

ARPES-Inspired Reciprocal-Space Crystal Property Predictor

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A critical contribution of artificial intelligence to materials physics is accurate and efficient predictions of crystal properties. Real-space graph neural networks are currently a mainstream choice for crystal property prediction, as reciprocal-space approaches have been commonly considered incapable of achieving comparable accuracy. Here, we develop an Angle-resolved-photoemission-spectroscopy-Inspired Reciprocal-space Crystal Property Predictor (AIRCPP), which combines spherical harmonics and Legendre polynomials as an orthogonal basis, sampled by a Lebedev grid for the reciprocal space. Using a large dataset of 95 700 materials, we demonstrate that AIRCPP achieves comparable or higher accuracy in predicting various crystal properties compared to the widely used crystal graph convolutional neural networks (CGCNN), but with much lower computational costs. Combining AIRCPP and CGCNN further enables a more powerful model termed AIRCPP-MIX that achieves comparable accuracy to the state-of-the-art advanced models. Our study demonstrates the giant potential of reciprocal-space approaches in highly accurate crystal property predictions, laying the foundation for computational materials design and discovery.

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Density functional theory (DFT) based first-principles calculations enable accurate predictions of material properties [1,2], which have profoundly advanced the development of condensed matter physics. However, their high computational costs are still a bottleneck that limits their applications in material simulations at extended time and length scales. Therefore, intense efforts have been devoted to the development of accurate and efficient methods for crystal property predictions in recent years [3–8], for which artificial intelligence (AI) has been a powerful booster [9–15].

Graph neural networks (GNNs), in particular, the crystal graph convolutional neural networks (CGCNN) [16] that employ graphs to describe crystals, have been extremely successful in accurately predicting crystal properties, becoming a highly active research field [17–22]. However, to accurately describe crystals, these methods require construction of the neighbor list to build the graph and descriptors, which is still a performance bottleneck in large-scale material simulations. Further, although real-space approaches can effectively describe short-range interactions, capturing long-range interactions has been a long-standing challenge [23].

In fact, due to the periodic nature of crystal structures, reciprocal-space approaches are a physically intuitive choice

for the representation of crystal information [24–26], and can rigorously capture the long-range interactions. There have indeed been such attempts in incorporating reciprocal-space descriptors into crystal neural networks [27–32]. Nevertheless, accurate continuous reciprocal-space features usually require costly methods like DFT due to the difficulty of reciprocal-space sampling. In contrast, machine-learning models often use atomic-coordinate-based Fourier transforms that are restricted to integer reciprocal-lattice points. While this captures the overall periodicity of the crystal, it misses higher-frequency features associated with local atomic arrangements, which are essential for an accurate description of the crystal and typically appear at noninteger points. As a result, it is commonly recognized that pure reciprocal-space approaches cannot achieve comparable or higher accuracy compared to their real-space counterparts.

In this article, we develop an angle-resolved photoemission spectroscopy (ARPES)-Inspired Reciprocal-space Crystal Property Predictor (AIRCPP). Using the Materials Project database with around 95 700 materials for training, testing, and validating, we show that this pure reciprocal-space approach achieves accuracy that is comparable or even higher compared to CGCNN in the prediction of various crystal properties. The computational cost of AIRCPP is significantly lower. This is because AIRCPP uses Lebedev grids for reciprocal-space sampling, which does not require expensive neighbor search in real space. Moreover, combining AIRCPP with CGCNN enables a hybrid model that we term AIRCPP-MIX, which achieves an accuracy that compares to the state-of-the-art advanced models. This advancement highlights the enormous potential of reciprocal-space methods for materials discovery, offering fruitful avenues for future research.

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Constructing reciprocal-space features requires performing a Fourier transform on the crystal, such as the structural factor, which is defined by

$$F(\mathbf{G}) = \sum_j f_j e^{-i\mathbf{G}\cdot\mathbf{r}_j}, \quad (1)$$

where f_j are the atomic form factors (i.e., the Fourier transform weights), $\mathbf{G}$ are reciprocal-lattice vectors, and $\mathbf{r}_j$ are the atomic coordinates in real space. The structure factor is used to describe the intensity distribution of x-ray diffraction [33–35].

As discussed above, traditional sampling with integer reciprocal-lattice points captures the periodicity, but misses key high-frequency features at noninteger points. Furthermore, the integer lattice grid depends on the choice of the lattice basis vectors. When the structure rotates with the basis vectors remaining fixed, this grid cannot maintain consistent sampling, and thus cannot achieve strict rotational invariance (see the Supplemental Material [36] for more detailed discussion).

