
DIELECTRIC TENSOR PREDICTION FOR INORGANIC MATERIALS USING LATENT INFORMATION FROM PREFERRED POTENTIAL

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ABSTRACT

Dielectrics are materials with widespread applications in flash memory, central processing units, photovoltaics, capacitors, etc. However, the availability of public dielectric data remains limited, hindering research and development efforts. Previously, machine learning models focused on predicting dielectric constants as scalars, overlooking the importance of dielectric tensors in understanding material properties under directional electric fields for material design and simulation. This study demonstrates the value of common equivariant structural embedding features derived from a universal neural network potential in enhancing the prediction of dielectric properties. To integrate channel information from various-rank latent features while preserving the desired SE(3) equivariance to the second-rank dielectric tensors, we design an equivariant readout decoder to predict the total, electronic, and ionic dielectric tensors individually, and compare our model with the state-of-the-art models. Finally, we evaluate our model by conducting virtual screening on thermodynamical stable structure candidates in Materials Project. The material Ba₂SmTaO₆ with large band gaps ($E_g = 3.36\text{eV}$) and dielectric constants ($\epsilon = 93.81$) is successfully identified out of the 14k candidate set. The results show that our methods give good accuracy on predicting dielectric tensors of inorganic materials, emphasizing their potential in contributing to the discovery of novel dielectrics.

Keywords SE(3), Graph neural networks, Inorganic materials, Dielectric tensor

1 Introduction

Dielectrics are an essential group of materials identified by their distinct electronic characteristics. They find extensive applications in various fields such as photovoltaics[1], energy storage[2, 3], microwave communication[4, 5], etc., in contemporary society. When subjected to an external electric field, a dielectric material is polarized by internally generating electric dipole moments. The dielectric constant ϵ , also known as permittivity, is a measure of such dielectric effect described by the proportionality between the externally applied electric field to the generated field within the material:

$$E_i^{\text{int}} = \sum_j \epsilon_{ij}^{-1} E_j^{\text{ext}} \quad (1)$$

where E^{int} and E^{ext} are the internal and external electric, respectively, and the indices $i, j \in \{1, 2, 3\}$ refer to the directions in the 3D space. The 3×3 dielectric tensor has a minimum of 1 and a maximum of 6 independent elements for various types of systems due to the crystal symmetry. It can be represented by a sum of two components: the electronic contribution (ϵ^∞) and ionic contribution (ϵ^0), which are generated by electron cloud distortion and atomic displacement, respectively, i.e., $\epsilon_{ij} = \epsilon_{ij}^\infty + \epsilon_{ij}^0$. Both high and low dielectric constants play an essential role in material design. For instance, high- κ dielectrics enable higher-density charge storage to shrink device sizes, while low- κ dielectrics are important to device packaging by minimizing the signal interference between neighboring interconnects.

As of the present, only a limited number of materials in few hundreds have had their dielectric constants measured[6] because of the requirement of huge experimental efforts. In the past decades, first-principle calculations played a critical

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role for accelerating the discovery of new materials[7]. Density functional theory (DFT)[8, 9] has gained significant popularity due to its commendable balance between computational speed and accuracy for simulating materials in silico. This has, in turn, facilitated the emergence of a wide range of diverse new materials.[10, 11]. Similarly, density functional perturbation theory (DFPT) serves as a simulation tool for establishing the relationship between structure and dielectric properties, and the calculated data in the order of thousands are publicly accessible for material exploration[12, 6]. However, the DFT-based methods entail significant computational cost, making them less feasible for high-throughput screening, and it is only applicable to small systems with the number of atoms typically less than 1000[13], since its complexity scales poorly with the number of particles. Alternatively, machine learning is becoming an important research tool, providing an alternative method for quantitative structure-property relationship (QSPR) analysis for material science. There are numerous successful works in designing materials for various applications, including fluorescent molecules[14], electrets[15, 16], DDR1 kinase inhibitors[17], thermal-electric materials[18], etc.

Several existing works made the efforts on making predictions for dielectric property directly from crystal/molecule descriptors by using the machine learning model. Umeda et al. adopted a random forest (RF) model to estimate experimental dielectric constants with the error range as large as 50% in the logarithmic scale on the purpose of developing ferroelectric material[19]. Takahashi et al. studied the prediction for static dielectric constants of metal oxides and analyzed importance of descriptors using RF models. Lin et al. employed a simple Gradient boosting regression (GBR) model to predict the electronic contribution of polycrystalline dielectric constants with RMSE of 0.824 and did analysis on feature importance for ABO_3 -type compounds[20]. Similarly, Kim et al. used a GBR model to predict both the electronic and ionic contribution of ABO_3 -type perovskites, achieving RMSE of 0.12 and 0.26 respectively[21]. Although these works proved the strong ability of machine learning models to rapidly estimate dielectric properties on unseen materials and are undoubtedly helpful to guide material designers before conducting wet experiments, there are still several limitations that hinder their full potential for exploration in the dielectric material space. Firstly, these tasks have mainly utilized simple machine learning models and manually selected descriptors for the models, thus unable to comprehensively showcase the structural characteristics of the materials which are crucial for more accurate dielectric tensor prediction. Additionally, these works only consider the specific types of inorganic materials (e.g. ABO_3 perovskite structures) or materials containing specific combinations of elements. This narrow scope restricts the generalizability of the models and hinders their applicability to a wider range of dielectric materials. Lastly, they use a simple average scalar to express the dielectric constant by

$$\epsilon = \sum_{i=1}^3 \lambda_i / 3 \quad (2)$$

where λ_i is the eigenvalue of ϵ . However, the off-diagonal elements in the dielectric tensor may reach large values and sometimes cannot be neglected in practical[22], thus prediction of the dielectric constants as tensors assists human researchers to understand the behavior of materials in the presence of a directed electric field. To distinguish, dielectric constants as scalars and as tensors are denoted with ϵ and ϵ , respectively. ϵ could provide crucial comprehensive measures for designs of electronic devices in various applications.

In recent years, graph neural networks (GNN) has been becoming a powerful tool for rapid atomic simulation in material science[23, 24] as graphs are a natural representation for crystals and molecules where nodes are atoms and edges are bonds between atom pairs. Many great GNN-based models[25, 26, 27, 28, 29, 30] are proposed and demonstrated their efficacy in accurately establishing a quantitative structure-property relationship. Recent works proposed the application of equivariant graph neural networks (EGNN) in materials science[31, 30] and discussed the necessity of equivariant representations to enhance model expressivity. TeaNet[31] is an EGNN architecture that satisfies special Euclidean group $E(3)$ equivariance including translation, rotation and reflection. Based on TeaNet with certain modifications, Preferred Potential (*PPF*)[32] is a universal neural network potential (NNP) model trained by massive data and has been released for multiple versions. What especially makes *PPF* robust for universal interatomic interactions is its enhanced representations of the local electronic environments centered around atoms and bonds by converting raw input data (atomic numbers and positions) to rank-0,1,2 tensors (i.e., scalars, vectors and tensors). Pretrained on the 22 million dataset (calculated by 1144 GPU years), the up-to-date *PPF* covers 72 elements in the periodic table for empirical universal interatomic potential simulation with strong transferability[33]. Its abundant intermediate interatomic information in pretrained layers of graph convolutional networks (GCN) and inclusion of equivariant rank-2 tensor features make it potentially suitable to transfer to diverse tensorial regression tasks with relatively limited datasets such as dielectric tensors.

In this study, we propose *Dielectric Tensor Neural Network(DTNN)* to predict the three types of dielectric tensors, ϵ_{ij}^∞ , ϵ_{ij}^0 and ϵ_{ij} , for inorganic materials across 72 supported elements with the equivariance to the input structure. By leveraging a pretrained *PPF* model as an efficient and expressive encoder, we demonstrated that the pretrained *PPF* processes a rich set of high-order latent compositional and structural information for tensorial property prediction. The ablation study shows that both latent atomic features and bond features from *PPF* contribute to the final prediction. To

evaluate the performance of *DTNN*, we compared it against existing methods, PaiNN[30], M3GNet[34] and MatTen[35], on the dataset obtained from Materials Project (MP)[36]. Finally, we employed our model to perform a virtual screening on the design of dielectric materials for the microelectronic manufacturing application.

