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# Artificial Intelligence-Driven Discovery of Magnetic Higher-Order Topological Corner States: A Review from Theoretical Framework to Large-Scale Screening

Chengtian Liang*, Zhaoyu Zhu, Yixuan Lin

School of Physics, Hangzhou Normal University, Hangzhou, China

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*Corresponding Author: Chengtian Liang (ctliang@meaworm.cn)

**Abstract.** This review explores the integration of artificial intelligence (AI) with condensed matter physics, specifically focusing on the prediction of magnetic higher-order topological corner states. We examine the theoretical foundations of higher-order topological insulators (HOTIs), the unique challenges posed by magnetic systems, and the application of equivariant graph neural networks in high-throughput screening. The article discusses active learning strategies for navigating vast chemical configuration spaces and addresses current limitations regarding data scarcity and strong electronic correlations.

## 1. Introduction: A New Paradigm in Computational Topological Physics

At the frontier of contemporary condensed matter physics, the discovery and manipulation of topological quantum states have become cornerstones for constructing future quantum computers, spintronic devices, and high-precision sensors. Since the discovery of the quantum Hall effect in the 1980s, topological physics has experienced a revolutionary evolution from first-order topological insulators to topological semimetals, and more recently, to higher-order topological insulators [1]. Traditional first-order bulk- boundary correspondence dictates that a d-dimensional bulk must correspond to gapless edge states of dimension $(d-1)$. However, higher-order topological insulators break this convention, revealing profound connections between d-dimensional bulk states and restricted boundary states of dimension $(d-n)$ where $n > 1$ [2]. In two-dimensional systems, second-order topological insulators exhibit insulating bulk and edge states, but host zero-dimensional confined corner states at geometric corners; in three dimensions, these may manifest as chiral or helical states confined to sample hinges [1].

The introduction of magnetic higher-order topological states opens new dimensions for controlling these topologically protected states by breaking time-reversal symmetry. Magnetic

order (ferromagnetic, antiferromagnetic, or non-collinear magnetic order) not only induces unique phenomena such as the quantum anomalous Hall effect and axion field responses but also enables real-time manipulation of corner state positions and properties through switching of magnetic moment directions [3]. However, locating and verifying magnetic higher-order topological corner states in real materials faces substantial computational barriers.

Traditional first-principles calculations, while highly accurate for small to medium-scale systems, exhibit computational costs scaling as $O(N^3)$ or higher with respect to atom number N [4]. The complexity of magnetic systems further exacerbates this challenge: researchers must screen across 1,421 magnetic space groups, considering complex exchange-correlation effects (such as Hubbard U corrections) and spin- orbit coupling [5]. Furthermore, determining magnetic ground states often requires traversing vast spin configuration spaces, becoming prohibitively time-consuming for large unit cells or non-collinear magnetic orders [6].

It is against this backdrop that artificial intelligence emerges as a powerful auxiliary tool. By lever- aging deep potential methods, graph neural networks, and equivariant neural networks, researchers can predict material magnetic properties and topological invariants at a computational cost thousands of times lower than traditional DFT [7]. The 2024 Nobel Prize in Chemistry awarded for AI-driven protein structure prediction exemplifies this trend, heralding a "Turing moment" for AI in molecular and mate- rials modeling [8]. In topological physics, AI is utilized not merely for accelerating energy calculations, but for efficiently mapping complex topological phase diagrams by learning symmetry indicators and electronic wave function distributions [2]. This article delves into the theoretical foundations, algorith- mic architectures, high-throughput screening workflows, and challenges of using artificial intelligence to predict magnetic higher-order topological corner states.

## 2. Theoretical Foundations

### 2.1. Physical Definition of Higher-Order Topological Insulators

Place the core characteristic of higher-order topological insulators (HOTIs) lies in their "missing" edge states. Taking two-dimensional second-order topological insulators as an example, both the bulk gap and one-dimensional edge gap is non-zero, yet zero-dimensional confined corner states exist at the corners of 2D samples [1]. Physically, this phenomenon is typically associated with the quantization of multipole moments. Analogous to how electric dipole moments in conventional insulators lead to edge charges, quantized electric quadrupole moments result in corner charges [9].

