Beyond Structure: Invariant Crystal Property Prediction with Pseudo-Particle Ray Diffraction

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Learnable diffraction probes • Reciprocal-space encoding • E(3)-invariant

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Representation Ambiguity in Crystal Graph Encoders

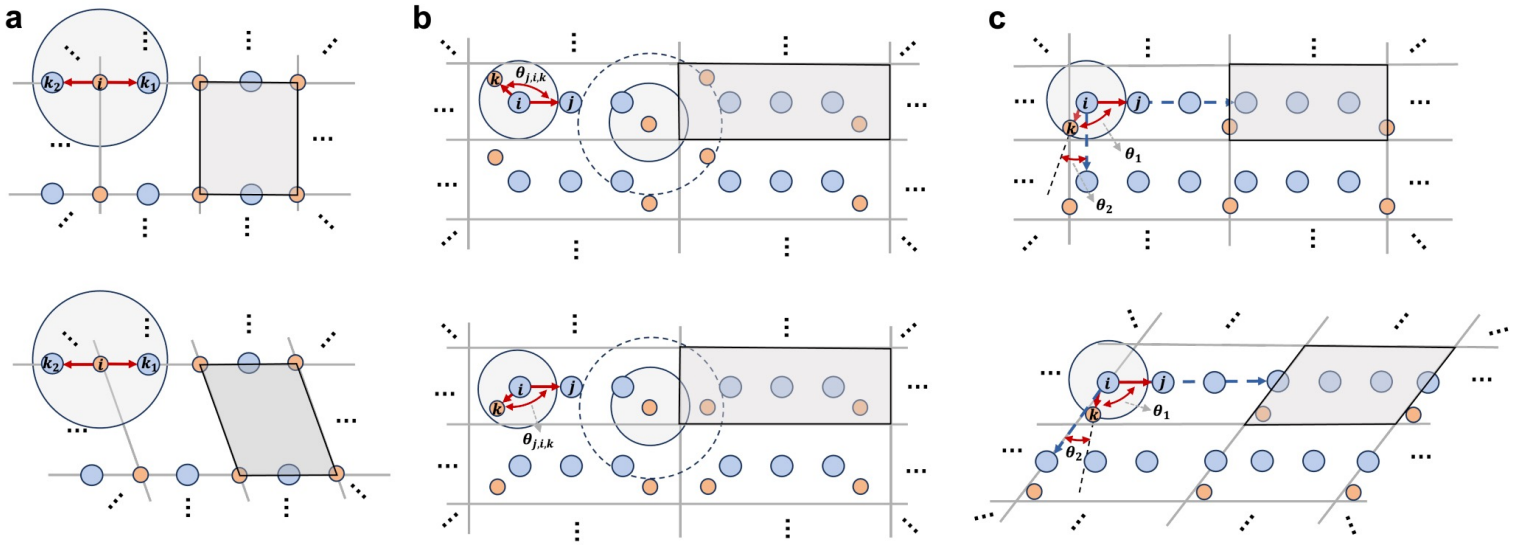
Finite Receptive Field Problem

GNNs **cannot distinguish** crystals differing only in long-range periodicity. Three failure modes:

- **(a)** Multi-edge: collapses periodicity
- **(b)** Angular: loses lattice-scale contrast
- **(c)** Periodic vectors: ambiguous patterns

Solution: Reciprocal Space

Diffraction encodes **complete** crystal information from a single unit cell — **lossless** and periodicity-preserving.



Three distinct crystal periodicities that produce **identical** graph representations under existing GNN methods.

Diffraction: From Atoms to Reciprocal Space

Structure Factor (Fourier Transform)

$$F(\mathbf{Q}) = \sum_{j=1}^{N} f_j(\mathbf{Q})\, e^{-i\mathbf{Q}\cdot\mathbf{r}_j}$$

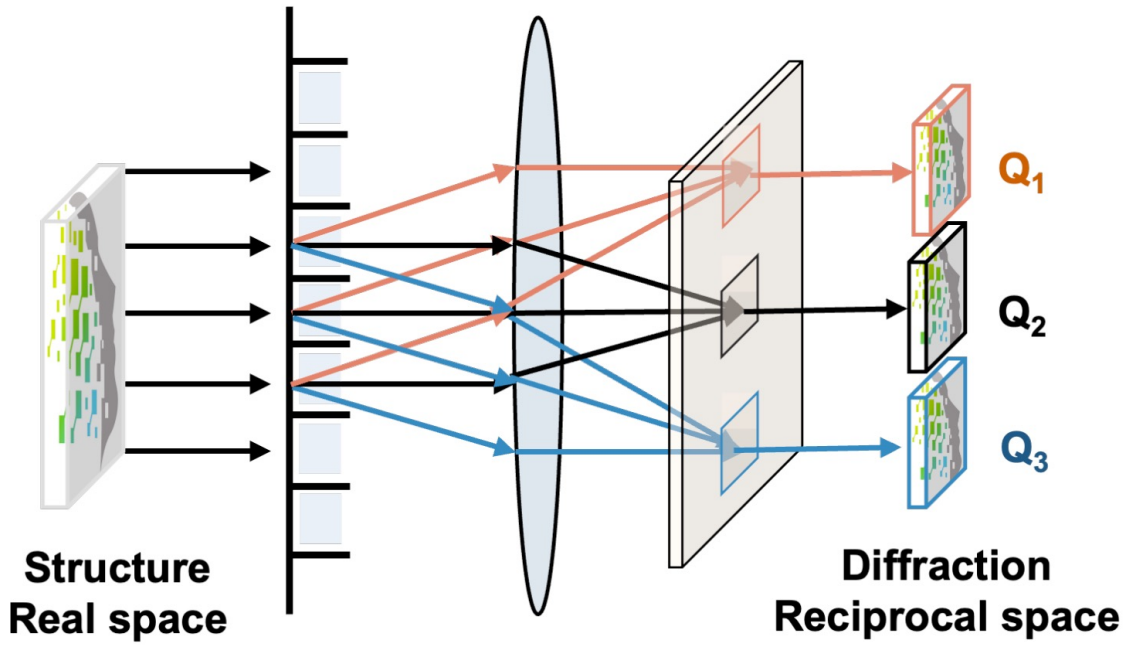
$f_j(\mathbf{Q})$: atomic form factor; $\mathbf{Q}$: reciprocal lattice vector.

