

# Lightweight equivariant model for efficient interatomic potential predictions

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## Article

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# **Lightweight equivariant model for efficient interatomic potential predictions**

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## Abstract

In modern computational materials science, deep learning has shown the capability to predict interatomic potentials, thereby supporting and accelerating conventional simulations. However, existing models typically sacrifice either accuracy or efficiency. Moreover, lightweight models are highly demanded for offering simulating systems on a considerably larger scale at reduced computational costs. Here, we introduce a lightweight equivariant interaction graph neural network (LEIGNN) that can enable accurate and efficient interatomic potential and force predictions for molecules and crystals. Rather than relying on higher-order representations, LEIGNN employs a scalar-vector dual representation to encode equivariant features. By extracting both local and global structures from vector representations and learning geometric symmetry information, our model remains lightweight while ensuring prediction accuracy and robustness through the equivariance. Our results show that LEIGNN consistently outperforms the prediction performance of the representative baselines and achieves significant efficiency across diverse datasets, which include catalysts, molecules, and organic isomers. Finally, we conduct a comparative analysis of LEIGNN against both classical molecular dynamics (MD) and *ab initio* MD simulations across solid, liquid, and gas systems. It is found that LEIGNN can achieve the accuracy of *ab initio* MD and retain the computational efficiency of classical MD across all examined systems, demonstrating its accuracy, efficiency, and universality.

## INTRODUCTION

In the field of computational materials, the calculation of interatomic potentials is critical for obtaining energy and then other energy-related physical quantities, such as forces and atomic trajectories. The computational methods, using pre-fitted empirical functions to form interatomic potentials such as classical molecular dynamics (MD), provide very fast but low-accurate material-property calculations. Meanwhile, methods based on high-fidelity quantum-mechanics calculations, such as density functional theory (DFT) and *ab initio* molecular dynamics (AIMD), provide highly accurate energies and forces but require high computational costs.

To address the above dilemma, deep learning techniques, such as graph neural networks (GNNs), have been proposed for predicting interatomic potentials or DFT Hamiltonian in

speed while preserving quantum mechanics-level accuracy[1–33]. To represent the molecule or crystal structure, GNNs typically use a graph where nodes are atoms and edges are chemical bonds between atoms. Atomic interactions are then simulated by graph convolution operations on the graph for passing message, where an atom can access its neighboring atoms during this process (**Fig. 1a**). Currently, the most widely used GNNs are under the Euclidean group  $E(3)$  *invariant* neural network architectures, which can effectively keep the crystal geometric symmetry and output energy with respect to  $E(3)$  translations, rotations, and reflections. This is achieved by leveraging invariant features, such as bond lengths and angles, which remain constant under these transformations. Early models like CGCNN[3], SchNet[13], and MEGNet[6] primarily incorporate bond lengths, leading to challenges in distinguishing structures with identical bond lengths but different overall configurations (**Fig. 1b**). Later iterations, like DimeNet[14], ALIGNN[15], and M3GNet[5], improve upon this by integrating bond angles (**Fig. 1c**). Recent models, such as GemNet[11] and SphereNet[34], propose considering dihedral angles in GNNs to unambiguously recognize the local structures (**Fig. 1d**). It is worth noting that distance and angular features are invariant representations which are only used to keep the geometric symmetry of crystals with respect to  $E(3)$  transformations, rather than utilize the geometric symmetries in a more profound manner for increasing the prediction accuracy and the sample efficiency. Actually, the idea to leverage crystal symmetry for effectively describing the electron wave function and material properties was proposed a century ago. Felix Bloch demonstrated a translation-symmetry-based structural function to maintain the equivariance of wave functions in 1928. Such an equivariant idea in crystals with periodic structures in 3D space provides a powerful framework for accurately understanding the material properties and significantly reduces the cost of computation, opening a new era for computational material science. **Fig. 1e-g** offer a concise elucidation of invariance and equivariance in the context of predicting energy and forces.