These topological properties are protected by crystal symmetries. For instance, systems with Cn rotational symmetry or mirror symmetry M restrict polarization strength to specific discrete values. When these symmetries are preserved, bulk band topological features manifest on boundaries through filling anomalies [10].

## 2.2. Magnetic Topological Quantum States and Time-Reversal Symmetry Breaking

In magnetic materials, endogenous magnetic order breaks T symmetry. Depending on the magnetic order type, systems may retain combined symmetries such as $C_nT$ or MT [5]. These residual symmetries can still protect specific topological states.

Table 1: Magnetic Order Types and Corresponding Topological States

| Magnetic Order Type | Symmetry Characteristics | Typical Topological States | Example |
|---|---|---|---|
| Ferromagnetic (FM) | Breaks T, retains lattice symmetry | Quantum anomalous Hall insulator, Weyl semimetal [4] | CrI3<br>CrO2<br>MnBi2Te4 (odd layers) |
| Type-A Antiferromagnetic (A-AFM) | Breaks T, may preserve $T_{\tau 1/2}$ (combined translation) | Topological antiferromagnetic insulator, Axion insulator [11] | MnBi2Te4<br>MnBi4Te7<br>EuSn2P2 |
| Non-collinear magnetic order | Complex space-rotation coupling | Topological textures, non-collinear HOTI [12] | Mn3Sn<br>Mn3Ge |
| Ferrimagnetic | Inequivalent magnetic sublattice spin flipping | ferrimagnetic-valley second-order topological insulator (ferrimagnetic-valley SOTI) | Mo2CSCl monolayer |

The influence of magnetic structure on corner states primarily manifests as a "mass term". When magnetic moment directions flip, they alter the mass domain walls of edge states, driving corner states to move between different positions or annihilate. This high degree of tunability makes magnetic HOTIs ideal materials for constructing topological quantum switches [11].

## 2.3. Symmetry Indicators and Topological Invariants

To avoid tedious Berry phase calculations or Wilson loop scanning, researchers have developed the Sym-metry Indicators (SIs) method. This approach requires only the extraction of irreducible representation character tables for bands at high-symmetry momentum points [13].

For the 1,421 magnetic space groups, magnetic topological quantum chemistry theory has established a complete mapping framework, directly connecting bulk symmetry eigenvalues to topological indices [5]. The advantage of AI models lies in their ability to learn these complex group-theoretic rules. By inputting crystal graph structures, GNNs can automatically extract

representation features at high-symmetry points and predict final topological invariants $Z_n$.

# 3. AI Methodology: From Atomic Coordinates to Topological Classification

## 3.1. Equivariant Neural Networks Based on Symmetry Learning

Due to strict symmetry requirements regarding rotation and translation for crystal physical properties, traditional deep neural networks often require massive data augmentation. To overcome this difficulty, equivariant neural networks have emerged. The core concept ensures that network operations (such as convolution and pooling) commute with specific group operations (such as the E (3) Euclidean group). E (3) Equivariant Graph Neural Networks (EGNN) explicitly process node position vectors $x_i$ and feature vectors $h_i$ during message passing. They ensure that output force vectors rotate synchronously with atomic rotation while energy scalars remain invariant [15]. MACE further introduces many-body inter-actions and higher-order equivariant features. When processing magnetic systems, magnetic moments $S_i$ are treated as axial vectors, with MACE capable of capturing fine symmetry constraints in spin-spin interactions [8].

These models can predict not only scalar properties (such as band gaps) but also vector fields and tensor fields, which are crucial for describing Wannier charge center offsets in magnetic HOTIs [7].

## 3.2. High-Throughput Screening: Feature Engineering and Model Integration

Table 2: Screening Stage Technologies and Functions

| Screening Stage | Key Technologies | Function |
|---|---|---|
| Input layer | Crystal graph convolution, Equivariant embedding | Preserves structural symmetry [19] |
| Intermediate layers | Attention mechanisms (GAT), Many-body interactions | Captures long-range magnetic coupling [20] |
| Output layer | Soft classification layer, Uncertainty quantification | Provides topological index pre dictions [14] |

AI-driven material screening typically follows a standard workflow. Step one: Obtain CIF structures from databases such as Materials Project or 2DMatPedia, combined with experimental magnetic con- figurations from MAGNDATA [16]; Step two: Convert crystals into graph structures. Node features include not only atomic numbers but also spin polarization information (such as local magnetic moment magnitude and direction) [4]. To enhance model

expressiveness, Universal Atom Embeddings (UAE) are typically introduced to capture chemical similarities [17]; Step three: Employ multi-task learning strategies, simultaneously training models to predict energy, band gaps, and topological invariants. Uti-lize ensemble learning to reduce overfitting risks and assess prediction uncertainty [18]; Finally: Based on model predictions of band inversion characteristics at high-symmetry points, subsequent SI logic de-termines the topological phase [14].

