Online ISSN: 3104-9338
Print ISSN: 3104-932X

Graph Neural Networks for Surface-State Prediction in Topological Semimetals: Principles, Architectures, and Emerging Applications

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Received: March 19, 2026

Revised: March 20, 2026

Accepted:March 21, 2026

Published online: March 30, 2026

To appear in: *International Journal of Advanced AI Applications,* Vol. 2, No. 4 (April 2026)

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Abstract. Topological semimetals—encompassing Weyl semimetals, Dirac semimetals, and nodal-line semimetals—host surface states whose existence is guaranteed by bulk topology rather than surface termination details. Predicting these surface states accurately and efficiently is essential for connecting theoretical classifications to experimental observables such as ARPES spectra, quantum oscillations, and anomalous transport coefficients. Classical first-principles approaches are accurate but computationally expensive; they struggle to scan parameter spaces, disorder effects, and heterostructure geometries at scale. Graph Neural Networks (GNNs) offer a compelling alternative: by encoding crystal structures as atom-bond graphs and learning symmetry-respecting representations, they can predict surface-state dispersions, Fermi arcs, and topological invariants at a fraction of the DFT cost. This review systematically examines the theoretical underpinnings of topological surface states, the design principles of GNN architectures suited to this task, benchmark comparisons with DFT, and case studies spanning Weyl semimetals, nodal-line systems, and magnetic topological semimetals relevant to spin transport. We identify open challenges—including disorder, strong correlations, and finite-temperature dynamics—and propose directions for next-generation models.

Keywords: *Graph Neural Networks; Topological Semi Metals; Surface States; Fermi Arcs; Weyl Semimetal; Nodal-line Semimetal; Spin Transport; Machine Learn ing*

1. Introduction

The past decade has witnessed a proliferation of topological semimetal phases that go well

beyond the initial paradigm of topological insulators. Weyl semimetals carry chiral bulk nodes whose topological charge (Chern number ±1) enforces open Fermi arc surface states connecting projected Weyl points on any surface termination [1]. Dirac semimetals host four-fold degenerate nodal points stabilized by nonsymmorphic or other crystal symmetries, while nodal-line semimetals exhibit one-dimensional band crossings whose drumhead surface states form nearly flat bands of high density of states [2]. In each case, the surface states are a direct manifestation of the bulk topological invariant and serve as the primary experimental signature accessible to ARPES measurements.

Predicting these surface states presents a distinct computational challenge compared to bulk property calculations. One must construct a semi-infinite slab geometry or employ iterative Green's function methods to obtain the surface spectral function, both of which multiply the computational cost relative to bulk DFT. For magnetic topological semimetals—where spin-orbit coupling, exchange splitting, and magnetic anisotropy must all be captured simultaneously—the problem becomes especially demanding. Furthermore, real surfaces exhibit reconstruction, chemical termination sensitivity, and adsorbate-induced modifications that are beyond reach of idealized periodic slab DFT [3].

Graph neural networks have emerged as a powerful framework for materials property prediction precisely because crystal structures are naturally represented as graphs: atoms as nodes and interatomic bonds as edges, with features encoding chemical identity, spin state, and local geometry. Unlike fixed-descriptor machine learning, GNNs learn hierarchical representations directly from structural data, capturing multi-body correlations at increasing length scales through successive message-passing layers [4]. When equipped with equivariance to the Euclidean group $E(3)$, these networks additionally respect the rotational and translational symmetries that physical observables must satisfy, enabling predictions of vectorial and tensorial quantities—including surface state dispersion and spin texture—without symmetry-breaking artifacts [5].

This review focuses specifically on the application of GNNs to the prediction of surface states in topological semimetals, a topic that has received less systematic attention than bulk property prediction despite its critical importance. We examine: (i) the theoretical framework for understanding surface states in different semimetal families; (ii) the design of GNN architectures tailored for surface-state learning; (iii) training strategies including transfer learning and active learning; (iv) key results from recent literature; and (v) the connection to spin transport in one-dimensional ferromagnetic chains coupled to topological semimetal

substrates.

2. Theoretical Framework: Surface States in Topological Semimetals

2.1. Bulk-Boundary Correspondence and Fermi Arcs

The existence of surface states in topological semimetals is a direct consequence of the bulk-boundary correspondence. In a Weyl semimetal, the Chern number C=±1 associated with each Weyl node acts as a source or sink of Berry curvature in the 3D Brillouin Zone (BZ). On a 2D surface, the projected Weyl points of opposite chirality are connected by open arcs in the surface BZ—Fermi arcs—whose existence cannot be removed without closing the bulk gap or breaking the relevant symmetry [1].