In this work, we integrate equivariance into GNNs for actively exploiting crystal symmetries and offering a richer geometrical representation compared to their invariant counterparts. Most importantly, our equivariant network is lightweight, which only incorporates scalar and vector features and manipulates them in a manner that preserves symmetry, resulting in robust representations that enhance both accuracy and sample efficiency. Our lightweight equivariant interaction graph neural network (LEIGNN) is significantly different

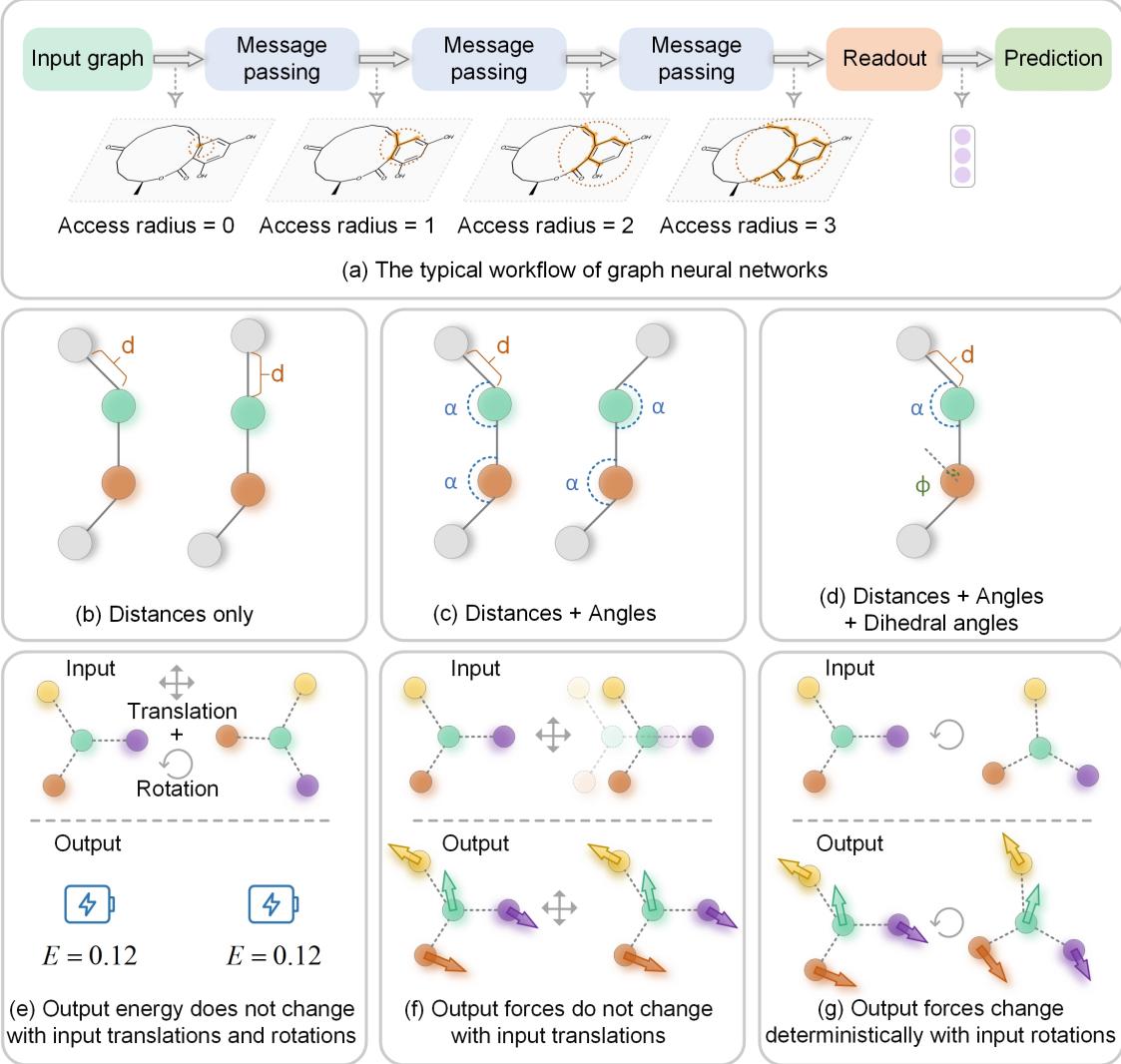


FIG. 1. Concepts of invariant GNNs. (a) A typical GNN workflow is illustrated, emphasizing how GNNs can include a wider range of interactions (or message passing) by stacking multiple layers to extend the accessible radius. (b), (c), and (d) underscore the importance of integrating structural features into GNNs, which include: (b) distance only, (c) both distance and angles, and (d) all distance, angles, and dihedral angles. (e), (f), and (g) elucidate the concepts of invariance and equivariance within the context of energy and forces prediction.

from previously reported equivariant GNNs which are on the basis of high-order functions, such as the spherical harmonic function. Their increased accuracy compared with invariant GNNs initially came at the cost of increased computational expense [19, 26–28, 35–40]. Cutting-edge models like NequIP[19], ScN[40], and eScN[39] employ tensor product operations to combine input features and filters equivariantly, which is extremely expensive in

practice computation [39–41].