From a physical perspective, as the Fourier transform of real space, reciprocal space associates each reciprocal-space vector with a specific periodicity in real space. For example, the atomic distribution and electronic structure in a given crystal exhibit inherent patterns in reciprocal space, which remain unchanged with the crystal size. Experimental techniques such as ARPES can directly probe the distribution of electronic states in reciprocal space, and their results are independent of the supercell selection [37–39]. Therefore, constructing features based on absolute reciprocal space can theoretically achieve good invariance.

Based on the physical insights described above, we illustrate the core physical representation of AIRCPP in Fig. 1. To fully capture the physical essence of the atomic form factor f_j , we introduce a modulation function in Eq. (2) that depends on both the wave vector amplitude $|\mathbf{k}|$ and the atomic species $\mathbf{A}_j$ to accurately model the variations of reciprocal-space features. This modulation is implemented via a learnable two-stage multilayer perceptron (MLP) architecture M :

$$\tilde{f}_j(\mathbf{k}) = M(|\mathbf{k}|, \mathbf{A}_j) \cdot f_j. \quad (2)$$

Inspired by the constant-energy surface windows used in ARPES (see Fig. 1), we extend the concept of atomic form factors. Unlike ARPES, which directly probes electronic energy levels, our approach introduces a multidimensional, learnable atomic embedding. Each dimension encodes a self-consistent reciprocal-space feature pattern, similar to the constant-energy windows used in ARPES. After applying the modulation in Eq. (2), this representation not only captures the electronic distribution, but also distinguishes between atomic species. Thus, we construct a physics-inspired, multidimensional, global reciprocal-space feature space that can be used to predict various crystal properties.

To accurately describe crystal properties, descriptors must possess strict translational, rotational, and permutation invariance [40]. The additive nature of the structure factor endows it with strict permutation invariance. Since the classical $F(\mathbf{G})$ is restricted to integer lattice points, we introduce $S(\mathbf{k})$ in AIRCPP, which is defined throughout the entire reciprocal

space. For translational invariance, we have

$$S'(\mathbf{k}) = \sum_j \tilde{f}_j e^{i\mathbf{k}\cdot(\mathbf{r}_j+\mathbf{d})} = S(\mathbf{k}) \cdot e^{i\mathbf{k}\cdot\mathbf{d}}, \quad (3)$$

$$|S'(\mathbf{k})| = |S(\mathbf{k})| \cdot |e^{i\mathbf{k}\cdot\mathbf{d}}| = |S(\mathbf{k})|, \quad (4)$$

where $\mathbf{d}$ is the translation vector. For any wave vector $\mathbf{k}$ in the reciprocal space, the amplitude of the structure factor satisfies translational invariance.

The spherical harmonics $Y_{lm}(\theta, \phi)$ serve as orthogonal basis functions for representing angular distributions on the sphere, while the radial dependence is captured by scaled and shifted Legendre polynomials $P_n(r)$. Together, these angular and radial functions constitute a spatially orthogonal basis. A spatial distribution $f(\theta, \phi, r)$ can thus be expanded as

$$f(\theta, \phi, r) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=0}^{\infty} a_{lmn} P_n(r) Y_{lm}(\theta, \phi), \quad (5)$$

where a_{lmn} are the expansion coefficients. To accurately compute a_{lmn} , the Lebedev quadrature and Gauss-Legendre quadrature are combined. A Lebedev grid is chosen to integrate spherical harmonics exactly up to degree l , while the Gauss-Legendre rule integrates radial polynomials exactly up to degree $2n - 1$. Using the orthogonality of the basis functions, the coefficients are then obtained via numerical integration [41–44]:

$$\begin{aligned} a_{lmn} &= \int_0^R \int_{\Omega} f(\theta, \phi, r) Y_{lm}^*(\theta, \phi) P_n(r) r^2 \sin \theta d\theta d\phi dr \\ &\approx \sum_{i=1}^{N_{\text{Leb}}} \sum_{j=1}^{N_{\text{Leg}}} w_i^{\text{Leb}} w_j^{\text{Leg}} f(\theta_i, \phi_i, r_j) Y_{lm}^*(\theta_i, \phi_i) P_n(r_j), \end{aligned} \quad (6)$$

