Novelty Assessment Report

Paper: A Single Architecture for Representing Invariance Under Any Space Group
PDF URL: https://openreview.net/pdf?id=8LZrXh9hhL
Venue: ICLR 2026 Conference Submission
Year: 2026
Report Generated: 2026-01-08

Abstract

Incorporating known symmetries in data into machine learning models has consistently improved predictive accuracy, robustness, and generalization. However, achieving exact invariance to specific symmetries typically requires designing bespoke architectures for each group of symmetries, limiting scalability and preventing knowledge transfer across related symmetries. In the case of the space groups—symmetries critical to modeling crystalline solids in materials science and condensed matter physics—this challenge is particularly salient as there are 230 such groups in three dimensions. In this work we present a new approach to such crystallographic symmetries by developing a single machine learning architecture that is capable of adapting its weights automatically to enforce invariance to any input space group. Our approach is based on constructing symmetry-adapted Fourier bases through an explicit characterization of constraints that group operations impose on Fourier coefficients. Encoding these constraints into a neural network layer enables weight sharing across different space groups, allowing the model to leverage structural similarities between groups and overcome data sparsity when limited measurements are available for specific groups. We demonstrate the effectiveness of this approach in achieving competitive performance on material property prediction tasks and performing zero-shot learning to generalize to unseen groups.

Core Task Landscape

This paper addresses: **Enforcing Invariance to Crystallographic Space Groups in Neural Networks**

A total of **50 papers** were analyzed and organized into a taxonomy with **20 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Space Group Equivariant Architectures for Property Prediction**
- **Space Group Constrained Generative Models**
- **Theoretical Foundations and General Equivariance Frameworks**
- **Representation Learning and Encoding Strategies**
- **Symmetry Breaking and Relaxed Equivariance**
- **Benchmarking, Evaluation, and Computational Methods**
- **Domain-Specific Applications and Extensions**
- **General Machine Learning Techniques for Symmetry**

Complete Taxonomy Tree

- Enforcing Invariance to Crystallographic Space Groups in Neural Networks Survey Taxonomy
- Space Group Equivariant Architectures for Property Prediction
  - Tensor Property Prediction with O(3) and Space Group Equivariance ★ (4 papers)
  - [0] A Single Architecture for Representing Invariance Under Any Space Group (Anon et al., 2026) View paper
  - [3] A space group symmetry informed network for o (3) equivariant crystal tensor prediction (Yan, 2024) View paper
  - [7] StrainTensorNet: Predicting crystal structure elastic properties using SE (3)-equivariant graph neural networks (T. Pakornchote, 2023) View paper
  - [12] Accurate piezoelectric tensor prediction with equivariant attention tensor graph neural network (Luqi Dong, 2025) View paper
  - Scalar Property and Symmetry Classification Prediction (4 papers)
  - [13] Composition based crystal materials symmetry prediction using machine learning with enhanced descriptors (Yuxin Li, 2021) View paper
  - [16] Equivariant networks for crystal structures (Kaba, 2022) View paper
  - [30] Material symmetry recognition and property prediction accomplished by crystal capsule representation (Chao Liang, 2023) View paper
  - [45] Formation Energy Prediction of Material Crystal Structures using Deep Learning (Virginio Torlao, 2024) View paper
  - Chemical Ordering and Compositional Disorder Modeling (1 papers)
  - [1] Learning ordering in crystalline materials with symmetry-aware graph neural networks (Peng, 2024) View paper
- Space Group Constrained Generative Models
  - Diffusion Models with Space Group Constraints (4 papers)
  - [2] Space Group Equivariant Crystal Diffusion (Chang, 2025) View paper
  - [9] Equivariant diffusion for crystal structure prediction (Peijia Lin, 2025) View paper
  - [20] Equivariant hypergraph diffusion for crystal structure prediction (Liu Yang, 2025) View paper
  - [21] WyckoffDiff - A Generative Diffusion Model for Crystal Symmetry (Kelvinius, 2025) View paper
  - Flow Matching and Continuous Normalizing Flows (3 papers)
  - [4] Space group conditional flow matching (Puny, 2025) View paper
  - [26] An equivariant flow matching framework for learning molecular crystallization (S Liu, 2024) View paper