2 Results

2.1 Overview

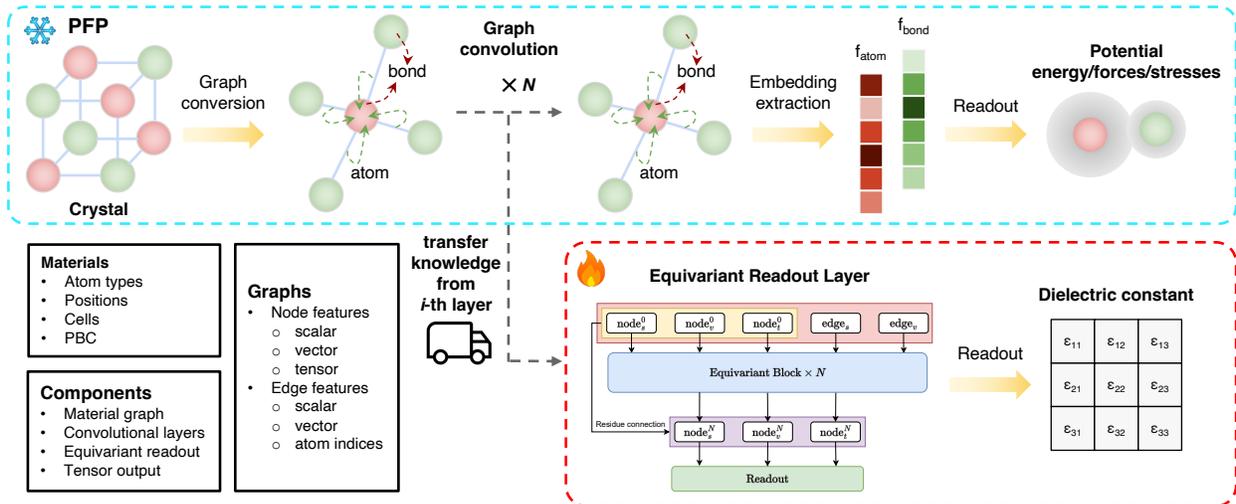


Figure 1: Diagram of the equivariant model for dielectric tensor prediction. The input graph is represented by initialized atom attributes $\mathcal{V} = \{(\mathbf{a}_s, \mathbf{a}_v, \mathbf{a}_t)_i\}_{i=1:N^a}^0$ and bond attributes $\mathcal{E} = \{(\mathbf{b}_{s\{i,j\}}, \mathbf{b}_{v\{i,j\}})_k\}_{k=1:N^b}^0$ between atoms with indices of i and j , where N^a and N^b are number of atoms and bonds. The intermediate knowledge output $\{(\mathbf{a}_s, \mathbf{a}_v, \mathbf{a}_t)_i\}_{i=1:N^a}^n$ and $\{(\mathbf{b}_{s\{i,j\}}, \mathbf{b}_{v\{i,j\}})_k\}_{k=1:N^b}^n$ from the n -th layer GCN of TeaNet/PFP is fed into an equivariant readout block to perform message interactions among different rank representations for a downstream task, i.e., dielectric tensor prediction here.

The challenge of GNN in materials science is that they usually require a large number of data to prevent models from overfitting, while such chemical data are generally expensive to collect either from simulation or experiments. Additionally, the numbers of calculated data for diverse properties can have large difference. For example, by the time of this work, there are more than $\sim 154\text{k}$ DFT-relaxed material structures with energies in MP, but only $\sim 7\text{k}$ ($<5\%$) of them are available with dielectric constant data. In this work, we took *PFP* as the parent encoder model, i.e., $N = 5$. And for convenience, we denote the *PFP* with the n ($1 \leq n \leq 5$)-th GCN layer as featurizer as *PFP-L*₁, ..., *PFP-L*₅. Our method leverages a *PFP* model consisting of 5 GCN layers, which was pre-trained on 22 million first-principle calculations of potential energies, as a multi-order feature encoder to generate universal compositional and structural information for the second-order dielectric property prediction (see Figure 1). We design a separate model (see Fig.2) to capture interactions among the intermediate knowledge from *PFP-L* _{n} and make predictions on downstream tasks without the need to finetune parameters in the parent *PFP* model. This design ensures the effective utilization of high-order common structural information, leading to improved performance even with a relatively small region of available training data. Details about the module implementation are available in the Methods Section.

2.2 Equivariance

Atomic systems are usually represented with coordinates in 3D Euclidean space. The same system could have transformations under the 3D symmetries: rotations, translations, and inversion. Under rotation in 3D space, certain properties of the system remain invariant, e.g., energy, meaning they do not change regardless of the rotation. Equivariant properties, including forces, stresses, and dielectric tensors, are expected to rotate accordingly with the system. In other words, as the system rotates, these properties undergo corresponding transformations to maintain their relationship with the system's new orientation. Formally, we consider a function $\phi : X \rightarrow Y$ and a group transformation G_T that acts on the vectors spaces X and Y . The function ϕ is equivariant to the transformation G_T if the following condition holds

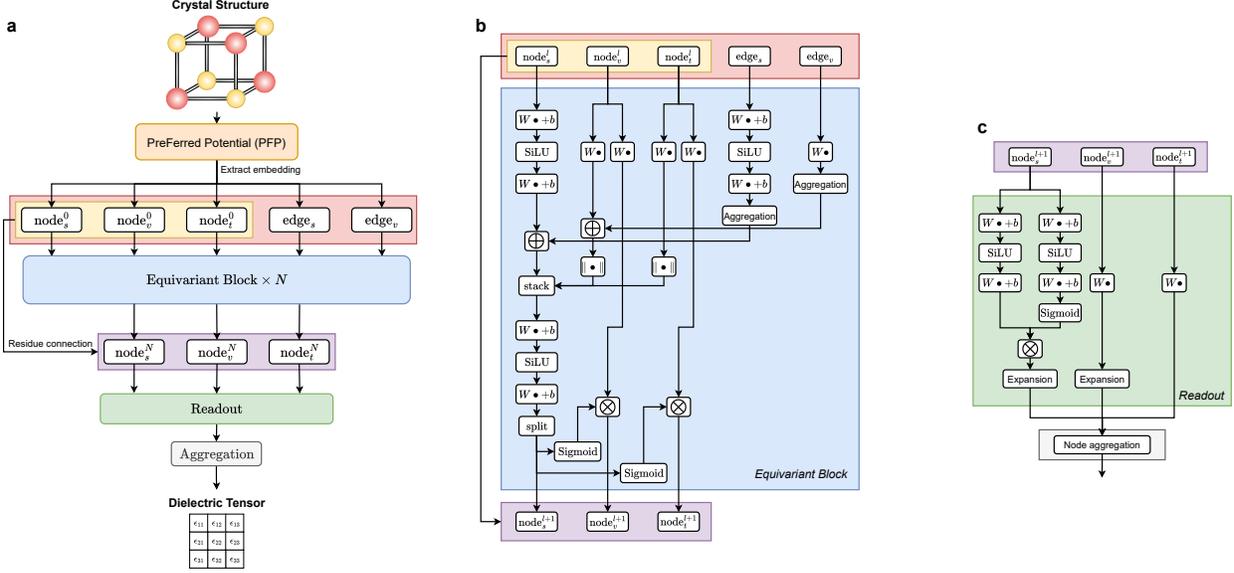


Figure 2: Schematic architecture of the equivariant dielectric model. (a) Overview of the *DTNN* framework; (b) Implementation of an equivariant block in *DTNN*; (c) Implementation of the readout block for dielectric tensor output.

for every element $x \in X$: $\phi(G_T(x)) = G'_T(\phi(x))$, where $G_T(x)$ represents the group transformation applied to the input x , and $G'_T(f(x))$ represents a related transformation applied to the output $\phi(x)$. Here, we focus on the rotational equivariance of the second-rank dielectric tensor ϵ with respect to the input vector space \mathcal{X} , (Fig.3), whose rotational equivariant condition is $R\Phi(\mathcal{X})R^T = \Phi(R\mathcal{X})$ where R is the arbitrary orthogonal rotation matrix and Φ is the neural networks to map \mathcal{X} to ϵ .

2.3 Dielectric Tensor Prediction Covering 72 Elements

2.3.1 Data preparation

We leverage on one of the largest open databases of DFT-calculated crystal structure properties, Materials Project[36], to obtain a wide range of training structures. The dataset (MP v2023.11.1) contains 7277 relaxed materials along with calculated dielectric constants. We clean up the dataset by restricting the element in total dielectric constants $\epsilon_{ij} \in [-10, 100]$ for $\forall i, j$ and filtering out structures that contain elements not supported by *PPF*. Finally there are 6,648 structures retained for model training. The data covers the electronic component ϵ_{ij}^∞ , ionic component ϵ_{ij}^0 , and total component ϵ_{ij} with a range of [1.0, 96.688], [0.0, 90.338] and [1.155, 98.889], respectively (Fig. 4(a)). Fig. 4(b) exhibits that all seven types of crystal systems are included in our dataset. Among them, the orthorhombic crystal system is the most prevalent, comprising 1,636 instances. In contrast, the triclinic and hexagonal systems are the least represented, with only 440 and 443 instances, respectively. The version of *PPF* architecture introduced in this work supports 72 elements in total, covering a wide range of elements across the periodic table. Excluding noble gases, He, Ne, Ar, and Kr, 68 elements are covered in the 6,648 available structures (Fig. 4(c)).