where R is the upper radial integration limit, N_{Leb} and N_{Leg} denote the number of Lebedev and Gauss-Legendre quadrature points, and w_i^{Leb} and w_j^{Leg} are the corresponding weights. Based on our systematic tests, the multilayer Lebedev grid employs 12 radial shells, spaced according to Gauss-Legendre quadrature, up to a cutoff of $2.4\pi \text{ \AA}^{-1}$ (see the Supplemental Material [36] for details of the tests). To ensure rotational invariance, we introduce angular power spectrum C_{ln} for each degree l by [45]

$$C_{ln} = \frac{1}{2l+1} \sum_{m=-l}^l |a_{lmn}|^2. \quad (7)$$

Since C_{ln} is SO(3)-invariant, the formulation is rotationally invariant. Thus, the descriptor is strictly invariant to translations, rotations, and atomic permutations.

AIRCPP includes two modules: descriptor construction and prediction (see the Supplemental Material [36] for more details). In the descriptor construction module, multidimensional complex-valued embedding features are initially generated by an embedding layer. These embedding features are then processed as Eq. (2) through a two-stage MLP to produce the modified atomic form factor $\tilde{f}_j$. Subsequently, the crystal feature representation is derived through structure factor calculations, basis functions expansion, and angular power spectrum computation. In the prediction module, the features are processed via an MLP, followed by adaptive weighting