- [50] Crystal Generative Modeling with Explicit Autoregressive Conditional Likelihoods and Nontrivial Space Group Stabilizers (R Chang, n.d.) View paper
- Autoregressive and Transformer-Based Generation (2 papers)
- [8] Space group informed transformer for crystalline materials generation (Zhendong Cao, 2025) View paper
- [14] Multi-property directed generative design of inorganic materials through Wyckoff-augmented transfer learning (Nong Wei, 2025) View paper
- Physics-Guided and Symmetry-Constrained Generation (3 papers)
- [6] Space group constrained crystal generation (Jiao Rui, 2024) View paper
- [15] Physics guided deep learning for generative design of crystal materials with symmetry constraints (Yong Zhao, 2023) View paper
- [41] Deep learning generative model for conditional crystal structure prediction of sodium amide (Rongfeng Guan, 2025) View paper

- Theoretical Foundations and General Equivariance Frameworks
  - Expressiveness and Completeness of Invariant Models (2 papers)
  - [5] On the Completeness of Invariant Geometric Deep Learning Models (Li Zian, 2024) View paper
  - [38] Fundamental Limits of Crystalline Equivariant Graph Neural Networks: A Circuit Complexity Perspective (Cao Yang, 2025) View paper
  - General Symmetry Group Equivariant Architectures (3 papers)
  - [18] Current symmetry group equivariant convolution frameworks for representation learning (Mishra, 2024) View paper
  - [24] Deep symmetry networks (Robert Gens, 2014) View paper
  - [35] Symmetry group equivariant convolutions for representation learning: a survey (R Basheer, 2026) View paper
  - Probabilistic and Functional Representations of Symmetry (2 papers)
  - [10] Probabilistic symmetries and invariant neural networks (Yw, 2020) View paper
  - [23] Representing and Learning Functions Invariant Under Crystallographic Groups (Adams, 2023) View paper
- Representation Learning and Encoding Strategies
  - Contrastive and Self-Supervised Learning for Crystals (3 papers)
  - [37] Structural Fingerprinting of Crystalline Materials from XRD Patterns Using Atomic Cluster Expansion Neural Network and Atomic Cluster Expansion (Xiao Zhang, 2025) View paper
  - [39] Deep Learning for XRD Structural Fingerprinting: E3NN Based Atomic Cluster Expansion Contrastive Learning (Xiao Zhang, 2025) View paper
  - [43] Data driven models for structure determination from powder diffraction measurements (Houben Andreas, 2025) View paper
  - Periodic Invariance and Conformal Encodings (2 papers)
  - [25] Conformal crystal graph transformer with robust encoding of periodic invariance (Gomes, 2024) View paper
  - [32] Equivariant message passing neural network for crystal material discovery (Bouraoui, 2023) View paper
  - Symmetry-Aware Fingerprinting and Descriptors (2 papers)
  - [40] Machine Learning Descriptors for Mapping Structureâ□□Propertyâ□□Performance Relationships of Perovskite Solar Cells (Y Su, 2025) View paper
  - [42] Symmetry-informed graph neural networks for carbon dioxide isotherm and adsorption prediction in aluminum-substituted zeolites (Petkovic, 2025) View paper
- Symmetry Breaking and Relaxed Equivariance (2 papers)
  - [29] Relaxed octahedral group convolution for learning symmetry breaking in 3d physical systems (Wang Rui, 2023) View paper
  - [33] Approximately Equivariant Quantum Neural Network for p4m Group Symmetries in Images (Su Yeon Chang, 2023) View paper
- Benchmarking, Evaluation, and Computational Methods
  - Multi-Task Benchmarks and Evaluation Frameworks (2 papers)
  - [31] Matsciml: A broad, multi-task benchmark for solid-state materials modeling (Miret, 2023) View paper
  - [49] PEROV-H3: Evaluating Generative Models under Size and Symmetry Shifts in Hydrogen-Storage Perovskites (C Polat, n.d.) View paper
  - Crystal Structure Prediction and Validation (2 papers)
  - [17] Efficient crystal structure prediction based on the symmetry principle (Yu, 2025) View paper
  - [19] Predictive crystallography at scale: mapping, validating, and learning from 1000 crystal energy landscapes (Christopher R. Taylor, 2024) View paper
- Domain-Specific Applications and Extensions
  - Quantum Materials and Spin Systems (3 papers)
  - [11] Spin- Kagome Heisenberg Antiferromagnet: Machine Learning Discovery of the Spinon Pair-Density-Wave Ground State (T Ä□uriÄ□, 2025) View paper
  - [28] Evidence for a Dirac spin liquid in the generalized Shastry-Sutherland model (A Maity, 2024) View paper
  - [47] Probing Entanglement and Symmetry Breaking Orders via Spectroscopies and Machine Learning (Tong-tong, 2023) View paper
  - Mechanical Metamaterials and Nonlinear Mechanics (1 papers)
  - [22] Designing Mechanical Meta-Materials by Learning Equivariant Flows (Mirramezani, 2024) View paper
  - Optical and Nonlinear Optical Materials Discovery (1 papers)
  - [44] Symmetryâ□□Aware Equivariant Network for Discovering SHGâ□□Active Materials (LA Klimova, 2025) View paper
- General Machine Learning Techniques for Symmetry (5 papers)
  - [27] Symmetry constrained machine learning (Bergman, 2019) View paper
  - [34] Group invariant machine learning by fundamental domain projections (Sheard, 2023) View paper
  - [36] Incorporating Symmetry and Constraints Into Machine Learning for Molecular and Solid-State Systems (Gong, 2025) View paper
  - [46] Generative Model-Based Exploration of Chemical Space for Crystals (Sultanov, 2024) View paper
  - [48] Deep Learning Based Generative Materials Design (Yong, 2022) View paper

