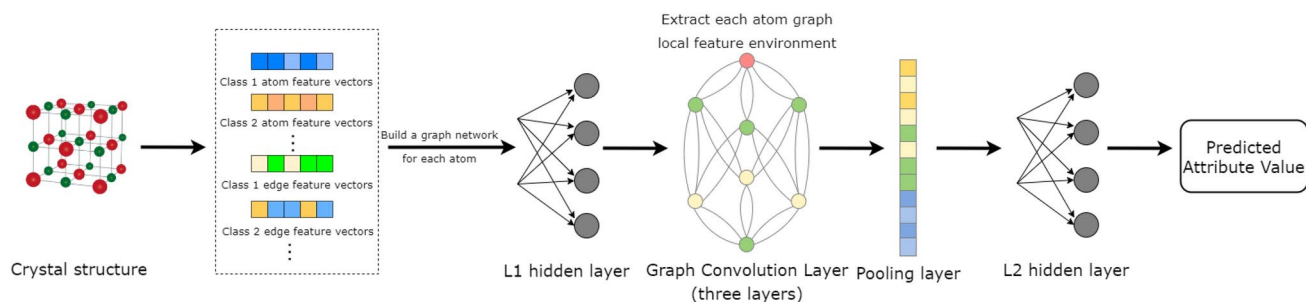


Fig. 2. Framework for tripartite interaction representation algorithm-enhanced crystal graph neural networks.

updates the structure-property model parameters through a fully connected layer(L2), and produces a highly accurate material property prediction model.

The structure graphs of crystals exhibit periodicity, allowing for multiple edges between the same pair of terminal nodes. In this framework, both node vectors and edge vectors are preserved to capture the inherent periodicity in crystal structures. Each node and edge within the crystal undergo feature extraction. The structure graph network utilizes graph convolutional layers to aggregate feature information between nodes and nodes, as well as nodes and edges. In a crystal graph network, each node, denoted as i , is represented by a feature vector v_i encoding the attributes of the corresponding atom. Similarly, each edge, represented as $(i, j)_k$, is associated with a feature vector $u(i, j)_k$ characterizing the k_{th} bond connecting atom i and atom j . This preservation of both node and edge vectors enhances the network's ability to represent the distinctive characteristics of the crystal structure.

Specifically, the structure graph neural network begins by extracting feature vectors for each atom and various types of chemical bonds present in the crystal structure. Subsequently, a local environment connection graph is created for each atom, and the atom graph is updated through the collaborative action of fully connected layers L1 and multiple graph convolutional layers. At this stage, the feature vectors obtained for each atom encapsulate information about its immediate surroundings. Considering the limited number of atoms within the crystal structure unit, the effects of a three-layer graph convolution can be extended to the entire graph, as depicted by the Eq. (5).

$$v_i^{(t+1)} = Conv(v_i^{(t)}, v_j^{(t)}, u_{(i,j)_k}^{(t)}), \quad (i, j)_k \in G \quad (5)$$

After this, a pooling layer synthesizes the distinct atomic local environment vectors into a comprehensive graph vector representing the overall crystal environment, as shown in Eq. (6).

$$v_c = Pool(v_0^{(0)}, v_1^{(0)}, \dots, v_N^{(0)}, \dots, v_N^{(R)}) \quad (6)$$

With the acquired crystal structure graph vectors, a fully connected layer (L2) for crystal structure and property prediction is established, ultimately leading to the prediction of target property values. Two fully connected hidden layers, L1 and L2, are utilized to capture the intricate relationship between crystal structures and properties. The output of L2 corresponds to the target property.