Our model aims to achieve both accurate and efficient predictions for interatomic potentials and forces. Specifically, we assign each node both scalars and vectors to represent equivariant features. LEIGNN combines these entities in a symmetry-preserving fashion to maintain equivariance. Equivariant LEIGNN surpasses scalar-only invariant models[3, 6, 13] in accuracy and generalization ability. It also offers an extremely lightweight structure compared to high-order tensor models[19, 40]. The model’s performance is further enhanced by a novel strategy for extracting global structural features from the vector representations. To validate the performance of our interatomic potentials, we conduct classical molecular dynamics and *ab initio* MD simulation across solid, liquid, and gas systems. LEIGNN can achieve the *ab initio* MD accuracy and computational efficiency of classical MD across all examined systems, showing its accuracy, efficiency, and universality.

## METHODOLOGY

The idea is to enhance GNNs by incorporating equivariance, offering a richer geometric representation while retaining a lightweight model. Each node in LEIGNN is assigned scalars and vectors to represent invariant and equivariant features, respectively. LEIGNN gradually updates the node representations through two key processes: message passing and message updating, as illustrated in **Fig. 2a**. The message passing phase aims at aggregating neighboring nodes to mimic two-body interactions, whereas the message updating is used to integrate  $N$  scalars and  $N$  vectors within a node to update node representations. LEIGNN consists of four layers, each comprising two phases: message passing and message updating, as illustrated in **Fig. 2b-d** and elaborated in Supplementary Materials.

In the message passing phase, a particular node  $v_i$  gathers messages from its neighbouring scalar  $\mathbf{x}_j$  and vector  $\vec{\mathbf{x}}_j$ , resulting in intermediate scalar and vector variables  $\mathbf{m}_i$  and  $\vec{\mathbf{m}}_i$  as follows:

$$\mathbf{m}_i = \sum_{v_j \in \mathcal{N}(v_i)} (\mathbf{W}_h \mathbf{x}_j^{(t)}) \circ \lambda_h(\|\vec{\mathbf{r}}_{ji}\|) \quad (1)$$

$$\vec{\mathbf{m}}_i = \sum_{v_j \in \mathcal{N}(v_i)} (\mathbf{W}_u \mathbf{x}_j^{(t)}) \circ \lambda_u(\|\vec{\mathbf{r}}_{ji}\|) \circ \vec{\mathbf{x}}_j^{(t)} + (\mathbf{W}_v \mathbf{x}_j^{(t)}) \circ \lambda_v(\|\vec{\mathbf{r}}_{ji}\|) \circ \frac{\vec{\mathbf{r}}_{ji}}{\|\vec{\mathbf{r}}_{ji}\|} \quad (2)$$

Here,  $\mathbf{W}_h, \mathbf{W}_u, \mathbf{W}_v \in \mathbb{R}^{F \times F}$  are learnable matrices. The functions  $\lambda_h$ ,  $\lambda_u$ , and  $\lambda_v$  are the linear combination of Gaussian radial basis functions [13].