Every atom contributes to a **global** crystal fingerprint.

Limitation of Prior Works

EwaldMP, PotNet, ReGNet use **fixed tabulated** X-ray form factors $f_j(|\mathbf{Q}|, \text{type})$ — blind to local chemical environment.

PRDNet replaces these with **learnable pseudo-particle** probes.



Reciprocal-space captures long-range periodicity invisible to GNNs.

Pseudo-Particle: Learnable Environment-Aware Scattering Probe

X-ray Photon (fixed, tabulated)

$$f_i^{\text{X-ray}} = f\left(|\mathbf{Q}|,\ f_i^{\text{type}}\right)$$

Blind to local chemical environment.
Same atom type $\Rightarrow$ same form factor.

Pseudo-Particle (learned)

$$f_i^{*} = f\left(|\mathbf{Q}|,\ \underbrace{G_\theta(\mathcal{G})}_{\text{local env.}},\ f_i^{\text{type}}\right)$$

Sensitive to: $|\mathbf{Q}|$, local bonding, and atomic species.

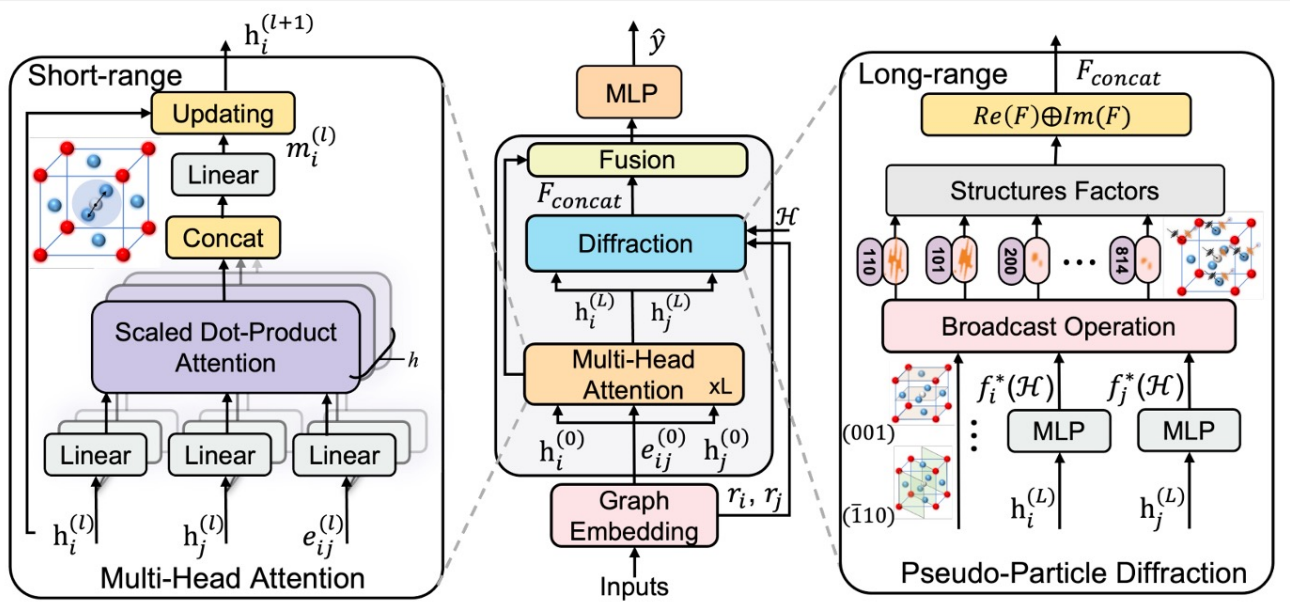
Two-Step Implementation

Step 1 — Graph encoder: $\mathbf{h}_i^{(L)} = \mathrm{MPNN}_\theta(\mathcal{G})$

Step 2 — Form-factor head: $f_i^*(\mathcal{H}) = \mathrm{MLP}_{\mathrm{form}}(\mathbf{h}_i^{(L)}) \in \mathbb{R}^{N_{\mathrm{hkl}}}$

- Fully differentiable end-to-end
- Covers all elements in the periodic table
- Outperforms tabulated X-ray on *every* task
- Not constrained by real-particle physics

PRDNet: Dual-Modality Architecture



Crystal graph (real space) + pseudo-particle diffraction

(reciprocal space).