During the training process, the Loss function $J(y, \hat{y})$ quantifies the disparity between the predicted attribute value($\hat{y}$) and the actual attribute value (y). The weights in the model are iteratively adjusted to optimize the model by minimizing the loss function using the training data. The entire model can be viewed as a function(f) that is parameterized by the weights(W), mapping crystals(C) to target attributes(y). Training the model can be conceptualized as the following optimization problem, as represented by Eq. (7).

$$\min_w J(y, f(C; W)) \quad (7)$$

Application of TiraGCNN on formation energy prediction

With this framework, the initial step involves representing the crystal structure using a graph neural network. This network encodes atomic information and depicts bonding interactions between atoms in the form of a crystal graph. Subsequently, a graph convolutional neural network is constructed based on this graph representation. Finally, target property predictions are obtained through the training process. In this experiment, data calculated by Density Functional Theory(DFT) serves as the training dataset, enabling the graph neural network framework to achieve an optimal representation of material structures and make precise predictions of target properties.

Dataset

The dataset for this work is sourced from the well-known open-access materials database, the Materials Project(MP)³¹. All the data are screened with three restrictions: (i) using GGA-PBE as the exchange-correlation functional, (ii) setting the kinetic energy cutoff to 520 eV, and (iii) ensuring the precision mode is set to Accurate or High. These restrictions make the data as reliable and comparable as possible. To ensure the generalization

ability of the model, inorganic crystals ranging from simple metals to complex compounds are included in the selected dataset. The dataset comprises a total of 23,744 data entries, encompassing 87 different elements, 7 crystal systems, and 230 space groups. In addition to the common binary, ternary, and quaternary compounds, the dataset includes complex compounds with more than 5 elements, within the range of atoms per unit cell from 1 and 200. The specific data distribution is illustrated in Fig. 3. The training, validation, and test sets were divided in a ratio of 8:1:1, with about 19,000 in the training set and about 2,400 in the test set. In addition, the test set covered the types of chemical element species in the training set (monocompounds to heptacompounds), and contained octacompounds (which did not appear in the training set). The test set also contains uncommon inert gases such as helium and other elements. We show the proportions of compounds in the dataset, with binary, ternary and quaternary compounds making up a large proportion, as well as containing more complex compounds. In addition, we show the distribution of the data in a scattered form in Fig. 3a and b, and a histogram plot in 3c. The quantile-quantile plots, which help assess if a set of data plausibly came from some theoretical distribution such as a normal or exponential, are shown in [Supplementary Figures](#).

Parameter setting and optimization

To construct the material graph neural network, we initially employ the One-hot encoding to initialize the input features of crystal structure and define the input for the graph neural network model. The feature vector dimensions are as follows, beginning with 19 bits for the elemental group number, 7 bits for the elemental periodic number, 10 bits for the covalent radius, 10 bits for the electronegativity, 10 bits for the first ionization energy, 10 bits for the electron affinity, a total of 4 bits for each orbital (s, p, d, and f), 12 bits for the atomic volume, and 10 bits for the valence electrons. In total, 92 bits are synthesized to encode the atomic input features. However, the edge vector feature differs, as it is based on the encoding of the interatomic distance. For the interatomic distance, we set the maximum radius of the atomic local environment set to 8 Å and the maximum number of nearest neighbor atoms set to 12. And the interatomic distance is encoded using the RBF (Radial Basis Function) thus obtaining the input edge feature vector to be 80 dimensional. For the atomic input feature encoding, we follow the 10 categories for continuous values based on the range and code the features separately. For continuous property values, the range of values is evenly divided into 10 categories, and then the vectors are encoded according to which range these property values fall within. To be precise, the range of values of the continuous values attribute is divided equally into ten categories, encoded in the form of one-hot encoding, with the position corresponding to the category encoded as 1 and the rest of the positions as 0. For discrete values, we directly code them based on the predefined categories. The following Table 1 presents the dimensions after encoding of atomic attributes.

In the training of neural network models, the choice of batch size plays a significant role in the outcomes. It directly affects training speed, memory usage, model convergence, and parameter update stability. Therefore, selecting the appropriate batch size is crucial. To achieve improved training results, we conducted tests on different batch sizes, and the test results are depicted in Fig. 4, more details can be reached from the [Supplementary Tables](#).