Table 1. Classification of topological semimetal surface states by bulk invariant, state character, protecting symmetry, and representative materials.

Semimetal Type	Bulk Invariant	Surface State	Key Symmetry	Examples
Weyl SM	Chern # C = ±1	Fermi arc	Broken T or P	TaAs, NbP, $Co_3Sn_2S_2$
Dirac SM	Z_2 or crystalline	Surface Dirac cone	Both T and P (+ crystal)	Na_3Bi, Cd_3As_2
Nodal-line SM	Berry phase π	Drumhead state	PT or mirror	ZrSiS, Cu_2Si, Ca_3P_2
Magnetic Weyl SM	C = ±1 (no T)	Spin-polarized arc	Broken T (magnetic)	Co_2MnGa, GdPtBi
Triple-point SM	Chern # C = ±2	Double Fermi arc	Cn (n≥3) rotation	MoP, WC, CoSi

The shape, length, and spin texture of Fermi arcs depend sensitively on the surface termination, the orbital character of the Weyl nodes, and the surface potential. For a material with N pairs of Weyl nodes, the net arc contribution on any surface is determined by summing Chern numbers of the occupied bands in the 2D momentum cut at each k_z value. This global constraint is topologically robust but leaves enormous freedom in the arc morphology—freedom that is determined by non-topological surface physics and is therefore highly sensitive to chemistry [6].

2.2. Surface Green's Function and Spectral Function

The standard computational approach to surface states is the iterative surface Green's function method. Starting from a tight-binding Hamiltonian H(k), one constructs the semi-infinite system by coupling a sequence of principal layers. The surface spectral function $A(k\|, \omega)=-(1/\pi)ImTrG_s(k\|, \omega)$ directly yields the ARPES intensity map observable in

experiment. This method scales as $O(N^2)$ in layer size and requires converged Wannier functions from DFT as input, placing it firmly in the first-principles regime [7].

GNN models offer a path to bypass the Wannier function construction step entirely, learning a direct mapping from crystal structure to surface spectral function—or equivalently, to a tight-binding Hamiltonian from which the spectral function can be computed cheaply. This two-stage approach (GNN → Hamiltonian → spectral function) separates the machine learning problem from the physics simulation, allowing physical consistency constraints to be imposed at the Hamiltonian level [8].

2.3. Spin Texture and Its Relation to Transport

Beyond the dispersion of surface states, their spin texture—the momentum-dependent expectation value $\langle S(k) \rangle$ on the surface Fermi arc or drumhead—is a central quantity for spintronic applications. In Weyl semimetals, the spin texture of Fermi arcs is helical and locked to momentum by spin-orbit coupling, giving rise to a large spin Hall angle and non-trivial spin-orbit torques when interfaced with ferromagnetic layers [9]. In nodal-line semimetals, the nearly flat drumhead states can develop spontaneous spin polarization through exchange interaction with an adjacent ferromagnetic chain, creating a topologically non-trivial interface state that is directly relevant to the quantum transport of spin-polarized currents.

Predicting spin textures with GNNs requires the network to output vector-valued quantities that transform correctly under spin rotations—precisely the capability provided by equivariant architectures processing atomic magnetic moments as $l = 1$ axial vectors under SO(3). This connection between equivariant GNN design and spin transport observables is one of the key themes of this review.

3. GNN Architectures for Surface-State Prediction

3.1. From Crystal Graph to Hamiltonian

The most physically grounded approach to GNN-based surface-state prediction is to learn the real-space Hamiltonian matrix elements H_{ij} rather than directly learning the surface spectrum. This strategy, implemented in frameworks such as DeepH and HamGNN, parameterizes the Hamiltonian as a sum of local contributions that respect crystal symmetry [8]. Each pair of atoms (i, j) separated by a lattice vector R contributes a block $H_{ij}(R)$ whose transformation properties under the site symmetry group are enforced by the equivariant architecture. The full Hamiltonian $H(k)=\Sigma_R H_{ij}(R)e^{ik\cdot R}$ then reproduces DFT band structures

with MAE typically below 10 meV across the full BZ.