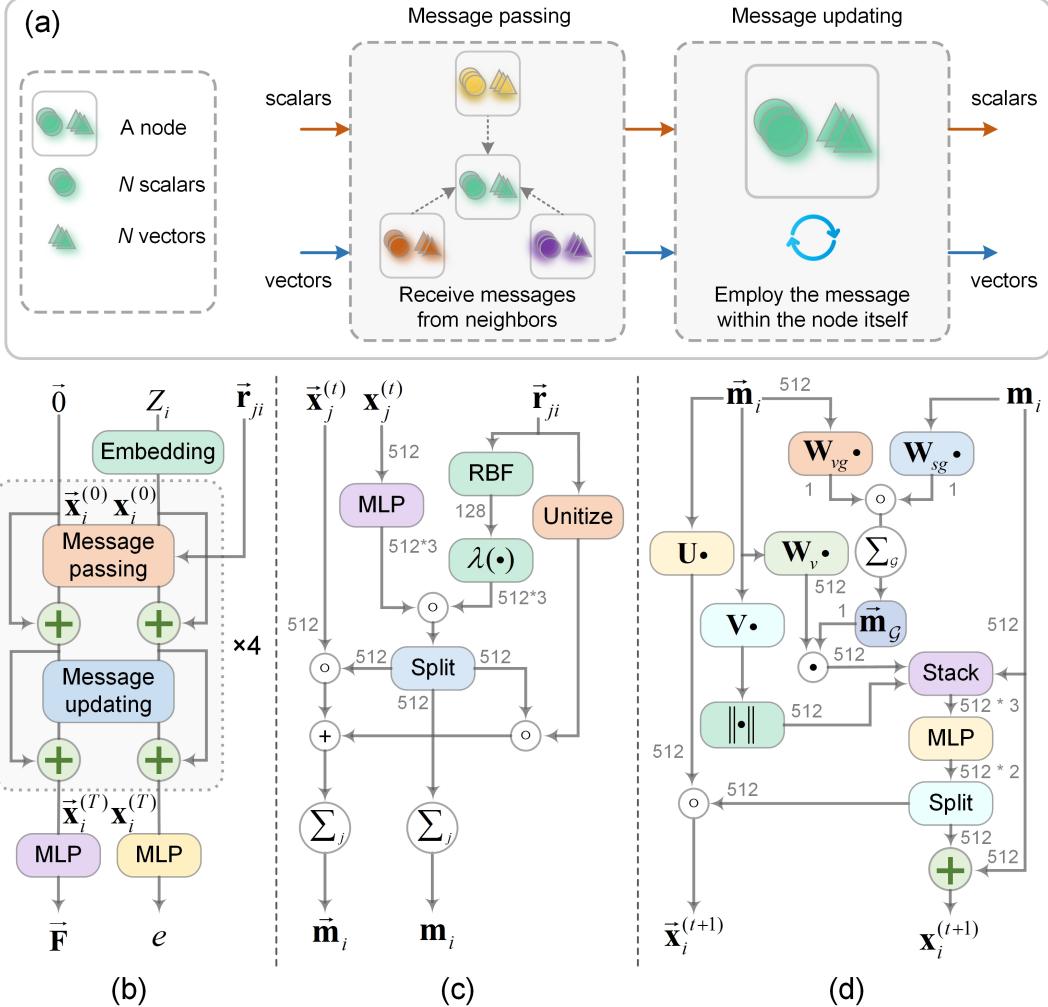


FIG. 2. The overall architecture of LEIGNN. (a) LEIGNN uses message passing and message updating to iteratively update node representations. (b) LEIGNN consists of four layers. (c) The message passing phase. (d) The message updating phase. The number of features after each operation is annotated in grey.

The message updating phase aims to aggregate  $F$  scalars and vectors within  $\mathbf{m}_i$  and  $\vec{\mathbf{m}}_i$ , respectively, to obtain new scalar  $\mathbf{x}_i^{(t+1)}$  and new vector  $\vec{\mathbf{x}}_i^{(t+1)}$ . Two strategies are employed to extract the local and global structures from the  $\vec{\mathbf{m}}_i$ . The local structure is extracted using vector norm  $\|\mathbf{V}\vec{\mathbf{m}}_i\|$  ( $\mathbf{V} \in \mathbb{R}^{F \times F}$ ), while the global structure is obtained by projecting each vector onto a global vector. Specifically, we first define the global vector  $\vec{\mathbf{m}}_G$  as follows:

$$\vec{\mathbf{m}}_G = \sum_{v_i \in \mathcal{G}} (\mathbf{W}_{sg} \mathbf{m}_i) \circ (\mathbf{W}_{vg} \vec{\mathbf{m}}_i) \quad (3)$$

where  $\mathbf{W}_{sg} \in \mathbb{R}^{1 \times F}$  and  $\mathbf{W}_{vg} \in \mathbb{R}^{1 \times F}$  are two learnable matrices compressing  $\mathbf{m}_i$  and  $\vec{\mathbf{m}}_i$  to

a scalar and a three-dimensional vector, respectively.  $\vec{\mathbf{m}}_{\mathcal{G}} \in \mathbb{R}^3$  is a global vector encoding the global structural information. We then use  $\vec{\mathbf{m}}_{\mathcal{G}}$  as a reference coordinate system and project each local vector onto it.