From Fig. 4, it becomes evident that, with the increase in the number of epochs on the same test set, the Mean Absolute Error(MAE) gradually decreases. Batch size has a substantial impact on both training time and accuracy. For instance, when running for 300 epochs, the MAE is minimized with a batch size of 64, whereas a batch size of 128 corresponds to a shorter training time. The best trade-off between training time and accuracy is achieved with a batch size of 128 for 400 and 500 epochs. Therefore, choosing a batch size of 128 appears to be the most suitable option.

Furthermore, the parameters relevant to the training process encompass the usage of the AdamW optimizer³², an improvement over Adam+L2 regularisation. The learning rate is set to 0.001, and the activation function employs the Tanh function, which enables the model to obtain better learning and representation capabilities. In terms of neural network size settings, the maximum radius of the atom's local environment is established at 8 Å and the maximum number of nearest neighbor atoms interacting with the central atom is limited to 12. The input atom embedding vectors are 92-dimensional, as previously described, and the input edge embedding vectors encompass 80 dimensions, reflecting a combined representation of inter-atomic distances and interactions. To accommodate the variability in the material dataset and minimize the influence of outliers

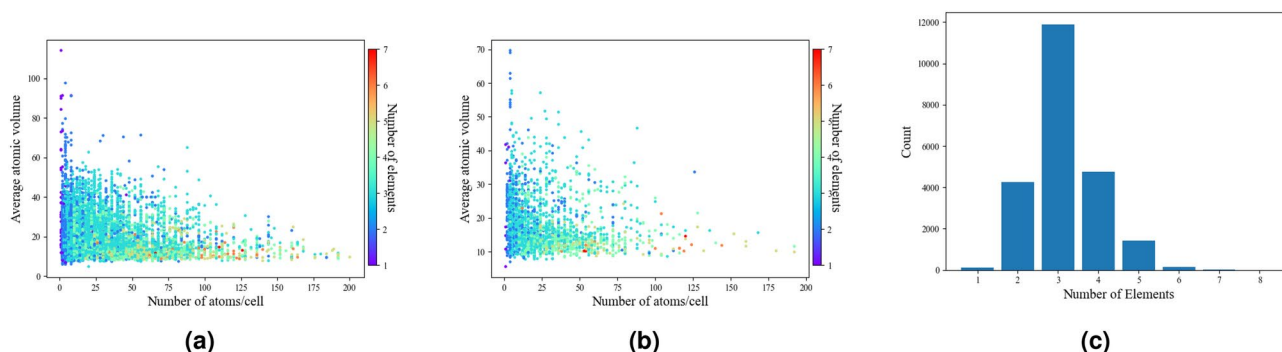


Fig. 3. Structural distribution of all data sets, (a) is for train set and (b) is for the test set. (c) is the distribution of the number of different elemental species.

Attribute	Unit	Dimension
Elemental group number	—	19
Elemental periodic number	—	7
Electronegativity	—	10
Covalent radius	pm	10
First ionisation energy	eV	10
Electron affinity	eV	10
Orbitals (s, p, d, and f)	—	4
Atomic volume	cm ³ /mol	10
Valence electrons	—	12

Table 1. Atomic attributes encoding and their dimensions.

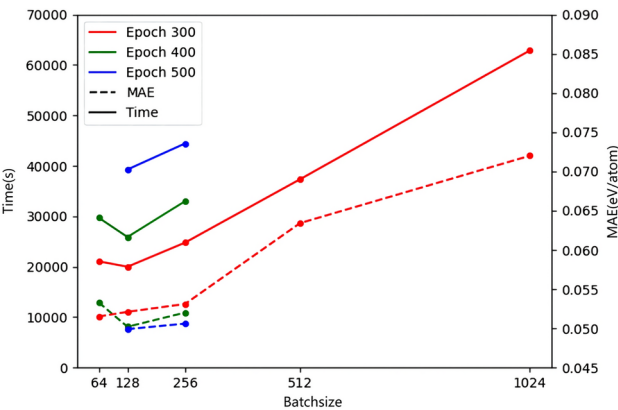


Fig. 4. The impact of batch size on training time and accuracy of model. A line graph shows the changes in training time and test results for different batch size. The impact of different batch sizes on training can be visualized.