To predict surface states, one extracts the Hamiltonian blocks corresponding to a chosen slab geometry—either through direct inference on a slab supercell graph or by assembling bulk Hamiltonian blocks into a finite slab—and subsequently diagonalizes numerically. This approach guarantees Hermiticity, time-reversal symmetry, and correct periodicity by construction, avoiding the unphysical artifacts that can arise when neural networks directly output spectral functions [8].

3.2. Equivariant Message Passing: Architecture Comparison

Table 2. Comparison of GNN architectures in terms of equivariance, key innovations, and suitability for topological semimetal surface-state prediction.

Architecture	Equivariance	Key Innovation	Surface-State Application	Accuracy vs. DFT
CGCNN	None (invariant only)	Crystal graph convolution	Band gap, not surface states	MAE ~0.24 eV (Eg)
SchNet	Translation + rotation (scalars)	Continuous-filter convolution	Limited: scalar properties	MAE ~0.014 eV/atom
NequIP / MACE	Full E (3)	Tensor product features	Force fields, partial Hamiltonian	DFT-level forces
DeepH	Site symmetry enforced	Local Hamiltonian learning	Full Hamiltonian → surface states	MAE < 10 meV (bands)
HamGNN	E (3)-equivariant	Orbital-resolved H blocks	Weyl/Dirac surface spectra	MAE < 15 meV
TopoNet	Crystallographic point group	Symmetry indicator heads	Topological invariant + arc topology	~91% class. accuracy

3.3. Multi-Task Learning: Simultaneously Predicting Bulk and Surface

A natural extension of the single-task Hamiltonian learning framework is multi-task training, in which the GNN is simultaneously supervised on bulk band structures, surface state dispersions, topological invariants, and magnetic properties. The rationale is that these targets are not independent: the topological invariant constrains whether a surface state must exist, the bulk Hamiltonian determines the arc connectivity, and the magnetic moment distribution shapes the spin texture. By leveraging these physical correlations, multi-task models generalize better from limited training data than single-task counterparts [10].

A practical challenge is that different tasks have incommensurable units and dynamic ranges. Gradient balancing techniques—such as GradNorm or uncertainty-weighted losses—adaptively reweight task gradients during training to prevent one task from dominating. In the

context of surface-state prediction, pairing the Hamiltonian regression loss with a classification loss on the topological invariant (Z_2, Chern number, or Berry phase) has been shown to improve Hamiltonian accuracy in topologically non-trivial materials by up to 20% compared to regression-only training [10].

3.4. Transfer Learning and Domain Adaptation

Labeled data for surface-state prediction is scarce: computing DFT surface spectral functions requires Wannier function construction, which fails for strongly entangled bands and is non-trivial to automate at scale. Transfer learning addresses this by pre-training GNN models on large databases of bulk DFT calculations—where training data is abundant—and then fine-tuning on a small dataset of surface-state calculations. The pre-trained model has already learned a chemical representation that encodes orbital hybridization, spin-orbit coupling strength, and band inversion tendencies; fine-tuning then adapts this representation to surface-specific features with minimal additional data [11].

Domain adaptation further extends this concept to account for systematic differences between training (DFT-PBE) and target (experimental ARPES) domains. By including a small number of experimentally resolved Fermi arc maps as fine-tuning targets, GNN models have been shown to predict arc morphologies that match ARPES measurements more closely than DFT itself—effectively learning the surface-potential correction that DFT neglects [12].

4. Training Strategies and Dataset Construction

4.1. Automated Wannierization Pipeline

The bottleneck for large-scale training of surface-state Graph Neural Networks (GNNs) is the generation of Wannier tight-binding models derived from Density Functional Theory (DFT) calculations. Traditional Wannier90 workflows often require manual selection of initial projectors and entanglement windows, which significantly limits throughput and efficiency. However, recent advancements in automated Wannierization tools—such as WannierTools AutoW, Wannier-Berri, and the AFLOW-Wannier module—have substantially reduced this barrier by combining heuristic orbital assignment with iterative disentanglement minimization techniques. When integrated with high-throughput DFT engines like VASP and Quantum ESPRESSO, these innovative pipelines can now generate Wannier Hamiltonians at an impressive rate of approximately 50 to 200 materials per day on a modern computing cluster. This capability provides the substantial volume of training data needed for robust and effective

GNN training, enabling researchers to explore and analyze material properties more comprehensively [7].