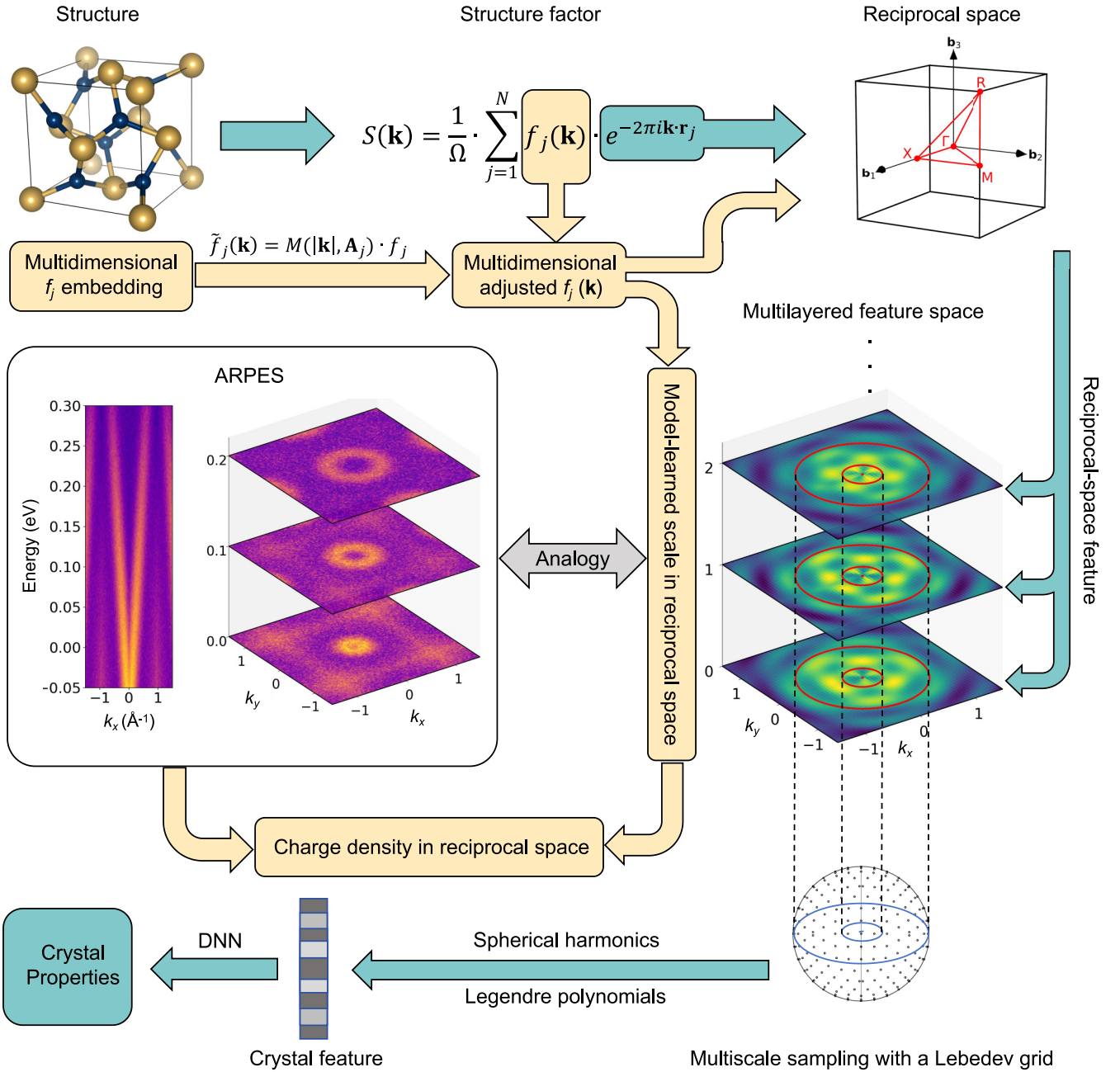


FIG. 1. Schematic illustration of the core physical representation and principle of AIRCPP.

or dimensionality reduction across two input dimensions. Finally, the features are mapped to the output via an MLP.

We evaluate the performance of AIRCPP against the widely used CGCNN on the Materials Project database [21,46,47]. The dataset comprises 95 700 crystal structures with total energy (E_t), formation energy (E_f), and band gap (E_g); a subset of 10 001 crystal structures includes bulk modulus (B) and shear modulus (G). More details of the model, hyperparameters, and datasets are provided in the Supplemental Material [36].

The model performance is summarized in Table I. Figure 2 shows a comparison of total-energy prediction accuracy on the large dataset between AIRCPP and CGCNN. For total-energy prediction, AIRCPP outperforms CGCNN, which can be attributed to its enhanced capability in modeling the global

electronic structure. In the case of formation-energy prediction, AIRCPP shows slightly lower accuracy than CGCNN, likely due to its limitations in capturing local structural details precisely for properties sensitive to local environments. The accuracy thus primarily depends on the accuracy of total-energy predictions, and still remains excellent for high-throughput materials discovery [48–51]. For band gap and elastic properties (B and G), AIRCPP achieves performance comparable to CGCNN, demonstrating robust representation of complex properties.

Compared with CGCNN, AIRCPP only requires atomic coordinates and species as input, avoiding the need for time-consuming real-space neighbor searches and graph construction. This gives AIRCPP a significant advantage in data preprocessing, especially over more complex real-space

TABLE I. Accuracy and efficiency of different models on the Materials Project dataset.

Property (MAE)	AIRCPP	AIRCPP-MIX	CGCNN	ALIGNN	CHGNet
Total energy (eV/atom)	0.059	0.031	0.094	0.071	0.030
Formation energy (eV/atom)	0.057	0.030	0.040	0.027	0.033
Band gap (eV)	0.310	0.228	0.291	0.235	0.297
B_v [lg(GPa)]	0.077	0.072	0.080	0.075	0.099
G_v [lg(GPa)]	0.125	0.113	0.116	0.105	0.141
Time per epoch (s)	18.7	24.0	19.8	326.4	386.5
Total time (h)	4.3	5.5	4.7	27.9	21.7
Number of parameters (M)	0.26	0.36	0.08	4.04	0.41

networks (see Fig. 3), which will thus be better suited for high-throughput materials screening and design.

To understand the origin of the excellent performance of AIRCPP, we analyze the reciprocal-space features it has learned. According to Fig. 4(a), the Brillouin zone lengths in the Materials Project dataset are mostly within $\pi/3 \text{ \AA}^{-1}$, allowing us to divide reciprocal space into three regions: near the Γ point ($|\mathbf{k}| \leq 0.1 \text{ \AA}^{-1}$) for the long-wavelength limit, an intermediate region ($0.1 < |\mathbf{k}| \leq \pi/3 \text{ \AA}^{-1}$) reflecting the crystal symmetry, and a large- $\mathbf{k}$ region ($|\mathbf{k}| > \pi/3 \text{ \AA}^{-1}$) capturing local atomic environments.

Since the modulation function $\tilde{f}_j(\mathbf{k})$ lacks periodicity, the reciprocal-space feature patterns also lose their periodic characteristics. A large sampling radius and dense Lebedev grid for the reciprocal space might help to improve the accuracy of AIRCPP, but it also increases the computational cost. Our careful tests demonstrate that using a sampling radius of $\sim 2.4\pi \text{ \AA}^{-1}$ can fully cover the Brillouin zone and captures the critical high-frequency Fourier components associated with local atomic arrangements, leading to high prediction accuracy with moderate computational demand (see the Supplemental Material [36]).