Layers	2	3	4	5
MAE (eV/atom)	0.095	0.080	0.084	0.091
Time (s)	1171	1523	1851	2165

Table 2. Effect of different numbers of convolutional layers on model prediction results for formation energy.

on the results, the MAE is used as the cost function, and the coefficient of determination R^2 is utilized to evaluate fitting performance of the model.

In the model, the graph convolutional layers encompass interactions involving the central atom and its immediate neighbors, allowing information to propagate through the convolution of the atom feature vectors and edge feature vectors, resulting in a more precise characterization of the central atom's local environment. In this experiment, interactions between the central atom with its 12 immediate neighbors are characterized and diffused through multiple convolution layers across the entire graph. The number of convolution layers directly impacts the extent of this diffusion, enabling the central atom to interact with atomic features at greater distances. Notably, in the crystal structure model, closer atoms have stronger interactions with the central atom, while more distant atoms have weaker interactions. To determine the optimal number of convolutional layers, a series of tests were conducted under the following conditions, 300 epochs, a test set size of 3000, and consistent hyper-parameters from previous settings. The results are presented in Table 2.

From Table 2, it is evident that with only 2 convolutional layers, while the training time is shorter, the performance of model is significantly poorer. On the other hand, as the number of convolutional layers increases from 3 onwards, training time also increases, but there is a diminishing return in terms of model performance. Therefore, the most favorable results are achieved with 3 convolutional layers.

Formation energy prediction

In this experiment, the previously optimized parameter set was used to train the model and predict the performance of formation energy property values for the inorganic compounds. The results, in terms of MAE and R^2 values, are presented in Fig. 5. As depicted in Fig. 5, the trained model achieved a Mean Absolute

Error(MAE) of 0.021 eV/atom with a coefficient of determination (R^2) of 0.9981. Meanwhile, the tested model exhibited MAE of 0.050 eV/atom, with an R^2 value of 0.9916.

Comparisons with existing methods

In order to assess the effectiveness of the proposed tripartite interactions graph neural network proposed in this paper, we compared it with widely-used high-precision models, such as CGCNN, Roost, and MEGNet. We calculated their prediction accuracy and studied the impact of training set size on the results. Our tests showed that Roost, CGCNN, and TiraCGCNN achieved excellent results with 400 epochs, while MEGNet achieved model convergence at 1000 epochs. The tests were conducted using a five-fold cross-validation method, wherein we randomized one seed at a time, totaling five seeds trained in each group. The final result is an average of the model's performance across all seeds. We focused on the formation energy related to structural stability as the target value for model training, and the results of the four models are depicted in Fig. 6.

TiraCGCNN exhibits significant advantages over the other three models across various sizes of training sets. Notably, the MAE of the prediction model reaches 50 meV/atom in the model trained on 20,000 pieces of test data, which is smaller than others. To assess the generalization ability of the models, the data selected for this experiment were unrestricted and uncleaned. In this test, the Roost, CGCNN, and MEGNet models do not achieve the highest reported prediction accuracy in this dataset, with Roost at 24 meV/atom²³, CGCNN at 39 meV/atom²², and MEGNet at 28 meV/atom²⁷. It is noticed that the MEGNet model shows a higher MAE, its higher precision can be obtained from a larger dataset (more than 20k from the benchmark test³³). However, under the same dataset conditions, the TiraCGCNN model developed in this work outperforms the existing models, thanks to the improvements made to address the limitations of the CGCNN model in this paper. These improvements include incorporating interactions of bond angles between three atoms and updating the features of edge vectors for two-body and tripartite interactions, resulting in a more accurate representation of the local atomic environment.

To further assess the generalization ability of the model more comprehensively, this experiment was supplemented with approximately 1000 additional test data which from different sources (Also from Material Project, randomly selected). The test results are depicted in Fig. 7.