$$\mathbf{s} = (\mathbf{W}_v \vec{\mathbf{m}}_i) \cdot \vec{\mathbf{m}}_{\mathcal{G}} \quad (4)$$

where  $\mathbf{W}_v \in \mathbb{R}^{F \times F}$ ,  $\mathbf{s} \in \mathbb{R}^F$  is the extracted global structure. Therefore, by projecting each local vector  $\vec{\mathbf{m}}_i$  onto the global vector  $\vec{\mathbf{m}}_{\mathcal{G}}$ , both the magnitude and angular information are implicitly extracted. This novel strategy for extracting global structural features from the vector representation sets LEIGNN apart from previous models[42, 43]. Finally, the scalar representation  $\mathbf{x}_i^{(t+1)}$  and vector representation  $\vec{\mathbf{x}}_i^{(t+1)}$  is updated according to:

$$\mathbf{x}_i^{(t+1)} = \mathbf{W}_{u1}(\mathbf{m}_i \oplus \|\mathbf{V}\vec{\mathbf{m}}_i\| \oplus \mathbf{s}) + \mathbf{W}_{u2}\mathbf{m}_i \quad (5)$$

$$\vec{\mathbf{x}}_i^{(t+1)} = (\mathbf{W}_h(\mathbf{m}_i \oplus \|\mathbf{V}\vec{\mathbf{m}}_i\| \oplus \mathbf{s})) \circ (\mathbf{U}\vec{\mathbf{m}}_i) \quad (6)$$

where  $\oplus$  is concatenation,  $\mathbf{W}_{u1}, \mathbf{W}_h \in \mathbb{R}^{F \times 3F}$  and  $\mathbf{W}_{u2}, \mathbf{U}, \mathbf{V} \in \mathbb{R}^{F \times F}$ . LEIGNN is strictly equivariant to rotation and translation, which is proved in **SM Section 2**.

To predict the potential  $e$ , we utilize an MLP layer  $\phi : \mathbb{R}^F \rightarrow \mathbb{R}^1$ . This layer learns atom-wise potentials  $e_i \in \mathbb{R}^1$  from the scalar representation  $\mathbf{x}_i^{(T)}$  which is obtained at the last graph convolution layer (referred to as the  $T$ -th layer). The total potential is then calculated as the sum of the atom-wise potentials:

$$e = \sum_{v_i \in \mathcal{G}} e_i \quad (7)$$

## RESULTS AND DISCUSSION

### Model Performance

We first evaluate LEIGNN in the structure to energy and forces (S2EF) task using Open Catalyst 2020 (OC20) dataset[44]. The purpose of this task is to predict energies and forces corresponding to each trajectory during structural relaxation. The OC20 dataset encompasses 1,281,040 density functional theory (DFT) relaxations with 264,890,000 single-point calculations and spans a vast range of materials, surfaces, and adsorbates. It has been reported that training a GNN model on the whole OC20 dataset requires hundreds or even

TABLE I. Comparison results of the proposed LEIGNN and baselines on S2EF task of four external validation sets of OC20 in terms of energy MAE (meV) and forces MAE (meV/Å), where all models are trained on the same OC20-50K. The ‘Improvement (%)’ row indicates the percentage by which LEIGNN outperforms the previous best model.

Model	ID		OOD Ads.		OOD Cat.		OOD Both	
	Energy	Forces	Energy	Forces	Energy	Forces	Energy	Forces
CGCNN	1125	75.3	1255	79.9	1111	74.4	1386	91.5
SchNet	1138	67.9	1255	73.3	1121	67.4	1394	84.9
PaiNN	680	66.6	877	72.1	671	66.2	973	83.3
DimeNet++	647	59.2	752	68.2	646	58.7	875	78.5
GemNet-dT	641	58.7	784	63.8	733	58.1	1029	75.4
LEIGNN (ours)	<b>543</b>	<b>55.4</b>	<b>655</b>	<b>60.2</b>	<b>585</b>	<b>54.9</b>	<b>778</b>	<b>71.0</b>
Improvement	15.3%	5.6%	12.9%	11.7%	12.8%	6.5%	11.1%	9.6%