Narrative

Core task: Enforcing invariance to crystallographic space groups in neural networks. The field has organized itself around several complementary directions. Space Group Equivariant Architectures for Property Prediction focuses on building models that respect crystallographic symmetries when predicting material properties, often leveraging O(3) equivariance and tensor representations (e.g., Crystal Tensor Network[3], StrainTensorNet[7]). Space Group Constrained Generative Models tackle the inverse problem of designing

new crystal structures while maintaining symmetry constraints (e.g., Space Group Diffusion[2], Space Group Flow[4]). Theoretical Foundations and General Equivariance Frameworks provide the mathematical underpinnings for these approaches, while Representation Learning and Encoding Strategies explore how to efficiently encode crystallographic information. Symmetry Breaking and Relaxed Equivariance address scenarios where strict invariance may be too restrictive, and Benchmarking, Evaluation, and Computational Methods ensure reproducibility and scalability across the field.

Within property prediction, a central tension exists between strict equivariance and computational efficiency. Works like Completeness Invariant Models[5] emphasize theoretical guarantees of completeness, while others prioritize scalability for large-scale screening. Invariant Space Group[0] sits within the tensor property prediction cluster, focusing specifically on O(3) and space group equivariance for predicting tensorial material properties. Its emphasis on rigorous symmetry enforcement aligns closely with Crystal Tensor Network[3] and StrainTensorNet[7], which similarly target tensor-valued outputs like elastic or piezoelectric tensors (Piezoelectric Tensor Prediction[12]). Compared to these neighbors, Invariant Space Group[0] appears to push further on the theoretical side of ensuring complete invariance, contrasting with approaches that might relax symmetry constraints for practical gains. The broader challenge remains balancing expressiveness, computational cost, and the physical correctness guaranteed by strict equivariance.

Related Works in Same Category

The following **3 sibling papers** share the same taxonomy leaf node with the original paper:

1. A space group symmetry informed network for o (3) equivariant crystal tensor prediction

Authors: Yan, Keqiang, Saxton, Alexandra, Keqiang Yan, et al. (14 authors total) | **Year/Venue**: 2024 | **URL**: View paper

Abstract

We consider the prediction of general tensor properties of crystalline materials, including dielectric, piezoelectric, and elastic tensors. A key challenge here is how to make the predictions satisfy the unique tensor equivariance to O(3) group and invariance to crystal space groups. To this end, we propose a General Materials Tensor Network (GMTNet), which is carefully designed to satisfy the required symmetries. To evaluate our method, we curate a dataset and establish evaluation metrics that ...