From Fig. 7, it can be seen that the TiraCGCNN model proposed in this work demonstrates superior generalization ability compared to the other three models, with a lower MAE. This enhanced performance indicates the robustness of the proposed tripartite interaction representation algorithm. Consequently, the model's adaptability to complex multi-element compounds, such as those with more than five elements, makes it a valuable tool for materials science researchers, especially in their pursuit of novel and unconventional materials with unique properties. The introduction of angular information can enhance accuracy, and models like M3GNet, which utilizes various angular information to implicitly encode higher-order three-body interactions, currently perform remarkably well. The reported training model of M3GNet uses the Materials Project dataset, consisting of approximately 60,000 items, with a prediction MAE of 0.019 eV/atom. We also tested M3GNet using the same dataset of 1,000 items mentioned above, with its reported pre-trained model, resulting in a prediction MAE of 0.069 eV/atom. Compared to the results from Fig. 7 for TiraCGCNN, the MAE of M3GNet is slightly higher, indicating that TiraCGCNN demonstrates better stability and generalization ability. This suggests that explicitly encoding higher-order multibody interactions can be beneficial.

Furthermore, the training time provides a visual depiction of the computational complexity differences among various models. The Roost model, despite its simple architecture and lower prediction accuracy, has a significant advantage in terms of training time. In contrast, the MEGNet model, which incorporates global

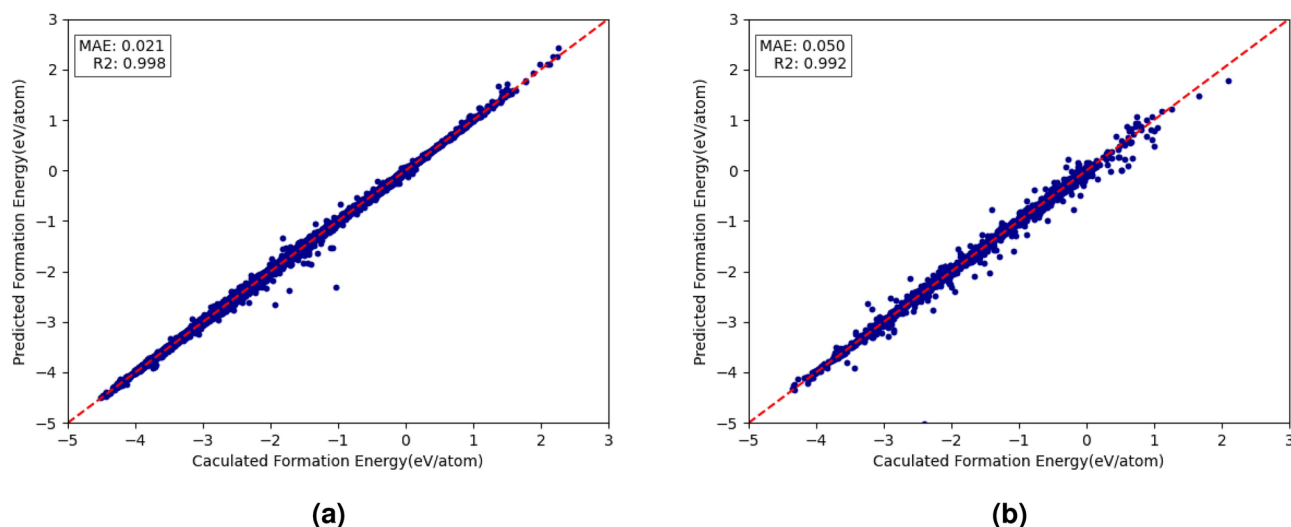


Fig. 5. Model performance on formation energy prediction of crystal compounds, (a) is for train set and (b) is for the test set.