Graph Stream

Multi-head gated attention.

$$\mathbf{e}_{ij} = \mathrm{RBF}(d_{ij}) \oplus \mathrm{SBF}(\theta_{ijk})$$

Captures *local* bond geometry.

Diffraction Stream

$$\mathrm{Re}(F_{hkl}) = \sum_i f_i^* \cos(2\pi \mathbf{h}\cdot\mathbf{r}_i^T)$$

Captures *long-range* periodicity.

Modality Fusion

$$\mathbf{z} = \mathrm{MLP}_{\mathrm{fuse}}([\mathbf{g} \oplus \mathbf{d}])$$

Global-level fusion (not atom-wise).

E(3) Invariance: Provably Correct by Construction

Proof Sketch (3 steps)

1. $\mathcal{H}$ is **closed**: $g \cdot \mathbf{h} = R_g \mathbf{h} \in \mathcal{H} \quad \forall g \in G, \mathbf{h} \in \mathcal{H}$

$$F_{g \cdot \mathbf{h}}(\{g \cdot \mathbf{r}_i\}) = e^{2\pi i \phi(g, \mathbf{h})} F_{\mathbf{h}}(\{\mathbf{r}_i\})$$

2. Phase $\phi(g, \mathbf{h}) = (R_g \mathbf{h}) \cdot \mathbf{t}_g \in \mathbb{Z} \Rightarrow e^{2\pi i \phi} = 1$
3. $|F_{\mathbf{h}}|^2$ is unchanged under all rotation, reflection, and translation operations. **QED.**

E(3) Guarantee

- **Rotation:** $R_g \mathbf{h} \in \mathcal{H}$
- **Reflection:** $\det R_g = \pm 1$
- **Translation:** phase cancels
- **Graph stream:** uses d_{ij}, θ_{ijk}

$\Rightarrow \mathbf{z}_{\text{fused}}$ is **exactly E(3)-invariant**

Provable — not just empirical.

State-of-the-Art on Materials Project (122,959 Crystals)

Method	Form.E eV/at.	Bandgap eV	Bulk log GPa	Shear log GPa	Young's log GPa	Metal% %
CGCNN	0.041	0.262	0.079	0.162	0.155	87.5
SchNet	0.038	0.344	0.092	0.129	0.143	82.8
MEGNET	0.053	0.307	0.134	0.206	0.189	86.6
Matformer	0.035	0.193	0.089	0.306	0.291	92.7
Crystalfarmer	0.030	0.216	0.047	0.118	0.106	87.5
eComFormer	0.033	0.153	0.088	0.269	0.311	82.5
EwaldMP	0.052	0.332	0.098	0.175	0.186	84.2
PotNet	0.035	0.251	0.104	0.175	0.151	88.9
ReGNet	0.047	0.331	0.088	0.172	0.204	85.1
PRDNet	**0.028**	**0.151**	**0.035**	**0.108**	**0.104**	**93.3**

SOTA on 6/6 Tasks

Best on form. energy, bandgap, all moduli, metal classification.

Bulk Modulus

↓25% vs. next best

(0.035 vs. 0.047 log GPa)

Form. Energy

0.028 eV/atom —

7% below prior SOTA

JARVIS-DFT Results & Ablation Study

JARVIS-DFT (75,993 crystals)

Method	Form.E eV/at.	Bgap eV	Bulk logGPa	Shear logGPa
CGCNN	0.038	0.144	0.125	0.163
Matformer	0.033	0.207	0.101	0.157
Crystalfarmer	0.048	0.208	0.065	0.144
PRDNet	**0.032**	**0.140**	**0.064**	**0.122**

Ablation — MP Formation Energy

Variant	Dif	MH	Res	EF	MAE
Default	✓	✓	✓	✓	**0.028**
NoDiff	×	✓	✓	✓	0.041
SingleHd	✓	×	✓	✓	0.040
NoRes	✓	✓	×	✓	0.038
NoEdge	✓	✓	✓	×	0.043

NoDiff ↑46% — diffraction is the most impactful component.

Conclusion

Four Contributions

Representation gap: first rigorous characterization of GNN ambiguity in crystal encoders.

Pseudo-particle probe: learnable, environment-aware form factors replace fixed X-ray tables.

E(3)-invariant module: reciprocal-space representation provably invariant under all space-group operations.

SOTA results: best on 6/6 tasks across MP, JARVIS-DFT, and Matbench.

Future Directions

- Equivariant representations for forces & stress.
- Aperiodic and defect structure modeling.
- Diffraction-guided crystal generation.
- Code release at camera-ready.

Thank you!

Questions welcome. ICLR 2026