4.2. Active Learning for Surface-Geometry Diversity

Topological semimetal surface states depend not only on the bulk crystal structure but also on the surface termination—cleavage plane, reconstruction, and adsorbate coverage. A training set composed exclusively of relaxed bulk structures will fail to capture this termination dependence. Active learning addresses this by iteratively selecting new surface geometries where the model predicts with high uncertainty, running DFT slab calculations for those geometries, and adding them to the training set. Uncertainty is quantified through GNN ensemble disagreement: the variance in predicted Hamiltonian matrix elements across an ensemble of five independently trained models provides a reliable proxy for prediction error [13].

In practice, this strategy has been applied to the TaAs family of Weyl semimetals, where four distinct surface terminations (Ta-terminated, As-terminated, and two reconstructed variants) exhibit qualitatively different Fermi arc morphologies. After five active learning cycles starting from 200 training structures, the GNN achieved sub-30 meV MAE on all four terminations, compared to sub-20 meV for the dominant termination alone—a significant improvement in transferability across surface chemistry [13].

5. Case Studies

5.1. Weyl Semimetal TaAs: Fermi Arc Topology

TaAs was the first experimentally confirmed Weyl semimetal, hosting 24 Weyl nodes and corresponding Fermi arcs. GNN models trained with the DeepH framework on a dataset of 1,400 bulk and slab calculations reproduced the characteristic "spoon-shaped" arcs on the (001) termination with a positional accuracy of ±0.02 $Å^{-1}$ in k-space relative to DFT. More importantly, the GNN correctly predicted the topological transition—disappearance of surface arcs—when the lattice parameter is strained beyond the critical value that annihilates two pairs of Weyl nodes, a prediction verified by subsequent slab DFT [8].

The spin texture of the TaAs Fermi arcs—which plays a critical role in determining the surface spin Hall conductivity and the overall efficiency of spin-orbit torque in TaAs/ferromagnet heterostructures—was successfully predicted by an equivariant Graph Neural Network (GNN) utilizing the NequIP variant. This advanced model achieved an

impressive average angular error of below 12° across the entire arc, which is comparable to the accuracy typically obtained from DFT+SOC calculations. Remarkably, this level of precision was accomplished at only 1/3,000 of the computational cost associated with traditional methods [5]. Such efficiency demonstrates the potential of GNNs in advancing our understanding of complex materials and their properties while significantly reducing the computational resources required for similar predictions.

5.2. Nodal-Line Semimetal ZrSiS: Drumhead States and Spin Coupling

ZrSiS and its isostructural analogs are archetypal nodal-line semimetals with a square-shaped nodal framework protected by non-symmorphic symmetry. Their drumhead surface states form a nearly flat band spanning a large region of the surface BZ, making them sensitive probes of surface magnetism and correlation effects. GNN-predicted surface Hamiltonians for the ZrSiX (X = S, Se, Te) series captured the systematic evolution of drumhead state bandwidth with increasing spin-orbit coupling, correctly reproducing the partial gapping of the nodal lines in ZrSiTe while preserving them in ZrSiS [14].

Of particular relevance to spin transport is the interaction of ZrSiS drumhead states with an adjacent one-dimensional ferromagnetic chain. When a GNN-predicted tight-binding model of ZrSiS is coupled to a Heisenberg ferromagnetic chain via exchange interaction, the resulting interface Hamiltonian supports a topologically non-trivial bound state at the chain endpoints whose spin polarization can be switched by reversing the chain magnetization. This prediction—enabled by the GNN's ability to provide an accurate surface Hamiltonian for an embedded geometry inaccessible to periodic DFT—directly connects to the quantum transport theme of controlling spin currents through topological semimetal surfaces [9].

5.3. Magnetic Weyl Semimetal $Co_3Sn_2S_2$: Anomalous Hall and Surface Arcs

$Co_3Sn_2S_2$ is a ferromagnetic Weyl semimetal with a large anomalous Hall conductivity ($\sigma_{xy} \sim 1130 \Omega^{-1} cm^{-1}$) arising from Berry curvature concentrated near Weyl nodes close to the Fermi level. GNN models incorporating magnetic moment vectors as equivariant node features predicted the anomalous Hall conductivity tensor with 8% relative error compared to DFT+SOC, while simultaneously predicting the (001) surface Fermi arc morphology with sub-20 meV accuracy [15].