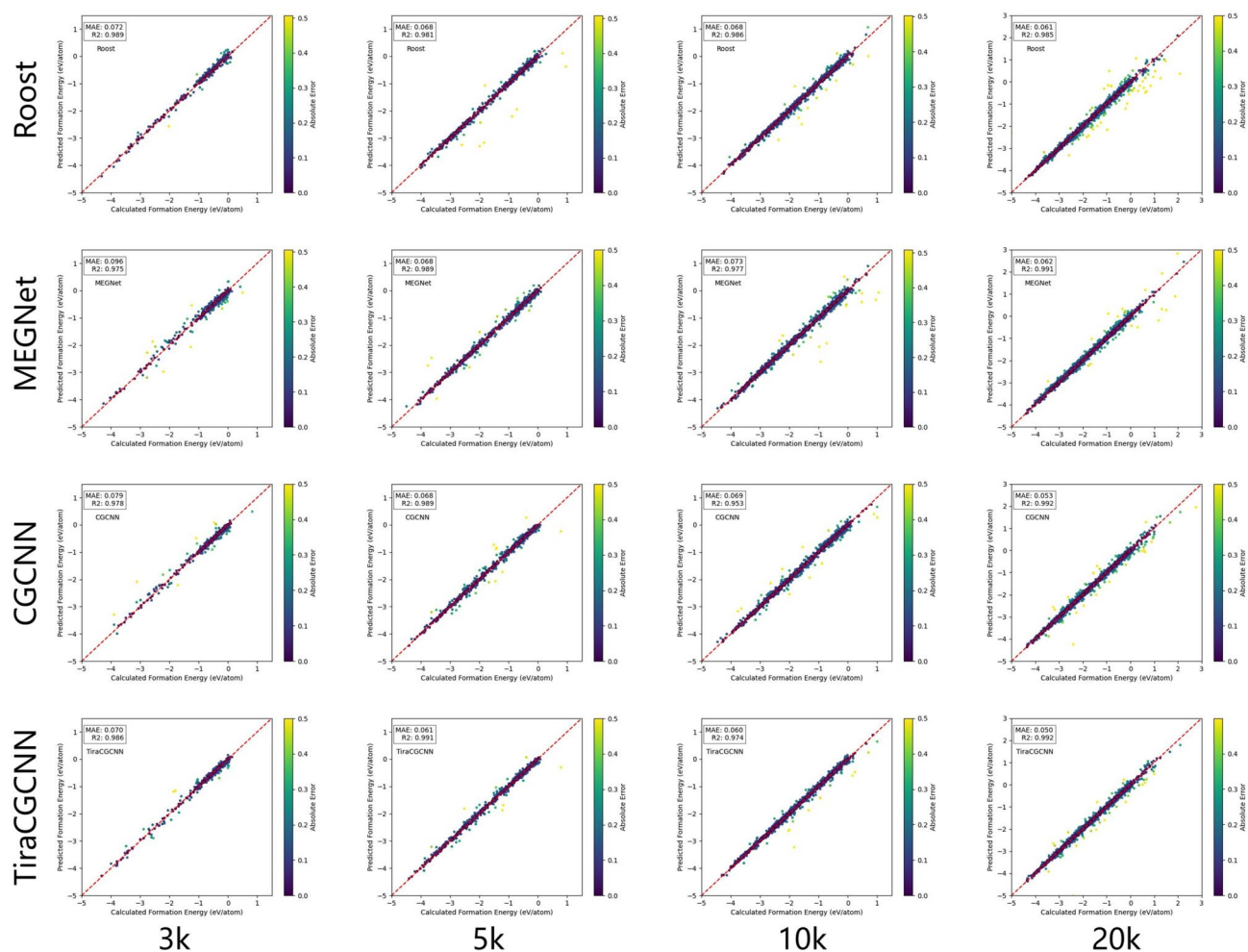


Fig. 6. The relationship between calculated values and predicted values with different train set sizes for four models. We can see the MAE and R^2 of each model under different sized datasets. Under the same dataset conditions, TiraCGCNN shows significant advantages, thanks to the improvements made in this paper.

Data size	Time(s)			
	Roost	MEGNet	CGCNN	TiraCGCNN
3k	1196	10257	959	2013
5k	1760	12396	1739	7018
10k	2560	14258	2659	11956
20k	4686	24373	5794	25884

Table 3. Training time for different models with different data sizes.