thousands of days [39]. Therefore, we only use a subset of it: OC20-50K ( $N = 50,000$ ). The dataset is split into a training set and an internal validation set with a ratio of 8:2, where the internal validation set is used to select the best model for testing. Finally, the select models are tested on four external validation sets provided by the OC20 project: in Domain (ID), out-of-domain adsorbate (OOD Ads.), out-of-domain catalyst (OOD Cat.), and OOD Both (both the adsorbate and catalyst are not seen in the training set). Each external validation set contains approximately 1M data points. We compare LEIGNN with five representative baseline models: CGCNN[3], SchNet[13], PaiNN[42], DimeNet++[14], and GemNet-dT[11]. All models are implemented using the source code provided by Open Catalyst Project[44] with recommended hyper-parameters (see **SM Section 3**). All models share the same training, internal validation, and external validation sets, and are trained to predict adsorption energy and per-atom forces simultaneously. The performance of the models is evaluated based on the mean absolute error (MAE).

As shown in **Table I**, LEIGNN consistently surpasses benchmark models in energy and force predictions across all external validation sets, especially the CGCNN and SchNet. LEIGNN’s implicit consideration of structural features can yield competitive performance

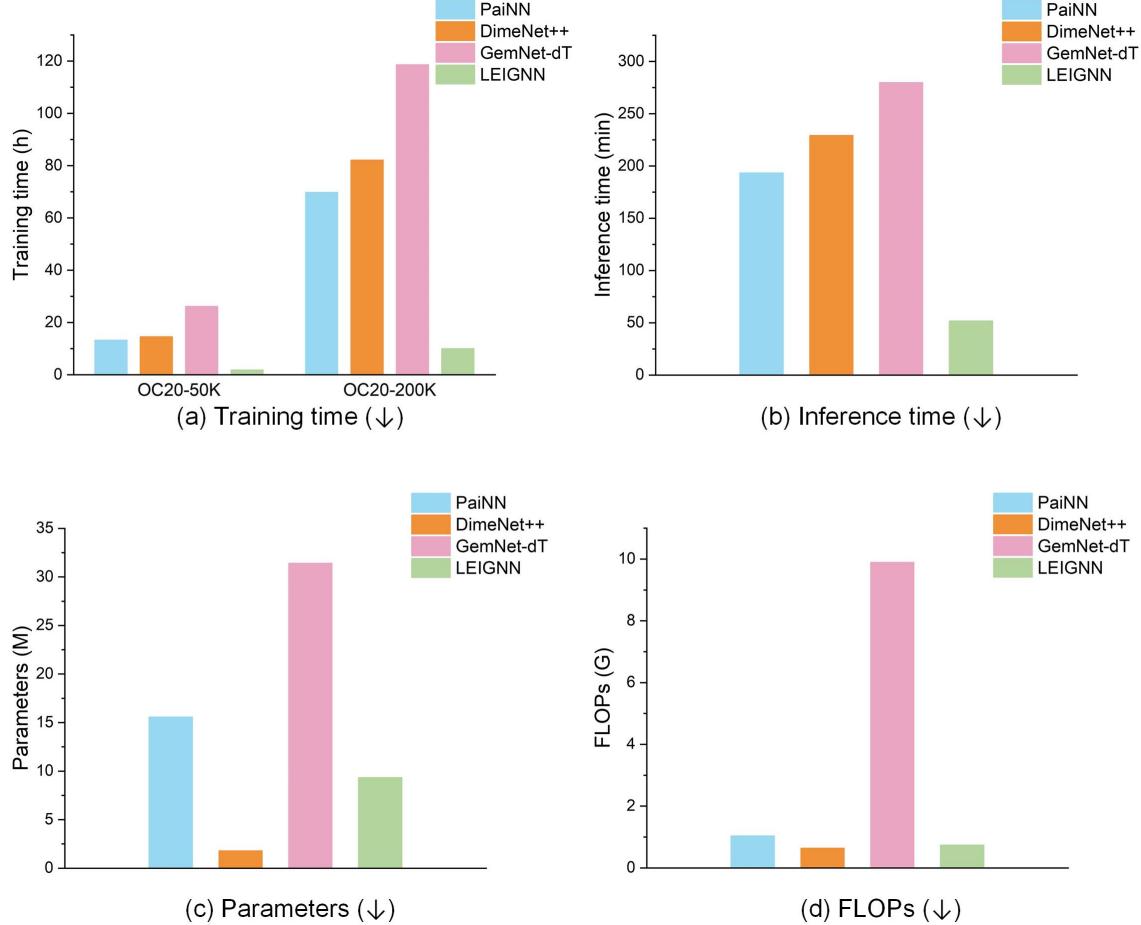


FIG. 3. Computational costs of the six models (the lower the better for all metrics). (a) Training time. (b) Mean inference time. (c) Number of parameters. (d) FLOPs.

compared to DimeNet++ and GemNet-dT which explicitly incorporate angular features. Furthermore, when evaluated on a larger dataset, OC20-200K ( $N = 200,000$ ), LEIGNN still demonstrates robust and competitive performance (see **SM Section 6**).