Relationship Analysis

Both papers belong to the same taxonomy category focusing on tensor property prediction with combined O(3) rotation equivariance and space group invariance. They overlap in addressing the challenge of predicting rank-2 and higher tensors (dielectric, piezoelectric, elastic) while respecting crystallographic symmetries. The key difference is that the original paper develops a single adaptive architecture using symmetry-adapted Fourier bases that can handle any of the 230 space groups with shared weights, while the candidate paper (GMTNet) uses tensor field networks with Wigner D-matrices and a symmetry enforcement module to achieve equivariance and space group constraints through graph-based representations.

---

2. StrainTensorNet: Predicting crystal structure elastic properties using SE (3)-equivariant graph neural networks

Authors: T. Pakornchote, A. Ektarawong, Teerachote Pakornchote, Thiparat Chotibut, Annop Ektarawong | **Year/Venue**: 2023 | **URL**: View paper

Abstract

Accurately predicting the elastic properties of crystalline solids is vital for computational materials science. However, traditional atomistic scale ab initio approaches are computationally intensive, especially for studying complex materials with a large number of atoms in a unit cell. We introduce a novel data-driven approach to efficiently predict the elastic properties of crystal structures using SE(3)-equivariant graph neural networks (GNNs). This approach yields important scalar elastic m...

Relationship Analysis

Both papers belong to the category of tensor property prediction with combined O(3) rotation equivariance and space group invariance for crystalline materials. They overlap in addressing the prediction of elastic properties (rank-2 tensors) while respecting crystallographic symmetries. However, the original paper develops a single adaptive architecture using symmetry-adapted Fourier bases that can handle any of the 230 space groups with shared weights, while the candidate paper (StrainTensorNet) uses SE(3)-equivariant graph neural networks to predict strain energy density and elastic constants without explicitly constructing a unified framework across all space groups.

---

3. Accurate piezoelectric tensor prediction with equivariant attention tensor graph neural network

Authors: Luqi Dong, Xuanlin Zhang, Ziduo Yang, Lei Shen, Yunhao Lu | **Year/Venue**: 2025 | **URL**: View paper

Abstract

Abstract The piezoelectric materials enable the mutual conversion between mechanical and electrical energy, which drive a multi-billion dollar industry through their applications as sensors, actuators, and energy harvesters. The third-rank piezoelectric tensor is the core matrices for piezoelectric materials and their devices. However, the high costs of obtaining full piezoelectric tensor data through either experimental or computational methods make a significant challenge. Here, we propose an ...

Relationship Analysis

Both papers belong to the same taxonomy category of tensor property prediction with O(3) and space group equivariance, addressing the challenge of predicting crystallographic tensors while respecting symmetries. The original paper develops a single adaptive architecture using symmetry-adapted Fourier bases that can enforce invariance to any of the 230 space groups through group-conditional routing matrices, enabling weight sharing and zero-shot generalization across groups. The candidate paper (EATGNN) focuses specifically on piezoelectric tensor prediction using equivariant graph attention networks with irreducible representation decomposition, achieving accurate predictions for both bulk and 2D materials but without the cross-group adaptability and weight-sharing framework of the original paper.

Contributions Analysis

Overall novelty summary. The paper proposes a single neural network architecture that can adapt its weights to enforce invariance to any of the 230 three-dimensional crystallographic space groups, rather than requiring bespoke designs for each group. It sits within the 'Tensor Property Prediction with O(3) and Space Group Equivariance' leaf, which contains four papers including the original work. This leaf focuses on predicting rank-2 or higher tensors (elastic, piezoelectric, dielectric) with combined rotation equivariance and space group invariance. The taxonomy reveals this is a moderately populated research direction within the broader property prediction category, suggesting active but not overcrowded exploration of tensor-valued predictions under crystallographic constraints.