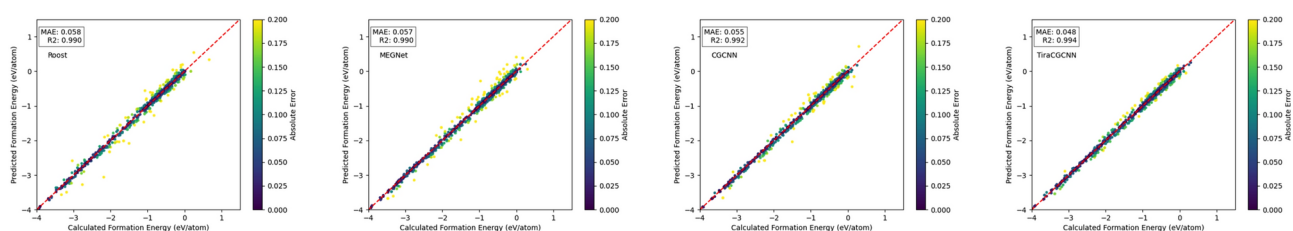


Fig. 7. Generalization performance of four models. We can see that for randomly supplemented additional test data, TiraCGCNN still maintains a low MAE with stronger generalization ability.

attribute computation on top of the CGCNN, experiences an increase in training time due to its added complexity. The TiraCGCNN model proposed in this work involves a more precise representation of the convolutional layer update process, resulting in increased computational effort and, consequently, a substantial rise in training time, as shown in Table 3. While the TiraCGCNN model's training time is longer, we consider it to be within acceptable limits. For larger datasets, additional parallel techniques and resources could be introduced to speed up the training process. Moreover, since machine learning models serve as surrogates for electronic structure computations, where inference time is critical, we conducted experimental tests to compare TiraCGCNN with M3GNet, using 1000 data points from this paper. The inference time for the M3GNet model is 24.8 seconds while the inference time for the TiraCGCNN model is 17.4 seconds. The inference times of TiraCGCNN and M3GNet are close, with TiraCGCNN being slightly faster. This indicates that the inference speed of the TiraCGCNN model is within a reasonable and acceptable range.

Discussion and conclusion

The precise characterization of crystal structures significantly influences the prediction of material structural properties. To attain a more accurate crystal structure characterization, this paper proposes a tripartite interactions representation algorithm enhanced crystal graph convolutional neural network model (TiraCGCNN). This model comprehensively unveils the correlations between atoms in crystals by capturing implicit structural information. In comparison to existing models, the TiraCGCNN model proposed in this paper demonstrates clear advantages in predicting crystal structure formation energy. Additionally, this paper establishes a framework for predicting crystal structure performance based on TiraCGCNN, further improving model efficiency through parallelization and process automation. The TiraCGCNN model shows improved performance in predicting formation energy. However, since certain information, such as calculation parameters, is not included in the model, fine-tuning is necessary to achieve high prediction accuracy for performance predictions that heavily depend on these parameters.

In terms of the research on the crystal graph structure representation model, there is still a need to explore the updating method of the graph convolutional layer. Particularly, it is essential to determine how to efficiently and accurately expand the network to encompass the entire crystal structure. Additionally, for the periodic features of crystals, integrating crystal structure-related principles and property information into the model can be explored to enhance accuracy and interpretability. Furthermore, to reduce the computational complexity of graph convolutional neural network models, the framework will seek to improve training efficiency through algorithm parallelism and process parallelization techniques.

Data availability

The data that support the findings of this study are available at <https://github.com/materialsCnicCas/TiraCG-CNN/tree/main/data>, or from the corresponding author upon reasonable request.

Code availability

The code that support the findings of this study are available at <https://github.com/materialsCnicCas/TiraCG-CNN>.

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Author contributions

Zongguo Wang and Yangang Wang contributed to design of the study. Yang Yuan, Ziyi Chen and Tianyu Feng performed the implementation and wrote the first draft of the manuscript. Zongguo Wang, Fei Xiong and Jue Wang reviewed and edited the manuscript. All authors reviewed the manuscript and approved the submitted version.

Declarations

Competing interests

The authors declare no competing interests.

Additional information

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