Next, we compare the computational costs among LEIGNN and the three accurate models of PaiNN, DimeNet++, and GemNet-dT in Table I. **Fig. 3** illustrates the model complexity in terms of training time, inference time, the number of parameters, and floating-point operations (FLOPs). As can be seen, LEIGNN offers approximately ten times faster training and inference speeds than GemNet-dT and is about five times faster than DimeNet++ and PaiNN. These findings highlight LEIGNN’s high efficiency. The lightweight feature of LEIGNN renders it a more suitable choice for large-scale simulation systems. Besides the OC20 database, we compare LEIGNN and other models on MD17 and ISO17 databases.

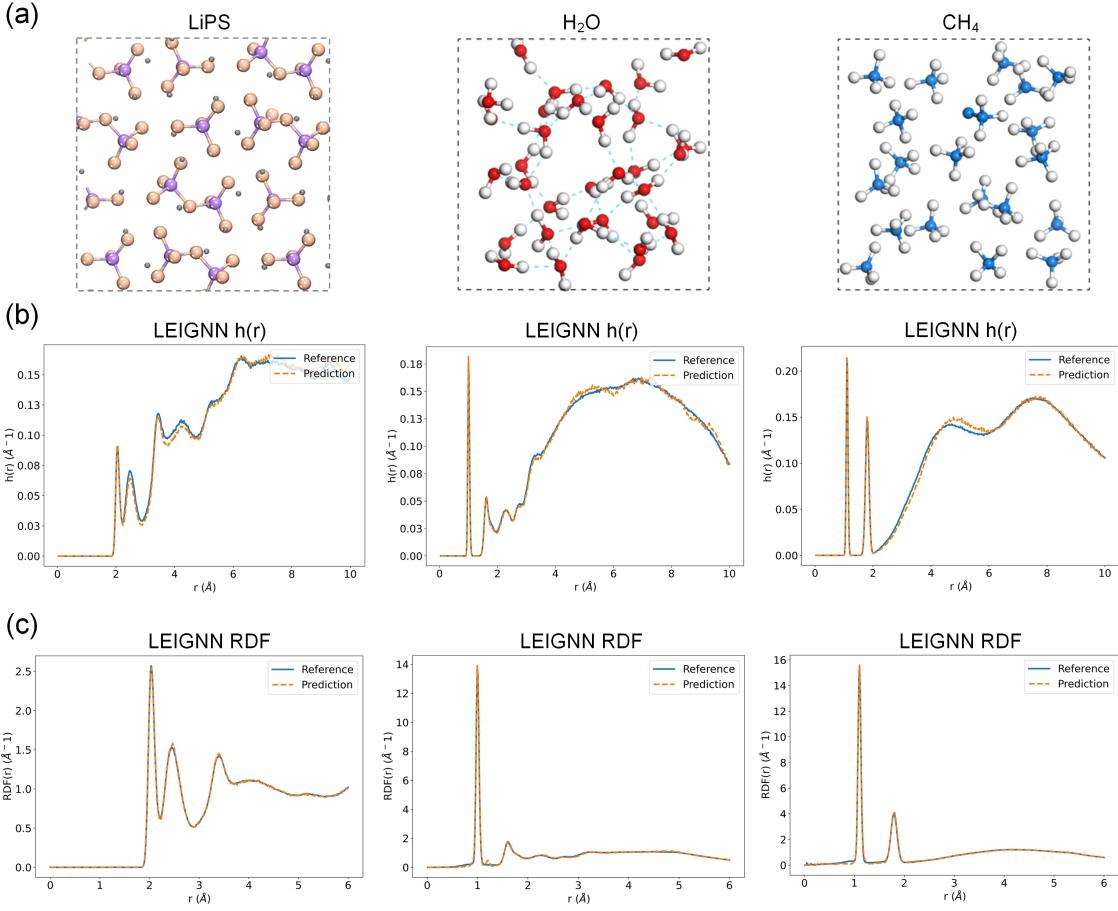


FIG. 4. MD simulations for LiPS, H<sub>2</sub>O, and CH<sub>4</sub>. (a) An overview of the three benchmark systems. (b)  $h(r)$  for trajectories predicted by the LEIGNN. (c) RDF for trajectories predicted by LEIGNN.