The taxonomy tree shows the paper's leaf is part of the 'Space Group Equivariant Architectures for Property Prediction' branch, which also includes scalar property prediction and chemical disorder modeling. Neighboring branches address generative models (diffusion, flow matching, autoregressive generation) and theoretical foundations (expressiveness, general equivariance frameworks). The scope note for the paper's leaf explicitly excludes generative models and scalar-only predictions, positioning this work at the intersection of rigorous symmetry enforcement and tensor-valued output prediction. The broader taxonomy reveals parallel efforts in representation

learning and symmetry breaking, indicating the field explores both strict equivariance and relaxed variants depending on application needs.

Among 15 candidates examined across three contributions, the analytical construction of symmetry-adapted Fourier bases shows one refutable candidate out of 10 examined, suggesting some prior work on Fourier-based symmetry encoding exists within the limited search scope. The single adaptive architecture contribution examined 2 candidates with no refutations, and the Crystal Fourier Transformer architecture examined 3 candidates with no refutations. The statistics indicate that within the top-15 semantic matches, the Fourier basis construction has the most substantial prior overlap, while the adaptive architecture and transformer components appear more distinctive. However, the limited search scope (15 candidates, not exhaustive) means these findings reflect only the most semantically similar work retrieved.

Based on the limited literature search of 15 candidates, the work appears to occupy a moderately novel position within tensor property prediction under space group constraints. The adaptive weight-sharing mechanism across all 230 space groups distinguishes it from sibling papers that may target specific groups or tensor types. The single refutable pair among 15 candidates suggests the Fourier basis approach has some precedent, but the overall architecture combining adaptive invariance with Fourier constraints may represent a synthesis not fully captured by prior work within the examined scope.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: Single adaptive architecture for any crystallographic space group invariance

Description: The authors introduce a unified neural network architecture that can adapt to enforce exact invariance to any of the 230 three-dimensional space groups by conditioning on the input group, rather than requiring separate architectures for each group. This enables weight sharing across different space groups and allows the model to leverage structural similarities between groups.

This contribution was assessed against **2 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

---

1. Prediction of the space group and cell volume by training a convolutional neural network with primitiveideal'diffraction profiles and its application toreal'experimental â¦

URL: View paper

Brief Assessment

Space Group CNN[63] focuses on space group classification from diffraction profiles using CNNs, not on creating a single adaptive architecture that enforces exact invariance to any space group through weight sharing. The candidate uses separate CNN models for classification tasks rather than a unified architecture that adapts weights to enforce group invariance.

---

2. Recognition of crystal lattice parameters using deep learning techniques

URL: View paper

Brief Assessment

Lattice Parameter Recognition[64] focuses on predicting lattice parameters from powder diffraction spectra using CNNs and transformers, not on developing adaptive architectures for space group invariance with weight sharing across groups.

Contribution 2: Analytical construction of symmetry-adapted Fourier bases via constraint characterization

Description: The authors derive analytical constraints that crystallographic group operations impose on Fourier coefficients and prove these constraints define a complete basis for group-invariant functions. They introduce a dual graph representation where nodes are reciprocal lattice frequencies and edges encode phase relationships, enabling algorithmic construction of the symmetry-adapted basis.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

---

1. DFT calculations of magnetic shielding and quadrupolar coupling in ordered systems: methods and applications to NMR crystallography

URL: View paper

Brief Assessment

NMR Crystallography DFT[58] focuses on cluster-based computational protocols for calculating NMR parameters in crystalline solids using symmetry-adapted cluster ansatz, not on constructing symmetry-adapted Fourier bases through constraint characterization of group operations on Fourier coefficients.

---

2. Three-Dimensional Multiorbital Flat Band Models and Materials.

URL: View paper

Brief Assessment

Multiorbital Flat Bands[59] focuses on constructing tight-binding models for flat band systems using group theory and crystallography, not on deriving Fourier basis constraints from crystallographic symmetries. The methodological approaches are fundamentally different.

---

3. WyCryst: Wyckoff inorganic crystal generator framework

URL: View paper

Brief Assessment

WyCryst[53] focuses on Wyckoff position-based representations for crystal generation using VAE models, not on constructing symmetry-adapted Fourier bases through analytical constraint characterization of group operations on Fourier coefficients.