The above dataset was partitioned into training, validation, and test subsets in an 0.8:0.1:0.1 ratio for the experimental analysis. To mitigate the impact of random variation, each experiment was independently performed five times with distinct random shuffle data splits. The outcomes are presented as the mean and standard deviation of these five iterations.

2.3.2 Performance of *DTNN*

We start by investigating the appropriate intermediate GCN layer of *PPF* as the input to *DTNN*. Note that neuron parameters related to \mathbf{a}_v^5 , \mathbf{a}_t^5 and \mathbf{b}_v^5 in the 5-th GCN layer are not trained in *PPF* because only \mathbf{a}_s^5 and \mathbf{b}_s^5 are used as readout features. Hence, for the multi-order features generated from the *PPF-L_n*, we take \mathbf{a}_s^n , \mathbf{a}_v^n , \mathbf{a}_t^n , \mathbf{b}_s^n , and \mathbf{b}_v^n for $1 \leq n \leq 4$, and we take \mathbf{a}_s^5 , \mathbf{a}_v^4 , \mathbf{a}_t^4 , \mathbf{b}_s^5 , and \mathbf{b}_s^4 for the *PPF-L₅*. We have performed hyperparameter optimization for the *DTNN* architecture via the optuna framework[37]. The hyperparameter configurations are detailed in Method

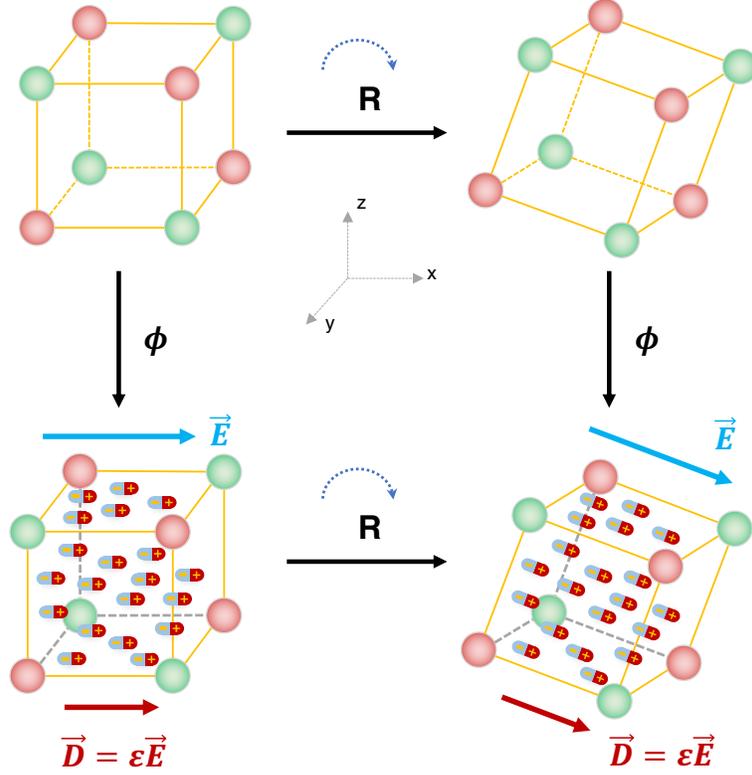


Figure 3: Rotational equivariance on dielectric constants of inorganic materials. \vec{E} is the external electric field, \vec{D} is the corresponding electric displacement, and ϵ is the 3×3 dielectric tensor.

Section. Finally, 2 equivariant blocks (see Fig. 2(b)) are stacked and concatenated with the $PPF-L_n$. For a batch of B test structures, four mean absolute error (MAE) metrics for the symmetric dielectric tensor, the tensor MAE_{ten} , mean diagonal $MAE_{\text{mean-diag}}$, diagonal MAE_{diag} , and off-diagonal $MAE_{\text{off-diag}}$, are defined respectively as:

$$MAE_{\text{ten}} = \frac{1}{6B} \sum_{1 \leq i \leq 3, i \leq j \leq 3}^B \left| \epsilon_{ij}^{\text{dft}} - \epsilon_{ij}^{\text{pred}} \right| \quad (3)$$

$$MAE_{\text{mean-diag}} = \frac{1}{B} \sum \left| \frac{1}{3} \sum_{1 \leq i=j \leq 3} \epsilon_{ij}^{\text{dft}} - \frac{1}{3} \sum_{1 \leq i=j \leq 3} \epsilon_{ij}^{\text{pred}} \right| \quad (4)$$

$$MAE_{\text{diag}} = \frac{1}{3B} \sum_{1 \leq i=j \leq 3}^B \left| \epsilon_{ij}^{\text{dft}} - \epsilon_{ij}^{\text{pred}} \right| \quad (5)$$

$$MAE_{\text{off-diag}} = \frac{1}{3B} \sum_{1 \leq i \leq 3, i < j \leq 3}^B \left| \epsilon_{ij}^{\text{dft}} - \epsilon_{ij}^{\text{pred}} \right| \quad (6)$$

These MAE metrics help assess the accuracy of the model predictions for the dielectric tensor properties. In this work, all models are trained using MAE_{ten} as the loss function. Due to structural symmetry, the number of independent elements in the dielectric tensor varies according to system type (see Table 1). Fig. 5(a) shows that generally the intermediate knowledge from the deeper GCN layer contributes more to the dielectric prediction. When $PPF-L_4$ and $PPF-L_5$ are taken as the feature generator for the child model, lower MAE_{ten} prediction errors are observed on the test structures. This could be explained by that the shallower layers only capture shorter-range local interactions. Meanwhile, quite close accuracy between $n = 4$ and $n = 5$ is because only their scalar representations are distinct. Considering the better computational efficiency, $PPF-L_4$ is taken as the feature generator and is utilized for the subsequent study. Fig. 5(b-d) showcases the performance of $DTNN$ on each crystal system for the prediction task of the electronic, ionic and total dielectric constants. Due to structural symmetry, Three models $DTNN-\epsilon^\infty$, $DTNN-\epsilon^0$ and $DTNN-\epsilon$ are separately