## 3.3. Active Learning in Large-Scale Search

Facing enormous chemical configuration spaces (such as over 10,000 possible 2D magnetic heterostruc-tures), exhaustive computation is infeasible. Active learning addresses this through "closed-loop iteration" [18].

In a typical active learning cycle, the AI model is first trained on a small labeled dataset (such as 1,000 DFT samples). The model then predicts over thousands of unlabeled candidate materials, calculating prediction entropy or variance (as metrics of uncertainty). The system automatically selects samples where the model is "most uncertain" or "most promising" for high-precision DFT verification [21]. This approach ensures limited computational resources are always invested in the most physically valuable regions, such as topological phase boundaries. According to recent research, this strategy has successfully identified 63 highly promising 2D magnetic topological materials, including CoO2 with rich higher-order phase transitions [18].

## 3.4. Case Analysis: AI Prediction vs. DFT Calculation

Table 3: Performance Comparison: Traditional DFT vs. AI Prediction

| Metric | DFT+SOC | AI (GNN/EGNN) | Source |
|---|---|---|---|
| Single material calculation time | ~10 hours (typical cell) | < 1 second | [7] |
| Large supercell (10k atoms) | Extremely difficult (> 106 core-hours) | Feasible (~103 core-hours) | [7] |
| Magnetic order prediction accuracy | 100% (theoretical baseline) | 77.8% – 91% | [6] |
| Topological invariant classification accuracy | N/A | ~91% | [14] |
| Magnetic moment prediction (MAE) | N/A | ~0.3 μB | [4] |

To illustrate AI efficacy, we compare various metrics in predicting magnetic higher-order topological states.

The core value of AI lies not merely in orders-of-magnitude speed improvements, but in

handling extreme problems such as twisted moir\'e superlattices that traditional methods cannot address, through "local configuration approximation" [7].

## 4. Deep Physical Origins of Prediction Errors

Current AI models exhibit approximately 9% error in topological classification. Understanding the sources of these errors is crucial for improving next-generation algorithms.

### 4.1. Limitations of Data and Physical Models

Topological properties depend on the band ordering at specific high-symmetry points in the Brillouin zone. For materials near critical points of topological phase transitions, extremely small lattice distortions or the choice of DFT functionals (such as fine-tuning of U values) can lead to changes in band ordering. AI models learn based on statistical features and often struggle to capture this near-singular physical sensitivity. The DFT calculations used as training labels for AI are not infallible. Due to numerical instabilities in DFT calculations (such as convergence to different magnetic metastable states), materials with identical stoichiometry and space groups may exhibit different topological properties. When AI models learn from these "noisy" labels, they naturally develop biases.

Contradiction between global topology and local environment: Topological invariants are global integrals over the Brillouin zone, whereas current graph neural networks primarily rely on message passing of local atomic environments. Although equivariant networks introduce symmetry constraints, when dealing with large-unit-cell systems, the models may not fully establish the complex mapping from local chemical bonds to global topological properties.

### 4.2. Influence of Environment and Microscopic Disorder

In the experiments, materials are seldom perfect ideal crystals. Crystallographic disorder, such as substitutional disorder where atoms randomly occupy lattice sites different from their intended positions, is exceedingly prevalent in practical materials. Nevertheless, the prevailing AI screening workflows predominantly operate based on idealized structural models that assume perfect periodicity and atomic ordering. Should an AI model fail to explicitly incorporate and account for such disorder effects during its training and prediction phases, the topologically protected states it predicts may, upon experimental validation, have already been obliterated or gapped out due to symmetry breaking induced by the inherent disorder present in real material samples. Furthermore, concerning magnetic materials characterized by strong electronic correlations, Density Functional Theory (DFT) exhibits inherent systematic

deviations and inaccuracies in describing the splitting of d and f orbitals, stemming from the limitations of approximate exchange-correlation functionals in capturing strong on-site Coulomb interactions. Consequently, if the training data itself, generated through these imperfect DFT calculations, fails to accurately capture the critical band inversion phenomena that define topological character, the AI models will inevitably and inextricably inherit, propagate, and amplify these fundamental errors in their subsequent predictions.