---

4. International Tables for Crystallography: Crystallographic Symmetry

URL: View paper

Brief Assessment

Crystallographic Symmetry Tables[54] is a reference work providing standard crystallographic group tables and symmetry operations, not a research paper proposing methods for constructing symmetry-adapted Fourier bases through constraint characterization.

---

5. -type antiferromagnetic is a multiferroic -wave altermagnet

URL: View paper

Brief Assessment

Multiferroic Altermagnet[55] focuses on magnetic symmetries in crystalline materials and constructs symmetry-adapted plane wave bases for spin-splitting functions in altermagnets, not general machine learning architectures for crystallographic group invariance.

---

6. Non-relativistic spin splitting above and below the Fermi level in a -wave altermagnet

URL: View paper

Brief Assessment

Spin Splitting Altermagnet[57] focuses on developing a symmetry-constrained adaptive basis (SCAB) for analyzing spin-split electronic states in altermagnetic materials, not on constructing symmetry-adapted Fourier bases for crystallographic groups using constraints from group operations.

---

7. Symmetry-adapted modeling for molecules and crystals

URL: View paper

Brief Assessment

Symmetry Adapted Modeling[52] focuses on multipole basis construction for molecules and crystals using point-group harmonics, not on Fourier bases for crystallographic groups via reciprocal lattice constraints as in the original paper.

---

8. Electron Tomographic Crystallography: Integrating Tomography and Fourier Synthesis for Real-Space Structural Analysis

URL: View paper

Brief Assessment

Electron Tomographic Crystallography[56] focuses on electron tomography and Fourier synthesis for structural analysis of crystals, not on constructing symmetry-adapted Fourier bases through analytical constraint characterization from crystallographic group operations.

---

9. Polaritonic Fourier crystal

URL: View paper

Brief Assessment

Polaritonic Fourier Crystal[51] focuses on physical polaritonic crystals with harmonic momentum modulation in hexagonal boron nitride, not on analytical construction of symmetry-adapted Fourier bases for crystallographic groups through constraint characterization.

---

10. Representing and Learning Functions Invariant Under Crystallographic Groups

URL: View paper

Prior Art Analysis

Crystallographic Functions[23] demonstrates that the analytical construction of symmetry-adapted Fourier bases through constraint characterization was previously established. The candidate paper derives the exact constraints that crystallographic group operations impose on Fourier coefficients (Proposition 3.1 and Theorem 3.2), introduces a dual graph representation where nodes are reciprocal lattice frequencies and edges encode phase relationships, and provides an algorithmic construction (Algorithm 1). These contributions directly overlap with the original paper's claimed novelty of deriving analytical constraints on Fourier coefficients and proving they define a complete basis, as well as introducing the dual graph representation for algorithmic construction.

Evidence

Evidence 1 - **Rationale**: Both papers claim to derive representations for crystallographically invariant functions with complete basis properties, establishing prior work on this contribution. - **Original**: we derive the analytical constraints that invariance to a crystallographic group imposes on a function's fourier series coefficients. second, we show how these constraints define a complete, g-invariant basis, which admits a dual representation in terms of graphs. - **Candidate**: we derive linear and nonlinear representations of functions that are (1) smooth and (2) invariant under such a group. the linear representation generalizes the fourier basis to crystallographically invariant basis functions. we show that such a basis exists for each crystallographic group, that it i...

Evidence 2 - **Rationale**: Both papers introduce graph-based representations to encode symmetry constraints, with the candidate's orbit graph construction predating the original's dual graph representation. - **Original**: the algebraic relationships and phase constraints from proposition 3.1 can be captured as a directed graph on the reciprocal lattice. in this graph, nodes represent frequenciesω ∈ l∗, and each symmetry operation ϕ(x) = ax + t induces a set of directed edges. - **Candidate**: algorithm 1 (constructing the orbit graph) . 1.) construct the ε-net γ. 2.) find local group elements aπ. 3.) for each pair x, y∈ γ, find dg(g(x), g(y)) = min {dn(x, ϕy) |ϕ ∈ aπ}. 4.) add an edge between x and y if dg(g(x), g(y)) < δ.