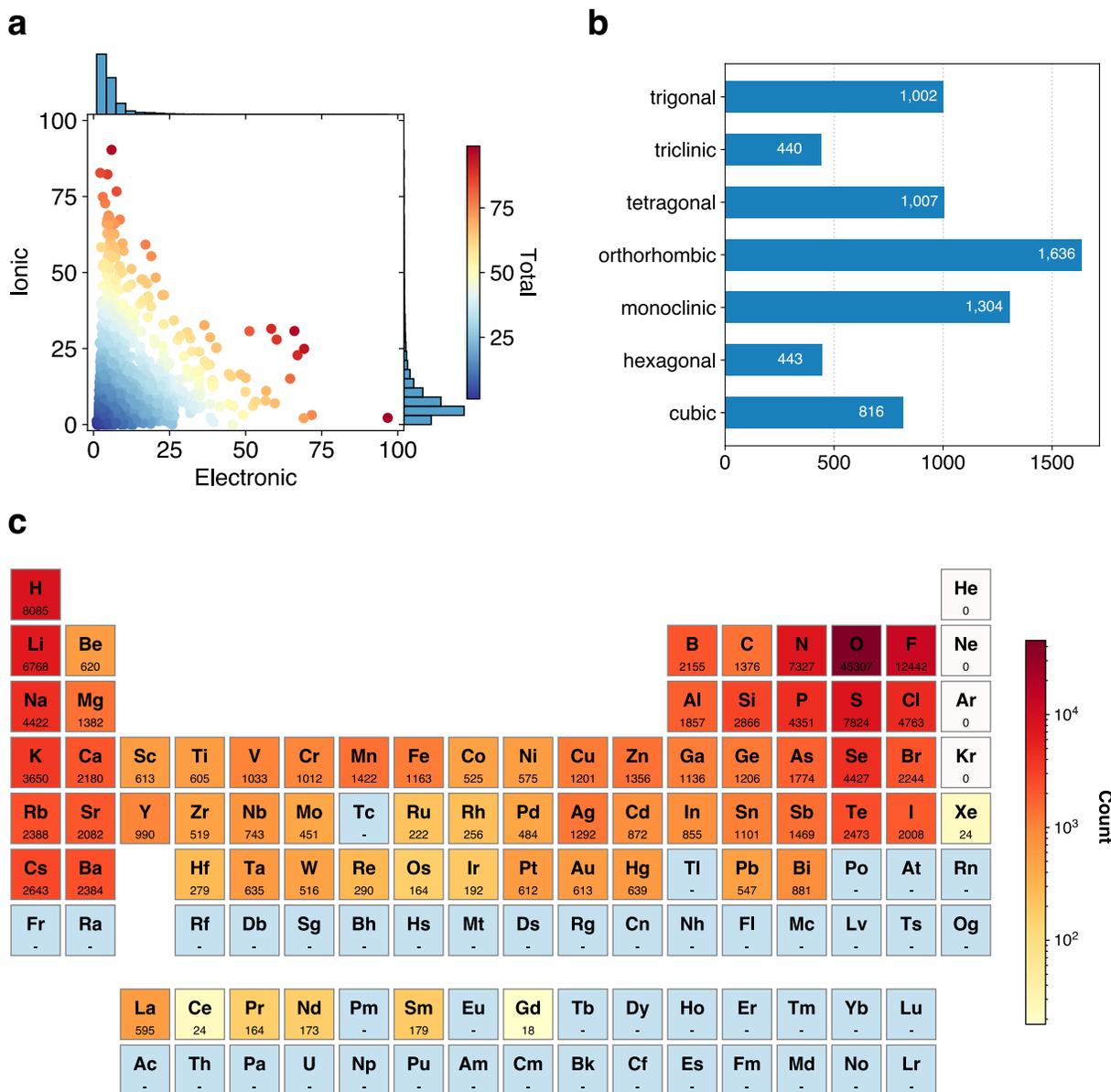


Figure 4: (a) $\epsilon^\infty - \epsilon^0$ map of structures in the dataset, colored by ϵ ; (b) Counts of crystal system types in the dataset; (c) Element counts for atoms in the structures with available dielectric properties on Materials Project. Elements under blue are not supported by PFP. Elements under white are supported by PFP but do not appear in the dataset.

trained with their MAE_{ten} , $\text{MAE}_{\text{mean-diag}}$, MAE_{diag} , $\text{MAE}_{\text{off-diag}}$ evaluated. Dielectric tensors of cubic, hexagonal, orthorhombic, tetragonal and trigonal systems hold 0 on their off-diagonal elements due to geometric symmetry. The zero off-diagonal errors for them demonstrates that our model keeps equivariance for correct prediction of 0 on all their off-diagonal elements. Additionally, the same MAE_{ten} and $\text{MAE}_{\text{mean-diag}}$ of the cubic system further confirm the output equivariance is guaranteed due to its symmetric structure along all three directions in the Euclidean space. The model performs uniformly for different crystal systems according to all MAE_{ten} in the range of $[0.27, 0.57]$ for ϵ^∞ , $[1.07, 1.93]$ for ϵ^0 and $[1.41, 2.14]$ for ϵ .

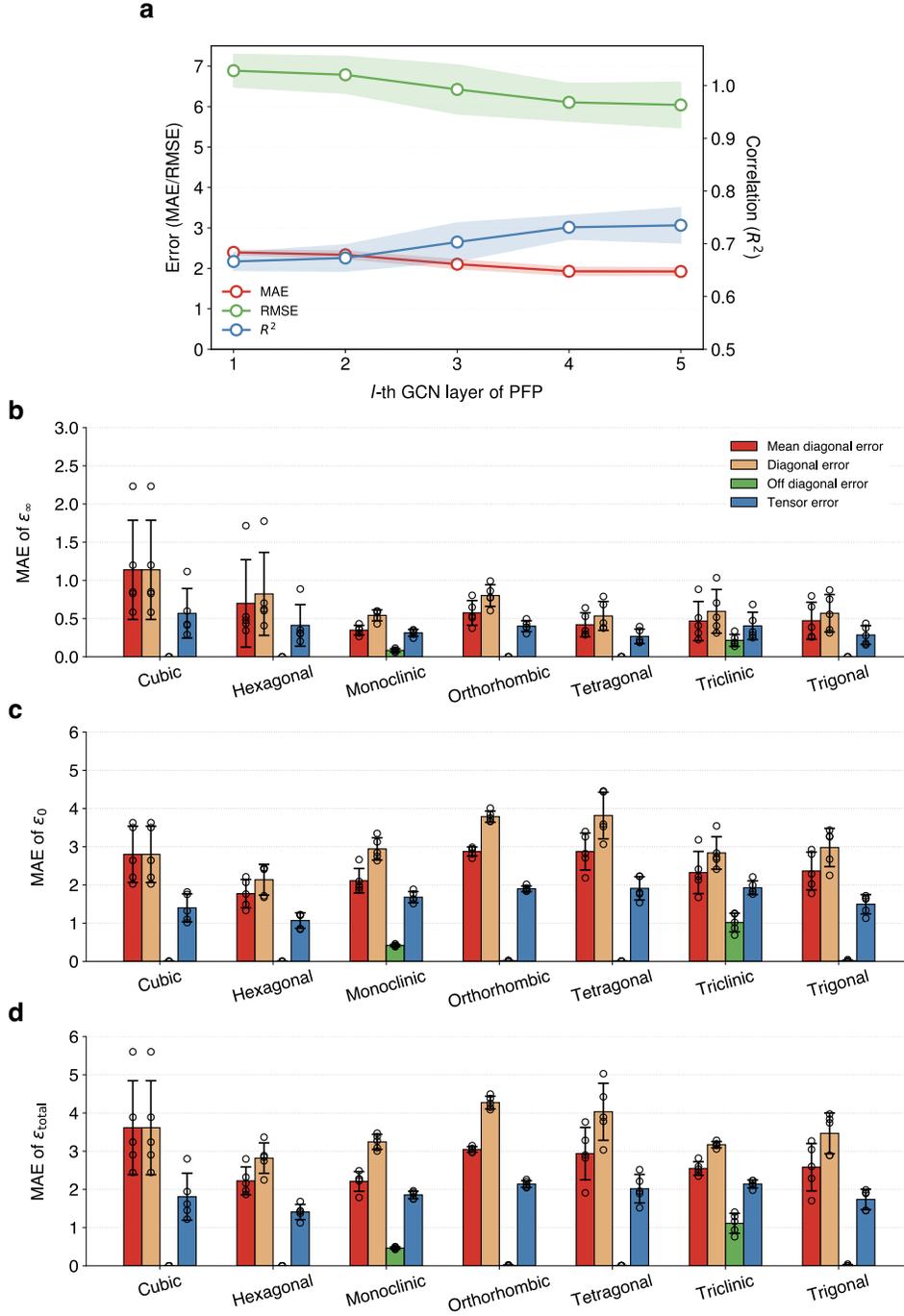


Figure 5: Performance of *DTNN* models on dielectric data from Materials Project. (a) Plot of the mean error (points) with standard deviation (shadow) for 5 runs against the intermediate embedding generated from the $PPF-L_n$ as *DTNN* inputs. (b) 5-run integrated plot of average MAE_{ten} for each element in the test set against the number of structures containing that element in the training set. (c-e) Multiple MAE metrics in the dielectric tensor for different crystal systems on the prediction of the electronic, ionic and total task.

| Crystal | Number of independent elements | Dielectric tensor |
|----------------------------------|--------------------------------|---|
| Cubic | 1 | $\begin{bmatrix} \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{bmatrix}$ |
| Tetragonal, Triagonal, Hexagonal | 2 | $\begin{bmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_1 & 0 \\ 0 & 0 & \epsilon_3 \end{bmatrix}$ |
| Orthorhombic | 3 | $\begin{bmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{bmatrix}$ |
| Monoclinic | 4 | $\begin{bmatrix} \epsilon_{11} & 0 & \epsilon_{13} \\ 0 & \epsilon_2 & 0 \\ \epsilon_{13} & 0 & \epsilon_{33} \end{bmatrix}$ |
| Triclinic | 6 | $\begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & \epsilon_{33} \end{bmatrix}$ |

Table 1: Number of independent components in the dielectric tensor for different crystal systems