Our LEIGNN model also surpasses those benchmark models (see **SM Sections 7 and 8**).

Finally, to showcase the efficacy of our novel approach for extracting global structural features from the vector representation, we conduct a comparative analysis between LEIGNN and a baseline variant, denoted as LEIGNN\_noG, which omits the integration of global structural information. The findings of this comparison are presented in **SM Section 9**, underscoring the significant role that global structure plays in our model's performance.

### Molecular Dynamics Simulations

Molecular dynamics simulations provide vital atomistic insights, but the accuracy versus efficiency trade-off has long been a challenge. Classical MD, which relies on empirical interatomic potentials, is computationally efficient but sacrifices accuracy. In contrast, *ab initio*

TABLE II. Evaluating LEIGNN and the classical Lennard-Jones (LJ) potential on MD simulations in terms of stability (ps), MAE of  $h(r)$  (unitless), MAE of RDF (unitless), and running time (min).

System	#Atoms	Method	Stability( $\uparrow$ )	$h(r)(\downarrow)$	RDF( $\downarrow$ )	Time
LiPS	83	LJ	0	0.42	12.34	<b>29.93</b>
		LEIGNN	<b>50</b>	<b>0.03</b>	<b>0.04</b>	43.85
H <sub>2</sub> O	96	LJ	0	0.61	9.58	<b>15.53</b>
		LEIGNN	<b>50</b>	<b>0.02</b>	<b>0.19</b>	26.95
CH <sub>4</sub>	100	LJ	0	0.48	9.85	<b>15.17</b>
		LEIGNN	<b>50</b>	<b>0.03</b>	<b>0.20</b>	26.53

molecular dynamics, which integrates first-principles methods such as density functional theory, provides higher accuracy but at a significant computational cost.

As the validation of our LEIGNN’s interatomic potentials, we finally demonstrate that our LEIGNN can have the computational efficiency of classical MD while retaining the AIMD-level accuracy. We benchmark LEIGNN against the classical MD potentials, evaluating stability, MAE of interatomic distances ( $h(r)$ ), MAE of radial distribution function (RDF), and running time. For a clear metric of stability, we deem simulations to be ‘unstable’ if deviations surpass predefined thresholds, indicating the sampling of highly nonphysical structures[41]. To test our model robustness, we consider various systems, including LiPS (solid), H<sub>2</sub>O (liquid), and CH<sub>4</sub> (gas), as shown in **Fig. 4a**, over a 50 ps simulation initiated from a randomly chosen test configuration. Refer to the **SM Sections 4 and 5** for detailed experimental settings and metrics.

Our results, summarized in **Table II**, reveal LEIGNN’s superiority over classical MD in both stability and accuracy for all systems. LEIGNN maintains consistent stability throughout the 50 ps simulations and demonstrates notably low MAEs for  $h(r)$  and RDF, suggesting its ability to accurately capture the structural properties of the system. Moreover, their running times are similar, highlighting LEIGNN’s efficiency. We further compare LEIGNN with high-fidelity AIMD. **Fig. 4 b-c** show the  $h(r)$  and RDF for AIMD and LEIGNN, revealing their strong alignment. Additional results are presented in **SM Section 10**. Overall, our results spotlight LEIGNN’s potential as a pivotal tool in computational materials science.

## CONCLUSION

In conclusion, we develop a lightweight, accurate, efficient, and universal equivariant graph neural network for predicting interatomic potentials and forces. Our LEIGNN consistently outperforms the prediction performance of the representative baselines across diverse molecular and crystal datasets. Moreover, our model can achieve the accuracy of *ab initio* MD and retain the computational efficiency of classical MD across all examined gas, liquid and solid systems.

## DATA AND CODE

Data and code for LEIGNN are available at <https://github.com/guaguabujianle/LEIGNN>.

## ACKNOWLEDGEMENTS

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