Evidence 3 - **Rationale**: Both papers prove the existence and completeness of symmetry-adapted Fourier bases through constraint characterization, with the candidate's Theorem 7 establishing this result prior to the original's Theorem 3.2. - **Original**: theorem 3.2. let g be a crystallographic group and l∗ be its reciprocal lattice. the rotational components (a) of the group's transformations (ϕ(x) = ax + t) partition l∗ into disjoint orbits o, where frequencies ω1, ω2 ∈ oif ω2 = aω1 for some ϕ ∈ g. - **Candidate**: theorem 7 (crystallographically invariant fourier basis) . let g be a crystallographic group that tiles rn with a convex polytope π. then the constrained problem (13) has solutions for countably many distinct values λ1, λ2, . . .of λ, and these values satisfy 0 = λ1 < λ2 < λ3 < . . . and λi i→∞- - -...

Contribution 3: Crystal Fourier Transformer architecture with group-conditional encoding

Description: The authors present a Transformer-based architecture that uses a group-conditional routing matrix to transform standard Fourier modes into provably invariant positional encodings. This encoding module can be integrated with existing ML models to capture exact symmetries while sharing weights across all 230 space groups.

This contribution was assessed against **3 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

---

1. A Symmetry-Aware Multimodal Transformer for Spin Hall Conductivity Prediction

URL: View paper

Brief Assessment

Spin Hall Transformer[62] focuses on spin hall conductivity prediction in spintronic materials using multimodal fusion of crystal structure and electronic band structure data. It does not address the group-conditional routing matrix or symmetry-adapted Fourier basis construction that forms the core of the original paper's contribution.

---

2. CLOUD: A Scalable and Physics-Informed Foundation Model for Crystal Representation Learning

URL: View paper

Brief Assessment

CLOUD Foundation Model[61] uses a symmetry-consistent ordered parameter encoding (SCOPE) with Wyckoff positions in a coordinate-free string representation, whereas the original paper develops a Fourier-based encoding with explicit group-conditional routing matrices that transform standard Fourier modes into invariant positional encodings through constraint graphs.

---

3. Wyckoff Transformer: Generation of Symmetric Crystals

URL: View paper

Brief Assessment

Wyckoff Transformer[60] focuses on generative modeling using Wyckoff positions as a discrete structure representation, not on Fourier-based positional encodings with group-conditional routing matrices for property prediction tasks.

Appendix: Text Similarity Detection

No high-similarity text segments were detected across any compared papers.