2.3.3 Model comparison

There are limited open-source works that discussed the prediction of tensorial properties of materials. The models of *PAINN*[30], *M3GNet*[34] and *MatTen*[35] are chosen for comparison in this work. They use different approaches to produce rank-2 equivariant tensors by incorporation of equivariant atomwise representations, partial derivative with respect to the Cartesian tensor, and spherical harmonics expansion, respectively. *PAINN* encodes each atom i with an invariant representation s_i and an equivariant vector representation v_i . Incorporating v_i has been demonstrated to be effective for structure recognition through ablation studies. The dielectric tensor in *PAINN* is constructed using a rank-1 tensor decomposition, and the atom positions are incorporated to hold the global structure information:

$$\epsilon = \sum_{i=1}^N \epsilon_0(s_i) I_3 + \vec{\nu}(\vec{v}_i) \otimes \vec{r}_i + \vec{r}_i \otimes \vec{\nu}(\vec{v}_i) \quad (7)$$

where I_3 is an identity matrix with size of three, ϵ_0 and $\vec{\nu}$ are invariant and equivariant nonlinearities, respectively. The *M3GNet* model is able to generate equivariant 3×3 tensor from the partial derivatives of its scalar output using the lattice matrix information. This scalar output is not directly trained as a target variable, and instead we train the model based on the loss computed from the derivative values of this output. Specifically, we calculate the loss of MAE_{ten} between these derivative results and labeled targets. After training, these derivative values are utilized for dielectric prediction. In *MatTen*, the atom feature contains a set of scalars, vectors, and high-rank tensors which are produced by spherical harmonics, namely, a geometric object consisting of a direct sum of irreducible representations of the $\text{SO}(3)$ rotation group. Its interaction blocks follow the design of Tensor Field Network[38] and NequIP[29]. The second-order features of all atoms are ultimately aggregated as the prediction of dielectric tensor. To investigate the necessity of including edge-related representations generated by *PFPL*₄, we trained two models, *DTNN* and *DTNN-simple*. *DTNN* leverages all latent embeddings $(\mathbf{a}_s^n, \mathbf{a}_v^n, \mathbf{a}_t^n, \mathbf{b}_s^n, \mathbf{b}_v^n)$, while *DTNN-simple* only utilizes $(\mathbf{a}_s^n, \mathbf{a}_v^n, \mathbf{a}_t^n)$ and the layers related to Eq.14 and Eq.17 are removed.

Table 2 provides a comparison of the three aforementioned models with *DTNN* and *DTNN-simple*. In the prediction task across different systems, the models are trained on the entire training data, while the test structures are categorized according to crystal systems. It is shown that *DTNN* performs best in 22 among all 24 tasks in comparison with all

| Models | <i>DTNN</i> | <i>DTNN-simple</i> | <i>PaiNN</i> | <i>M3GNet</i> | <i>MatTen</i> |
|--------------|----------------------------------|----------------------|---------------|----------------------|---------------|
| Task | Electronic (ϵ_∞) | | | | |
| Cubic | 0.570 ± 0.325 | 0.714 ± 0.449 | 1.811 ± 0.900 | 0.971 ± 0.498 | 1.012 ± 0.340 |
| Hexagonal | 0.412 ± 0.272 | 0.430 ± 0.260 | 0.893 ± 0.537 | 0.469 ± 0.310 | 0.548 ± 0.274 |
| Monoclinic | 0.314 ± 0.045 | 0.319 ± 0.047 | 0.515 ± 0.115 | 0.382 ± 0.070 | 0.447 ± 0.025 |
| Orthorhombic | 0.401 ± 0.071 | 0.391 ± 0.088 | 0.749 ± 0.200 | 0.420 ± 0.059 | 0.523 ± 0.086 |
| Tetragonal | 0.268 ± 0.095 | 0.268 ± 0.095 | 0.665 ± 0.224 | 0.456 ± 0.191 | 0.415 ± 0.092 |
| Triclinic | 0.405 ± 0.179 | 0.404 ± 0.170 | 0.722 ± 0.282 | 0.431 ± 0.079 | 0.564 ± 0.214 |
| Trigonal | 0.285 ± 0.122 | 0.311 ± 0.133 | 0.737 ± 0.327 | 0.371 ± 0.103 | 0.494 ± 0.191 |
| All | 0.368 ± 0.063 | 0.391 ± 0.063 | 0.836 ± 0.125 | 0.489 ± 0.085 | 0.554 ± 0.049 |
| Task | Ionic (ϵ_0) | | | | |
| Cubic | 1.400 ± 0.368 | 1.383 ± 0.329 | 3.217 ± 1.025 | 1.901 ± 0.321 | 1.819 ± 0.621 |
| Hexagonal | 1.068 ± 0.201 | 1.028 ± 0.121 | 2.168 ± 0.479 | 1.359 ± 0.206 | 1.572 ± 0.308 |
| Monoclinic | 1.679 ± 0.147 | 1.711 ± 0.130 | 2.351 ± 0.272 | 1.827 ± 0.175 | 1.982 ± 0.178 |
| Orthorhombic | 1.898 ± 0.074 | 1.915 ± 0.114 | 3.120 ± 0.171 | 1.957 ± 0.150 | 2.156 ± 0.173 |
| Tetragonal | 1.910 ± 0.305 | 1.867 ± 0.348 | 3.14 ± 0.398 | 2.058 ± 0.192 | 2.092 ± 0.265 |
| Triclinic | 1.926 ± 0.179 | 1.901 ± 0.144 | 2.523 ± 0.229 | 1.783 ± 0.267 | 2.172 ± 0.201 |
| Trigonal | 1.494 ± 0.253 | 1.571 ± 0.315 | 2.745 ± 0.600 | 1.742 ± 0.230 | 1.769 ± 0.333 |
| All | 1.677 ± 0.050 | 1.685 ± 0.049 | 2.823 ± 0.180 | 1.862 ± 0.131 | 1.969 ± 0.052 |
| Task | Total (ϵ) | | | | |
| Cubic | 1.808 ± 0.615 | 1.898 ± 0.621 | 4.834 ± 1.443 | 2.627 ± 0.702 | 2.548 ± 0.845 |
| Hexagonal | 1.409 ± 0.199 | 1.419 ± 0.271 | 3.151 ± 0.498 | 1.671 ± 0.557 | 1.954 ± 0.266 |
| Monoclinic | 1.854 ± 0.098 | 1.890 ± 0.148 | 2.784 ± 0.344 | 2.047 ± 0.160 | 2.267 ± 0.184 |
| Orthorhombic | 2.141 ± 0.089 | 2.178 ± 0.068 | 3.535 ± 0.152 | 2.228 ± 0.153 | 2.461 ± 0.180 |
| Tetragonal | 2.018 ± 0.373 | 2.036 ± 0.284 | 3.325 ± 0.544 | 2.403 ± 0.345 | 2.351 ± 0.434 |
| Triclinic | 2.142 ± 0.105 | 2.218 ± 0.181 | 3.103 ± 0.624 | 1.906 ± 0.284 | 2.488 ± 0.136 |
| Trigonal | 1.739 ± 0.269 | 1.624 ± 0.280 | 3.265 ± 0.709 | 1.984 ± 0.259 | 2.040 ± 0.371 |
| All | 1.911 ± 0.094 | 1.927 ± 0.104 | 3.427 ± 0.265 | 2.185 ± 0.114 | 2.320 ± 0.153 |

Table 2: Performance comparison of models across all crystal systems. Models are trained separately for 3 tasks: the electronic component, ionic component and total dielectric constants. The results are shown by the MAE_{ten} and standard deviation of 5 runs using different random split. The 5 trained *DTNN* models will be employed as ensemble models for virtual screening in the next section.

models. The aggregation of potential edge information showcases significant improvements in accuracy, as evidenced by *DTNN* beating *DTNN-simple* in 18 out of the 24 tasks. It should be noted that *DTNN-simple* still gives much better accuracy than the other 3 models, outperforming 22 tasks. Only two tasks lost to *M3GNet* when making ionic and total dielectric tensor predictions on triclinic systems. Hence, the latent edge scalar and vector features provide additional useful geometric information which benefits the dielectric prediction.

2.4 Discovery of Dielectric materials

2.4.1 Potential application

Dielectrics are crucial functional materials for in microelectronic device manufacturing. Materials with high dielectric constants have the potential to enable higher energy density storage, leading to performance enhancement and device miniaturization.[39]. Meanwhile, large band gaps (E_g) are also desirable as they prevent leakage currents when materials are exposed to large electric fields, especially at nanoscale thicknesses.. Hence, novel dielectric materials with both high dielectric constants ϵ and large band gaps E_g are highly preferred for such applications. The *DTNN* model has been proven effective predicting dielectric tensors which account for the direction and magnitude of the electric field. To represent the capacity of electric energy storage, dielectric tensors ϵ can be simplified to scalar quantities by Eq.2. To prepare the candidate set for screening, we downloaded 14,375 non-metal materials from the MP database. These materials are specifically selected based on the energy above convex hull $E_{\text{hull}} = 0$ to estimate their thermodynamic stability, so that only stable materials are included in the candidate set. The candidates have unknown dielectric constant properties, and there is no overlap between this candidate set and our training dataset. We attempt to leverage our models for virtual screening on all these candidates to identify potential materials suitable for dielectric applications in microelectronic device manufacturing. To improve the accuracy, we use the ensemble results from the 5 *DTNN* models trained in the previous section.