Taking SiO_2 as an example, we plot its reciprocal-space feature distribution on the $k_x k_y$ plane ($k_z = 0$) in Fig. 4. These reciprocal-space features can be categorized into three types: features primarily composed of Si atom Fourier transform results, features dominated by O atoms, and mixed features from both elements. This indicates that AIRCPP can effectively identify the relative spatial arrangements of different elements by learning patterns in reciprocal space, which are difficult to capture using traditional integer grids. Furthermore, AIRCPP can directly sample the features in the near- Γ region, as the

smallest sampling radius is approximately $0.07 \text{ \AA}^{-1}$. This capability is crucial for accurately describing long-range interactions, especially when predicting physical quantities that depend on material behaviors in the long-wavelength limit, e.g., the elastic properties.

AIRCPP alone already demonstrates the giant potential of reciprocal-space approaches in predicting crystal properties. Still, its accuracy is lower than the most advanced machine-learning models with more sophisticated architectures. However, in the following we show how straightforward it is to achieve even higher accuracy by making use of AIRCPP. We concatenate reciprocal-space features from AIRCPP with real-space features from CGCNN before the final output layer, leading to a much more powerful model termed AIRCPP-MIX (see details in the Supplemental Material [36]). As shown in Table I, AIRCPP-MIX outperforms ALIGNN [20] in band gap prediction and matches its formation energy accuracy, while reaching total energy accuracy equivalent to CHGNet [52]. Crucially, AIRCPP-MIX maintains exceptional computational efficiency, with an end-to-end cost only $\sim 25\%$ higher than the base model, yet several times faster than advanced frameworks like CHGNet and ALIGNN. Notably, AIRCPP-MIX matches the accuracy of ALIGNN and CHGNet with fewer parameters, indicating a physically more direct approach.

Physically, although both real-space and reciprocal-space descriptions encompass the entire crystal, they emphasize different aspects: Real-space representations focus on local chemical bonding, while reciprocal space naturally captures

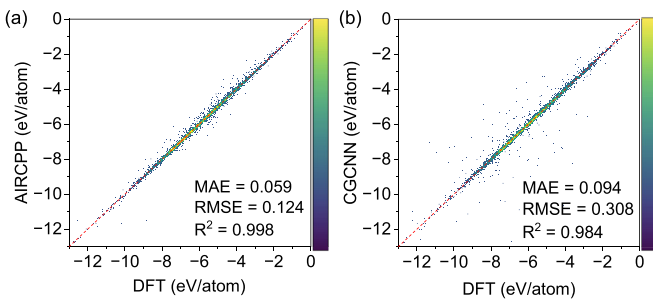


FIG. 2. Comparison of (a) AIRCPP and (b) CGCNN in predicting total energies of different crystal structures.

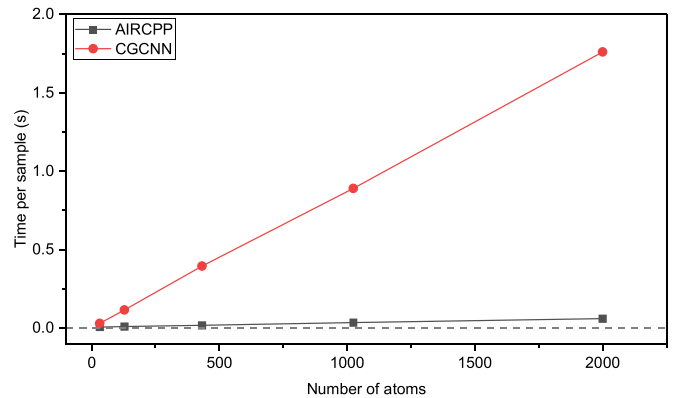


FIG. 3. Comparison of AIRCPP and CGCNN in the efficiency of data preprocessing.