References

- [0] A Single Architecture for Representing Invariance Under Any Space Group View paper
- [1] Learning ordering in crystalline materials with symmetry-aware graph neural networks View paper
- [2] Space Group Equivariant Crystal Diffusion View paper
- [3] A space group symmetry informed network for o (3) equivariant crystal tensor prediction View paper
- [4] Space group conditional flow matching View paper
- [5] On the Completeness of Invariant Geometric Deep Learning Models View paper
- [6] Space group constrained crystal generation View paper
- [7] StrainTensorNet: Predicting crystal structure elastic properties using SE (3)-equivariant graph neural networks View paper
- [8] Space group informed transformer for crystalline materials generation View paper
- [9] Equivariant diffusion for crystal structure prediction View paper
- [10] Probabilistic symmetries and invariant neural networks View paper
- [11] Spin- Kagome Heisenberg Antiferromagnet: Machine Learning Discovery of the Spinon Pair-Density-Wave Ground State View paper
- [12] Accurate piezoelectric tensor prediction with equivariant attention tensor graph neural network View paper
- [13] Composition based crystal materials symmetry prediction using machine learning with enhanced descriptors View paper
- [14] Multi-property directed generative design of inorganic materials through Wyckoff-augmented transfer learning View paper
- [15] Physics guided deep learning for generative design of crystal materials with symmetry constraints View paper
- [16] Equivariant networks for crystal structures View paper
- [17] Efficient crystal structure prediction based on the symmetry principle View paper
- [18] Current symmetry group equivariant convolution frameworks for representation learning View paper
- [19] Predictive crystallography at scale: mapping, validating, and learning from 1000 crystal energy landscapes View paper
- [20] Equivariant hypergraph diffusion for crystal structure prediction View paper
- [21] WyckoffDiff - A Generative Diffusion Model for Crystal Symmetry View paper
- [22] Designing Mechanical Meta-Materials by Learning Equivariant Flows View paper
- [23] Representing and Learning Functions Invariant Under Crystallographic Groups View paper
- [24] Deep symmetry networks View paper
- [25] Conformal crystal graph transformer with robust encoding of periodic invariance View paper
- [26] An equivariant flow matching framework for learning molecular crystallization View paper
- [27] Symmetry constrained machine learning View paper
- [28] Evidence for a Dirac spin liquid in the generalized Shastry-Sutherland model View paper
- [29] Relaxed octahedral group convolution for learning symmetry breaking in 3d physical systems View paper
- [30] Material symmetry recognition and property prediction accomplished by crystal capsule representation View paper
- [31] Matsciml: A broad, multi-task benchmark for solid-state materials modeling View paper
- [32] Equivariant message passing neural network for crystal material discovery View paper
- [33] Approximately Equivariant Quantum Neural Network for p4m Group Symmetries in Images View paper
- [34] Group invariant machine learning by fundamental domain projections View paper
- [35] Symmetry group equivariant convolutions for representation learning: a survey View paper
- [36] Incorporating Symmetry and Constraints Into Machine Learning for Molecular and Solid-State Systems View paper
- [37] Structural Fingerprinting of Crystalline Materials from XRD Patterns Using Atomic Cluster Expansion Neural Network and Atomic Cluster Expansion View paper
- [38] Fundamental Limits of Crystalline Equivariant Graph Neural Networks: A Circuit Complexity Perspective View paper
- [39] Deep Learning for XRD Structural Fingerprinting: E3NN Based Atomic Cluster Expansion Contrastive Learning View paper
- [40] Machine Learning Descriptors for Mapping Structureâ□□Propertyâ□□Performance Relationships of Perovskite Solar Cells View paper
- [41] Deep learning generative model for conditional crystal structure prediction of sodium amide View paper
- [42] Symmetry-informed graph neural networks for carbon dioxide isotherm and adsorption prediction in aluminum-substituted zeolites View paper
- [43] Data driven models for structure determination from powder diffraction measurements View paper
- [44] Symmetryâ□□Aware Equivariant Network for Discovering SHGâ□□Active Materials View paper
- [45] Formation Energy Prediction of Material Crystal Structures using Deep Learning View paper
- [46] Generative Model-Based Exploration of Chemical Space for Crystals View paper
- [47] Probing Entanglement and Symmetry Breaking Orders via Spectroscopies and Machine Learning View paper
- [48] Deep Learning Based Generative Materials Design View paper
- [49] PEROV-H3: Evaluating Generative Models under Size and Symmetry Shifts in Hydrogen-Storage Perovskites View paper
- [50] Crystal Generative Modeling with Explicit Autoregressive Conditional Likelihoods and Nontrivial Space Group Stabilizers View paper
- [51] Polaritonic Fourier crystal View paper
- [52] Symmetry-adapted modeling for molecules and crystals View paper
- [53] WyCryst: Wyckoff inorganic crystal generator framework View paper
- [54] International Tables for Crystallography: Crystallographic Symmetry View paper
- [55] -type antiferromagnetic is a multiferroic -wave altermagnet View paper

- [56] Electron Tomographic Crystallography: Integrating Tomography and Fourier Synthesis for Real-Space Structural Analysis View paper
- [57] Non-relativistic spin splitting above and below the Fermi level in a -wave altermagnet View paper
- [58] DFT calculations of magnetic shielding and quadrupolar coupling in ordered systems: methods and applications to NMR crystallography View paper
- [59] Three-Dimensional Multiorbital Flat Band Models and Materials. View paper
- [60] Wyckoff Transformer: Generation of Symmetric Crystals View paper
- [61] CLOUD: A Scalable and Physics-Informed Foundation Model for Crystal Representation Learning View paper
- [62] A Symmetry-Aware Multimodal Transformer for Spin Hall Conductivity Prediction View paper
- [63] Prediction of the space group and cell volume by training a convolutional neural network with primitiveideal'diffraction profiles and its application toreal'experimental â View paper
- [64] Recognition of crystal lattice parameters using deep learning techniques View paper