2.4.2 Inversely related E_g and ϵ

It is known that there exists inverse relationship between the electronic part of dielectric constants ϵ^∞ and band gaps E_g . On the other hand, the ionic contribution ϵ^0 does not show a clear correlation with E_g . The theoretical background of this phenomenon is explained in reference[40]. This trend is also observed in the materials present in the training set as shown in Fig. 6(a) and Fig. 6(b). To showcase the capability of our model in capturing such latent quantum mechanism knowledge underlying chemical structures, we employ the $DTNN-\epsilon^\infty$ and $DTNN-\epsilon^0$ models to predict the two dielectric constant components for the 14,375 candidates, respectively. The density of data points are drawn in contours for structures in the training set (red) and candidate set (blue) using the kernel density estimation. Despite the fact that the model does not learn explicitly from band gap data, the distribution of model-predicted electronic dielectric constants of the candidates and their DFPT-computed band gaps from MP indicates the model’s capacity to comprehend this negative relationship between the two properties through materials’ graph representations. This phenomenon can be explained by the interplay between electronic polarization and electronic excitations. Materials with smaller band gaps allow for easier excitation of electrons to higher energy levels, leading to higher electronic polarizability and larger electronic dielectric constants. Conversely, materials with larger band gaps hinder electron excitation, resulting in lower electronic dielectric constants [41]. In contrast to the case of ϵ^∞ , no discernible correlation is observed between $DTNN-\epsilon^0$ -predicted ionic part and band gaps. From a microscopic perspective, the ionic dielectric constant is influenced by the displacement of cations and anions from their equilibrium positions under the influence of electric fields. The strength of bonds or phonon frequencies is highly sensitive to variations in bond lengths. Consequently, materials with similar compositions can exhibit a wide range of ϵ^0 due to differences in bond lengths [42]. The weak constraint of E_g to ϵ^0 along with the broad value spectrum of ϵ^0 present the opportunity for the exploration and discovery of novel dielectric materials characterized by both high ϵ and E_g .

2.4.3 Virtual screening & DFPT validation

We conducted the virtual screening by predicting total dielectric constant scalar ϵ for all structures in the candidate set. Following the previous work[42], $E_g \cdot \epsilon$ is assigned as the figure of merit (FOM) to quantify the performance of dielectrics, since E_g and ϵ are approximately proportional to the logarithm of the leakage current density[43]. After prediction, we ranked the structures according to FOM and investigated the compositions of the top-100 materials subset compared to all materials in Fig.6(c). Excluding common non-metallic elements like oxygen and fluorine, we found tantalum (Ta) to be the most frequently occurring metallic element among the top candidate materials, followed closely by lead (Pb), bismuth (Bi), and niobium (Nb). To validate the promising materials identified by $DTNN$, we selected 12 candidates from the top 100 materials based on computational budget constraints. These candidates were chosen to have a unit cell size with a maximum of 20 atoms to enable efficient computation of their dielectric constants using DFPT. The details of DFPT configurations are available in the Method section.

Fig. 6(d) illustrates the distribution of the figure of merit (FOM) for stable materials in both the training set and candidate set. The thermodynamically stable material with the highest FOM in the training dataset is Sn_2ClF_3 (mp-29252, $E_g = 3.56\text{eV}$, $\epsilon^\infty = 3.81$, $\epsilon^0 = 72.77$, $\epsilon = 76.55$). We successfully identified a new material $\text{Ba}_2\text{SmTaO}_6$ (mp-1214622, $E_g = 3.36\text{eV}$, $\epsilon^\infty = 4.85$, $\epsilon^0 = 88.96$, $\epsilon = 93.81$) with structural visualized in Fig. 6(e). Its FOM score is higher than any calculated stable structures in our database that are used for model training. Three of the constituent elements present in $\text{Ba}_2\text{SmTaO}_6$ (O, Ta, and Ba) are among the most commonly occurring elements in the compositions of materials within the top 100 candidates. This observation further supports the compatibility of these elements in forming high-performance dielectric materials.

3 Discussion

Transfer learning is the most popular approach to tackle the data bottleneck which is common in materials science. Previous studies have utilized transfer learning in GNN models, both for the same properties and across different properties, to demonstrate enhanced accuracy in materials science[44, 45, 15]. For example, Chen et al. developed the AtomSets framework[46], which employs a straightforward model architecture to process structure-embedded scalar information read from a pretrained MEGNet model[25], enabling high accuracy predictions with limited datasets. However, the feasibility of transfer learning for properties across different tensorial orders has been less explored. Our study indicates that more than scalar features, it is also possible to transfer higher-rank equivariant compositional and structural information from a pretrained EGNN energy model to a different tensorial property prediction with a small amount of available data, while maintaining the equivariance. These equivariant representations may hold shared structural or even electronic-level information, since the TeaNet/PFP model aims to emulate iterative electronic relaxation. This is evident through the accurate predictions our model achieved for both electronic and ionic dielectric constants, which are produced by different microscopic mechanisms. Furthermore, the pretrained TeaNet/PFP serves as

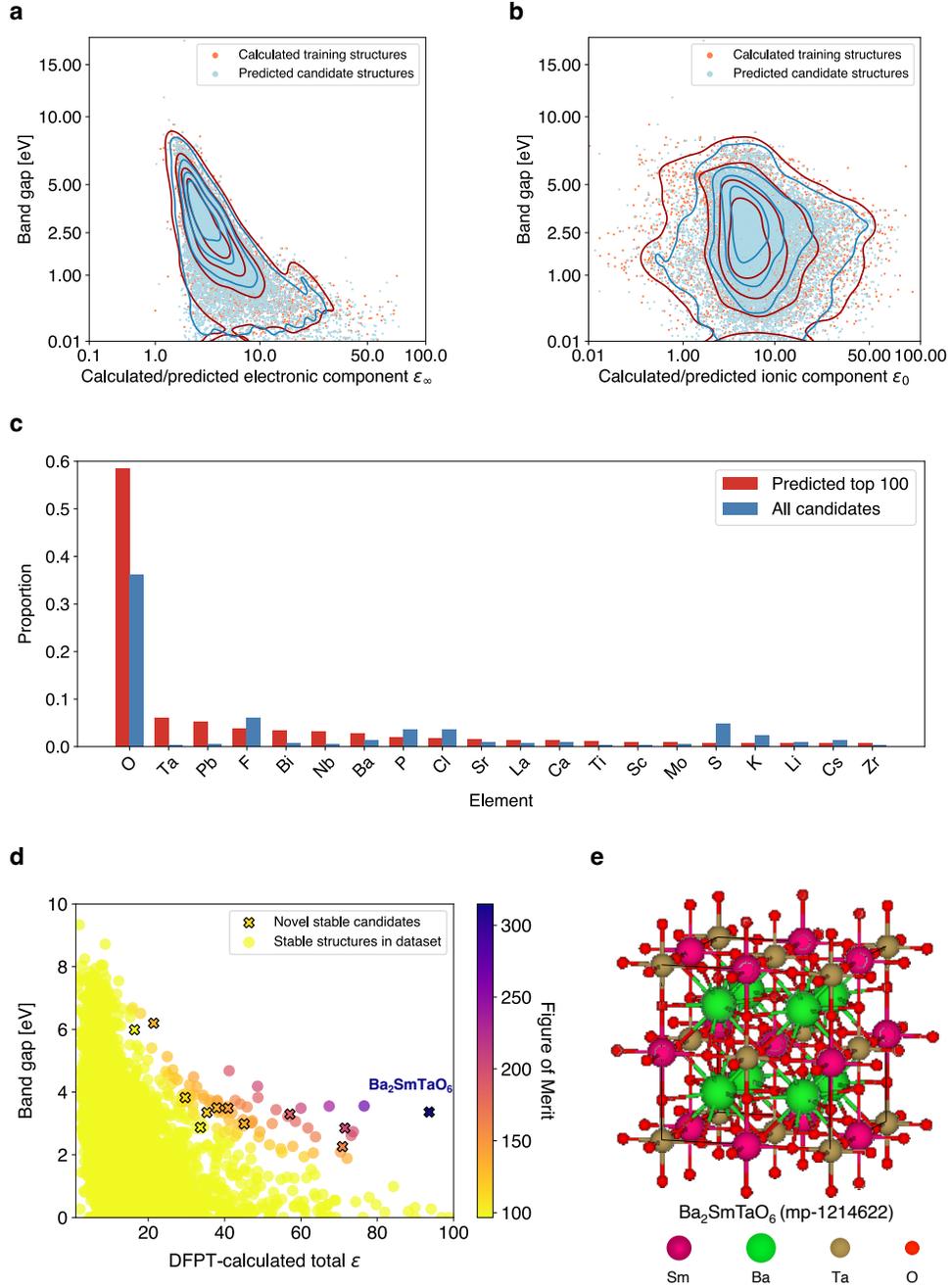


Figure 6: (a-b) The joint distribution of band gaps E_g and electronic dielectric constants ϵ^∞ (a) or ionic dielectric constants ϵ^0 (b) for 6,648 training structures and 14,375 stable candidate structures. ϵ^∞ and ϵ^0 of training structures and E_g of all structures are obtained from computational results in MP, while ϵ^∞ and ϵ^0 of candidate structures are predicted by *DTNN*- $\epsilon^\infty/\epsilon^0$. The 5-level densities of data points are drawn in contours using the kernel density estimation for structures both in the candidate set and original set. (c) The top 20 most frequently occurring elements in the top 100 high-quality candidate materials screened from 14,375 candidate structures. (d) DFT-calculated $E_g - \epsilon$ data points colored by their figure of merit defined by $E_g \cdot \epsilon$ for 4,146 stable structures in training data and 12 new stable structures screened by *DTNN*. (e) Structure visualization of $\text{Ba}_2\text{SmTaO}_6$ as the top-tier candidate validated by DFPT calculation.