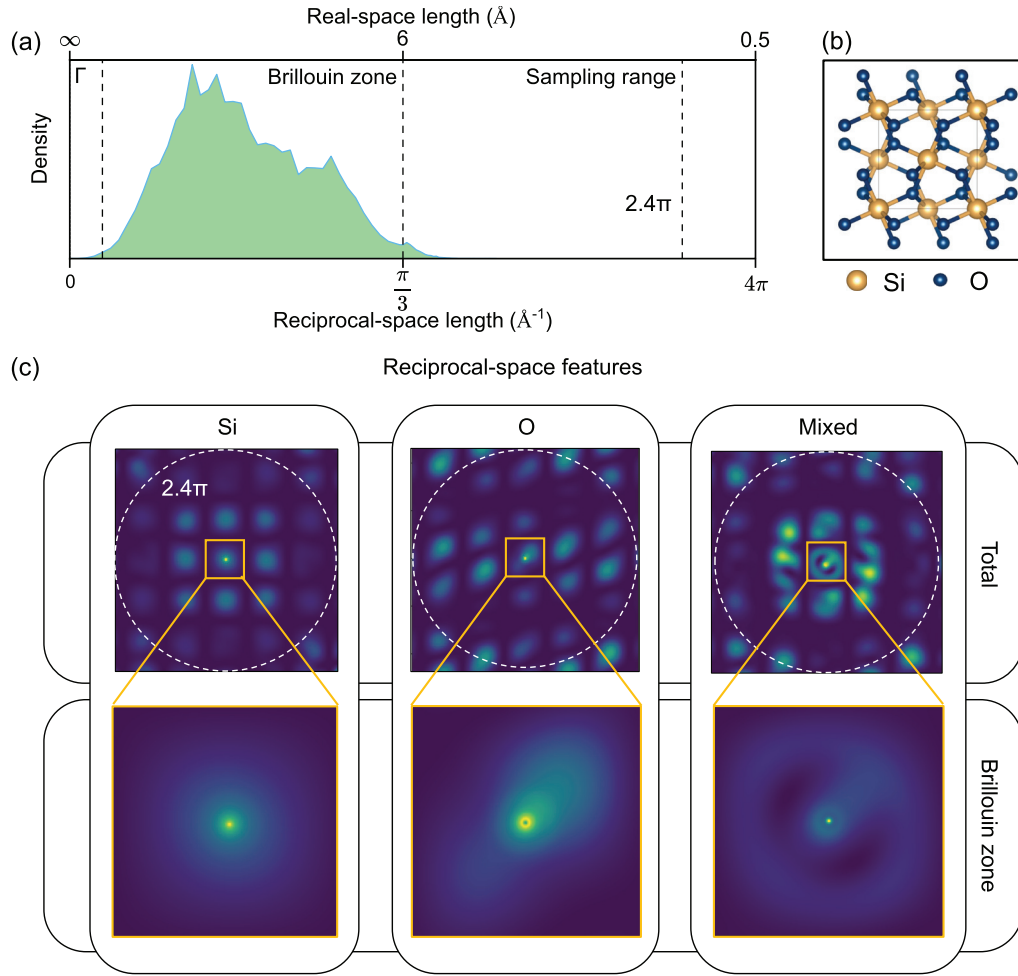


FIG. 4. Analysis of the reciprocal-space features learned by AIRCPP. (a) Brillouin zone distribution in the Materials Project database. (b) Crystal structure of SiO_2 . (c) Reciprocal-space feature patterns on the $k_x k_y$ plane ($k_z = 0$) for SiO_2 , showing both the fully sampled space and the first Brillouin zone.

long-range periodic correlations. Together, they form a complete and orthogonal structural representation. Fusing these features enables a giant leap in the accuracy, highlighting the rich physical information embedded in reciprocal space and the effectiveness of AIRCPP in extracting it—particularly for reciprocal-space properties like band gaps. Crucially, we intentionally selected CGCNN as the real-space part to isolate architectural gains, implying that integrating AIRCPP with more advanced frameworks holds significant promise for pushing the boundaries of accuracy.

To conclude, we have developed a pure reciprocal-space crystal property predictor named AIRCPP. With the large database of Materials Project for various properties, we have shown that AIRCPP exhibits comparable or even higher accuracy in comparison with the widely used CGCNN. However, the computational costs are drastically reduced through efficient and accurate multiscale sampling of the reciprocal space using Lebedev grids, getting rid of the time-consuming neighbor search in real-space approaches. Furthermore, AIRCPP-MIX, a hybrid model combining AIR-

CPP with CGCNN, achieves an accuracy compares to the advanced models while remaining highly efficient. This study demonstrates the promise of reciprocal-space descriptors for material property prediction, establishing a new paradigm for developing efficient and high-precision machine-learning models to boost the development of condensed matter physics.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [54].

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