# 5. Case Studies: From MnBi2Te4 to Novel SOTI Candidates

## 5.1. Magnetic and Topological Evolution of the MnBi2Te4 Series

The MnBi2Te4 family serves as a paradigmatic platform for studying magnetic topology. These materials consist of alternating stacking of MnBi2Te4 septuple layers (SL) and Bi2Te3 quintuple layers (QL). Their magnetic properties exhibit clear layer dependence: the bulk form shows A-type antiferromagnetism (intralayer ferromagnetic, interlayer antiferromagnetic), while thin samples with odd numbers of layers display uncompensated ferromagnetism, supporting the quantum anomalous Hall effect. Recent AI-assisted research predicts that several members of this family (such as MnBi4Te7 and Mn2Bi2Te5) are mirror-symmetry-protected topological crystalline insulators (TCI) under specific magnetization directions and may host second-order topological corner states. Using active learning, researchers discovered that through subtle Mn-Bi site mixing, the interlayer coupling strength can be effectively tuned, and even a transition from antiferromagnetic to ferromagnetic ground states can be achieved.

## 5.2. Emerging 2D Magnetic SOTI Candidates

Beyond the classic telluride series, AI models have identified other high-potential magnetic SOTIs.

- CrSBr Monolayer and Bilayer: CrSBr possesses a highly anisotropic structure. The monolayer is a ferromagnetic SOTI, while the bilayer is an antiferromagnetic SOTI. Its corner states exhibit fully spin-polarized characteristics and demonstrate exceptional robustness against SOC and small symmetry-breaking perturbations.
- Mo2CSCl Monolayer: This is a newly predicted "ferrimagnetic-valley" SOTI, combining ferrimagnetism, second-order topological corner states, and valley polarization, providing an ideal platform for multi-field controlled spintronic devices.
- $2H-VX2$ ($X = S, Se, Te$) Series: These transition metal dichalcogenides have been identified as 2D SOTIs with ferromagnetic ground states, whose corner states carry a

quantized fractional charge of $e/3$.

## 6. Challenges and Future Perspectives

Compared to non-magnetic materials, experimentally verified magnetic configuration data is extremely scarce. The MAGNDATA database contains only hundreds of finely described magnetic structures [16]. Furthermore, topologically trivial materials far outnumber non-trivial ones in nature, causing severe class imbalance problems during AI model training [6]. Future development requires advanced generative models (such as crystal GANs) to produce high-quality simulated magnetic data [22].

The accuracy ceiling of AI models is fundamentally limited by the source of their training data—DFT functionals. For magnetic materials with strong electronic correlations, DFT exhibits inherent biases in describing $d/f$ orbital splitting [11]. If training data itself fails to accurately capture band inversions, AI models inherit these errors. Developing "Δ-machine learning" techniques that predict differences between low-precision DFT and high-precision experimental data (or DMFT calculations) represents an important future direction [15].

Furthermore, current research mostly focuses on static structures at 0 K. However, magnetic systems possess rich excited states (such as magnons). AI needs to further integrate temperature effects and disorder influences to predict corner state coherence lengths and lifetimes at finite temperatures [2].

## 7. Conclusion

Artificial intelligence is injecting unprecedented momentum into magnetic higher-order topological physics research. Through equivariant neural networks' deep characterization of symmetry, AI has become not merely an acceleration tool, but a "microscope" for exploring new physical phenomena. From predicting magnetic phase transitions in the MnBi2Te4 family to locating corner states in large-scale moir\'e systems, AI demonstrates the capability to handle ultra-high-dimensional parameter spaces [11]. Despite challenges regarding data scarcity and insufficient description of correlation effects, as active learning loops mature and high-quality magnetic databases expand, artificial intelligence will undoubtedly lead magnetic higher-order topological corner states from theoretical prediction toward experimental application.

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