an encoder that integrates electron density information, assisting in comprehending the electronic-level relationship between the E_g and ϵ^∞ . Apart from dielectric constants, several works attempted to predict tensorial properties of

materials such as the polarizability[47], quadrupole[48], by using equivariant architectures. The accuracy of such tasks could potentially be improved by fixing parameters in the shallower layers of an EGNN model pretrained on commonly computed properties like energy.

The *PPF* model is pretrained on over 22 million structures covering the diverse chemical space. It is efficient and expressive to take a pretrained *PPF* as the parent model to generate locally-interacted features as the input to a much simpler child model. In the current readout architecture, it consists of only 0.6 million trainable parameters for the downstream tasks of dielectric constant prediction. The model performing best on the validation accuracy appears at the average epoch of 263 out of 5 training runs for total dielectric constants. By stopping the training after 200 epochs without improvement in validation accuracy, the model training can be efficiently completed within approximately 2 hours using about 6GB memory on an Nvidia Tesla-V100 GPU. We proved that such efficient training on encodings from the parent model can bring a promising property predictor even on a small data region as demonstrated in Table 2. The incorporation of second-order equivariant features in our model may also contribute to high data efficiency as the symmetry of the dielectric tensors is automatically guaranteed due to the model architecture. Based on only 6.6k sample structures with labeled tensor containing up to 6 independent elements from MP, our model achieved a mean tensor prediction error of 0.368 for ϵ^∞ , 1.677 for ϵ^0 and 1.911 for ϵ .

After validating the screening results with DFPT computations, our model successfully identified $\text{Ba}_2\text{SmTaO}_6$ out of massive data with over 14k structures directly based on its structural graph. Thanks to widely-supported elements in the pretrained *PPF*, our model can also give relatively good prediction on rare earth elements, e.g., the Sm element in $\text{Ba}_2\text{SmTaO}_6$. The rare earth elements have diverse industrial applications such as glass, lights, magnets, batteries, and catalytic converters and so on[49], due to their unique physical and chemical properties. Our model has the potential to make predictions about properties concerning rare elements, which typically suffer from limited data availability.

In this study, we shows the applicability of our model to a problem in microelectronic device manufacturing, where only the simplified scalar dielectric constant is taken to evaluate the charge storage ability. Accurate predictions of dielectric constants as tensors can contribute to understanding material behavior in the presence of electric fields and their interactions with other materials. This knowledge can facilitate the development of new materials with tailored properties for specific applications, such as energy storage, signal transmission, and electronic component design.

4 Conclusion

An equivariant model is introduced to predict the second-order tensorial property, dielectric constants, for inorganic materials across 72 supported elements. By leveraging transfer learning, the TeaNet/PPF was treated as the frozen base model to encode material graphs with integrated elemental and structural information. A light-weight trainable equivariant readout module is connected to integrate information in different orders for the final outputs. It was discovered that embedded features from deeper GCN layers in TeaNet/PPF contribute to better accuracy in predicting total dielectric constants. After efficiently training the equivariant readout module, our *DTNN* model achieved higher accuracy in predicting the electronic, ionic, total dielectric tensors compared with state-of-the-art models, PaiNN, M3GNet and MatTen, across various crystal system types. To test the model’s capability in discovering novel dielectric materials for microelectronic manufacturing with large band gaps and high dielectric constants, we observed that our model can comprehend the electronic-level inverse correlation between band gaps and electronic dielectric constants. Finally, the virtual screening conducted by the model identified one dielectric material that contains a combination of high-dielectric constant and large band gap, $\text{Ba}_2\text{SmTaO}_6$ ($E_g = 3.36\text{eV}$, $\epsilon = 93.81$) from a vast pool of over 14k candidates with only 12 DFPT calculations.

Our work highlights that pretrained equivariant graph neural networks, which capture higher-order tensor representations, can incorporate common compositional and structural information, leading to improved accuracy in predicting properties of different orders. This approach also represents a viable alternative for enhancing prediction accuracy for other higher-order properties such as polarizability, multi-poles, and elasticity, thereby accelerating new material discoveries for specific applications.

5 Methods

5.1 Data Source

The Materials Project (v2023.11.1) contains a dataset of 7,277 dielectric tensors. The dielectric properties are calculated using the Vienna Ab-Initio Simulation Package (VASP version 5.3.4), employing the generalized gradient approximation GGA/PBE exchange-correlation functional[50] with the +U correction[51, 52] to account for electron-electron interactions within the transition metal orbitals. Projector Augmented Wave pseudopotentials[53, 54] were also

included. In the majority of cases, the dielectric constants obtained from these calculations exhibit a relative deviation of less than +/- 25% when compared to experimental values at room temperature. For each structure, it contains the value of the two components, namely, the electronic component and the ionic component. The total dielectric tensor can be calculated by summing up the two components. We clean up the dataset by filtering out dielectric constants that contain any element out of the range of $[-10, 100]$. Structures that contain elements not supported by PFP (shown in Fig.4(c)) are cleaned up, and finally there are 6,648 structures retained for model training.

The dataset is randomly split into the training, validation and test data in the ratio of 80%, 10% and 10%, respectively. For each experiment conducted in the present study, we do 5 different random splits first and we report their average performance as well as the deviation of the 5 runs to reduce the impact of random.

5.2 Model Architectures

Once the model is trained on large potential data, we extract the intermediate knowledge \mathbf{a}_s^n , \mathbf{a}_v^n , \mathbf{a}_t^n , \mathbf{b}_s^n , and \mathbf{b}_v^n , from a pretrained *PFP-L_n* as the input for our equivariant readout layers.

Overview The input materials are preprocessed to identify appropriate neighbor atoms under the periodic boundary conditions for graph construction. Each material is represented by a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. The initialized atom attributes contain three types of information with different ranks: $\mathcal{V} = \{(a_s^{(0)}, a_v^{(0)}, a_t^{(0)})_i\}_{i=1:N^a}$, where $a_s^{(0)} \in \mathbb{R}^{C_s^a}$, $a_v^{(0)} \in \mathbb{R}^{C_v^a \times 3}$, $a_t^{(0)} \in \mathbb{R}^{C_t^a \times 3 \times 3}$, and N^a is the number of atoms. a_s is initialized by looking up the table, in which each element is mapped to a high-dimension encoding with summation equal to the atomic number divided by 2. Both atom vector a_v and atom tensor a_t are initialized to be zeros. Two types of bond attributes are prepared: $\mathcal{E} = \{(b_s^{(0)}, b_v^{(0)})_k\}_{k=1:N^b}$, in which $b_s^{(0)} \in \mathbb{R}^{C_s^b}$, $b_v^{(0)} \in \mathbb{R}^{C_v^b \times 3}$, N^b is the number of bonds between atom pairs within the cutoff radius R_c , and C_s^a , C_v^a , C_t^a , C_s^b , C_v^b are the corresponding number of channels for each feature. Both $b_s^{(0)}$ and $b_v^{(0)}$ are filled with zeros initially in this work.

TeaNet[31] is used as the base GNN architecture in *PFP*[32, 33]. The TeaNet architecture incorporates a second-order Euclidean tensor for high-order geometry interaction and performs equivariant graph convolutions using its information. The original material[31] provides a step-by-step explanation for TeaNet implementation, please check it for more details. *PFP* has several modifications on TeaNet, such as introducing the Morse-style two-body potential term and so on, see the corresponding material[32] for details. *PFP* hold the scalar features a_s , b_s invariant and the vector/tensor features a_v , a_t , b_v equivariant to 3D rotations. *PFP* calculates local interactions in each of its GCN layers. 5-layer GCN layers are constructed with the cutoff radius R_c as 3, 3, 4, 6 and 6Å, respectively. In other words, latent embeddings in the earlier convolutional layers hold less distant information. As a result, the maximum distance of atomic interactions counted in *PFP* is 22Å after the 5-layer information propagation. The intermediate atom/bond features $a_s^{(l)}$, $a_v^{(l)}$, $a_t^{(l)}$, $b_s^{(l)}$, and $b_v^{(l)}$ extracted from the l -th GCN layer are used as the input to the designed *DTNN* which contains N equivariant blocks and a readout neural network.

Neural network definition We denote the one-layer linear transformation without the bias term as

$$\mathcal{L}^k : x \mapsto \mathbf{W}_k x \quad (8)$$

and one layer of the perceptron model as

$$\mathcal{L}_g^k : x \mapsto g(\mathbf{W}_k x + \mathbf{b}_k) \quad (9)$$

where \mathbf{W}_k and \mathbf{b}_k are learnable parameters, $g(x)$ is the activation function which can be substituted by $s(x)$ as the SiLU activation function and $\sigma(x)$ as the sigmoid activation function. The SiLU activation function $s(x)$ [55, 56, 57] is defined by the sigmoid function $\sigma(x)$ multiplied by its input x

$$s(x) = x * \sigma(x) = \frac{x}{1 + e^{-x}} \quad (10)$$

Thus the K -layer MLP with $s(x)$ in the intermediate layers and without the activation function in the final layer can be expressed as

$$\xi^K(x) = (\mathcal{L}^K(x) \circ \mathcal{L}_s^{K-1} \circ \dots \mathcal{L}_s^1)(x) \quad (11)$$

And the K -layer gated MLP[58] is represented by

$$\phi^K(x) = ((\mathcal{L}^K(x) \circ \mathcal{L}_s^{K-1} \circ \dots \mathcal{L}_s^1)(x)) \odot ((\mathcal{L}_\sigma^K(x) \circ \mathcal{L}_s^{K-1} \circ \dots \mathcal{L}_s^1)(x)) \quad (12)$$

where \odot denotes the element-wise product. It comprises two networks, i.e., a normal MLP defined as defined in Eq.11 and a gate network with the final layer activated by a sigmoid function.

Equivariant block The equivariant block takes $a_s^{(l,n)}$, $a_v^{(l,n)}$, $a_t^{(l,n)}$, $b_s^{(l)}$, and $b_v^{(l)}$ as inputs, where l denotes the GCN layer number of *PF*, and n denotes the layer number of the equivariant block. The perceptron models are applied to the atom scalar features $a_s^{(l,n)}$ and edge scalar features $b_s^{(l)}$, respectively,

$$a_{s1}^{(l,n)} = \xi_{a_{s1}}^K(a_s^{(l,n)}) \quad (13)$$

$$b_{s1}^{(l,n)} = \xi_{b_{s1}}^K(b_s^{(l,n)}) \quad (14)$$

To keep the equivariance of vector features and tensor features, the linear transformations without the bias term are applied to the atom vector features $a_v^{(l,n)}$, atom tensor features $a_t^{(l,n)}$, and bond vector features $b_v^{(l)}$.

$$a_{v1}^{(l,n)} = \mathcal{L}_{a_{v1}}(a_v^{(l,n)}) \quad (15)$$

$$a_{t1}^{(l,n)} = \mathcal{L}_{a_{t1}}(a_t^{(l,n)}) \quad (16)$$

$$b_{v1}^{(l)} = \mathcal{L}_{b_{v1}}(b_v^{(l)}) \quad (17)$$

The neighbor set of atom i is denoted as \mathcal{N}_i . Let $a_{s1,i}^{(l,n)}$ denote the scalar feature of atom i , and $b_{s1,\{i,j\}}^{(l)}$ denote the scalar feature of the bond connecting atom i and atom j . Other vector and tensor features are represented in a similar manner. The bond scalar features $b_{s1}^{(l)}$ and vector features $b_{v1}^{(l)}$ are aggregated to atom scalar features $a_{s1}^{(l,n)}$ and vector features $a_{v1}^{(l,n)}$ accordingly, thus for each atom i

$$a_{s2,i}^{(l,n)} = a_{s1,i}^{(l,n)} + \sum_{j \in \mathcal{N}_i} b_{s1,\{i,j\}}^{(l)} \quad (18)$$

$$a_{v2,i}^{(l,n)} = a_{v1,i}^{(l,n)} + \sum_{j \in \mathcal{N}_i} b_{v1,\{i,j\}}^{(l)} \quad (19)$$

Then the norm of node vector features and tensor features are combined with the node scalar features and fed into another perceptron model.

$$a_{s3}^{(l,n)} = \xi_{a_{s3}}^K(\text{concat}(a_{s2}^{(l,n)} + \text{norm}(a_{v2}^{(l,n)}) + \text{norm}(a_{t2}^{(l,n)}))) \quad (20)$$

Inspired by the gate nonlinearity design[59], the interaction output of different-rank node features are split, and the vector and tensor components are multiplied by the sigmoid activation function to form a gate equivariant nonlinearity for the transformed input of the vector feature and tensor feature, respectively.

$$a_{s4}^{(l,n+1)}, a_{v3}^{(l,n)}, a_{t3}^{(l,n)} = \text{split}(a_{s3}^{(l,n)}) \quad (21)$$

$$a_{v4}^{(l,n+1)} = \sigma(a_{v3}^{(l,n)}) \odot \mathcal{L}_{a_{v2}}(a_v^{(l,n)}) \quad (22)$$

$$a_{t4}^{(l,n+1)} = \sigma(a_{t3}^{(l,n)}) \odot \mathcal{L}_{a_{t2}}(a_t^{(l,n)}) \quad (23)$$

Finally, the updated $a_{s4}^{(l,n+1)}$, $a_{v4}^{(l,n+1)}$ and $a_{t4}^{(l,n+1)}$ are used as the input for the next equivariant readout block.

Readout The final layer output, i.e., layer N , of the equivariant blocks $a_s^{(l,N)}$, $a_v^{(l,N)}$ and $a_t^{(l,N)}$ are aggregated for the tensorial property prediction. Since the dielectric constant is an intensive property, we take the average aggregation of the atom features in the graph representation of materials. The gated MLP applied to the scalar features $a_s^{(l,N)}$ is found to help improving the accuracy compared with the normal MLP. Therefore, the atom scalar features is processed by

$$a'_s = \phi^K(a_s^{(l,N)}) \quad (24)$$

The channels of atom vector and tensor features are compressed to 1 by

$$a'_v = \mathcal{L}_{a_{v3}}(a_v^{(l,N)}) \quad (25)$$

$$a'_t = \mathcal{L}_{a_{t3}}(a_t^{(l,N)}) \quad (26)$$

Finally, we construct the dielectric tensors using

$$\epsilon = \frac{1}{N} \sum (a'_s \mathbf{I}_3 + a'_v \otimes a'_v + a'_t) \quad (27)$$

where \mathbf{I}_3 is the 3×3 tensor with ones on the diagonal and zeros elsewhere, and \otimes represents the outer product operation. The first models isotropic, and the final two terms add the anisotropic components of the dielectric tensor. Therefore, the final output of our model is the 3×3 dielectric tensor following the equivariance of the materials input.

5.3 Hyperparameters

The *DTNN* model contains 2 equivariant blocks (Fig. 3(a)). All the latent dimensions in MLP in Fig. 3(b) and (c) are set to 128 with a dropout rate of 0.2. The batch size is set to 64 during training. The AdamW optimizer[60] is utilized to optimize parameters with $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\lambda = 0.01$. The learning rate starts at 1×10^{-4} and a cosine annealing schedule is applied for tighter convergence. The gradient norm is clipped at 2.0 to stabilize the training. Early stopping is applied during training if no improvement on the validation accuracy is observed after 200 epochs.

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Competing interests

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Zetian Mao was an intern/part-time employee at Preferred Networks, Inc. during this study. Jethro Tan and Wenwen Li are full-time employees working at Preferred Networks, Inc.

Data availability

The materials with dielectric constants are freely accessible using The Materials Project API (<https://next-gen.materialsproject.org/api>).

Code availability

The code implementation of *DTNN* will be publicly available after submission to the journal.

Author contribution

Z. M. implemented the codes and conducted experiments. W. L, J. T. and Z. M. conceived the idea. W. L. and J. T. provided technical support of *PPF*, and supervised the research. All authors wrote and confirmed the manuscript.

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