A key insight from this case study is that the GNN correctly captured the sensitivity of arc morphology to the direction of the Co magnetic moment—a property invisible to non-magnetic

GNN models. When the magnetization is rotated from the easy axis (c-axis) to the hard axis (ab-plane), the Weyl nodes shift in momentum space and the arc connectivity changes, a prediction the GNN reproduced without additional DFT calculations through equivariant propagation of the rotated moment vector [15].

Table 3. Summary of GNN case studies for surface-state prediction in topological semimetals.

Material	Semimetal Type	GNN Task	Key Result	Error vs. DFT
TaAs	Weyl SM	Fermi arc morphology + spin texture	Topological transition predicted under strain	±0.02 $Å^{-1}$; 12° spin angle
ZrSiS/Se/Te	Nodal-line SM	Drumhead state bandwidth	SOC-driven gapping trend reproduced	MAE < 18 meV
$Co_3Sn_2S_2$	Magnetic Weyl SM	AHC tensor + arc under M rotation	Arc connectivity change with moment rotation	8% AHC, < 20 meV arc
Cd_3As_2	Dirac SM	Surface Dirac cone dispersion	Fermi velocity within 5% of DFT	MAE < 12 meV
MoP	Triple-point SM	Double Fermi arc topology	Both arcs simultaneously predicted	MAE < 25 meV

6. Challenges and Error Analysis

6.1. Entangled Bands and Wannier Obstruction

A fundamental difficulty arises in materials where topological bands are strongly entangled with trivial bands across a wide energy window. In such systems, the construction of maximally localized Wannier functions is obstructed by the topology itself—a phenomenon known as Wannier obstruction. This forces the use of symmetry-indicated non-Abelian Wannier representations that are harder to automate and produce training labels of lower quality. GNN models trained on such data exhibit higher errors (MAE 30–50 meV) in the entangled window and may misclassify topological invariants near phase boundaries [7].

6.2. Surface Reconstruction and Chemical Termination

Experimentally observed surfaces of topological semimetals frequently undergo complex reconstruction into supercells that break the surface translational symmetry typically assumed by slab Density Functional Theory (DFT) calculations. Accurately predicting these reconstructed-surface states using advanced Graph Neural Networks (GNNs) necessitates training data derived from supercell slabs, which are often computationally expensive and time-consuming to generate. As a result, current models tend to be most reliable for ideal cleavage-plane terminations; however, their accuracy diminishes significantly when applied to surfaces that exhibit substantial reconstruction or are covered with adsorbate layers. This degradation in predictive performance occurs under precisely the conditions most commonly encountered in

Angle-Resolved PhotoEmission Spectroscopy (ARPES) experiments conducted in non-UHV environments, where surface conditions can vary considerably and introduce additional complexities and uncertainties [3]. Consequently, developing more versatile and robust models that can accommodate these variations remains a critical challenge in the field of material science, as it is essential for enhancing our understanding of electronic properties and behaviors in real-world applications.

6.3. Surface Reconstruction and Chemical Termination

Several magnetic topological semimetals—including EuB_6 and GdPtBi—contain rare-earth f electrons whose Kondo-like correlations are beyond standard DFT+U. In these materials, the surface states are Kondo-screened at low temperature and their spectral function acquires a sharp Abrikosov-Suhl resonance at the Fermi level. GNNs trained on DFT+U data inherit the systematic errors of the DFT+U approximation and cannot reproduce this resonance. Delta-machine-learning approaches—predicting the correction between DFT+U and DFT+DMFT spectral functions—represent the most promising path toward GNN-level accuracy in this regime [16].

7. Outlook and Future Directions

Several research frontiers will define the next generation of GNN-based surface-state prediction. First, the integration of experimental ARPES data as training targets—through physics-informed domain adaptation—will allow models to self-correct for surface potential and many-body effects that DFT systematically misses, moving the accuracy ceiling above DFT itself.

Second, the extension of surface-state GNNs to heterostructure geometries is urgently needed. When a topological semimetal is interfaced with a ferromagnetic layer or a superconductor, the proximitized surface state acquires properties—exchange gap, induced pairing—that depend on the interface atomic structure in ways that bulk GNNs cannot capture. Training GNNs directly on interface geometries, with graph representations that include both materials and the interfacial bonding region, will enable predictions of proximity-induced topological superconductivity and spin-orbit torque efficiency that are directly relevant to device design.

Third, the incorporation of thermal fluctuations and phonon effects will connect zero-temperature GNN predictions to finite-temperature experimental observables. The coherence of surface Fermi arcs and drumhead states at room temperature is limited by electron-phonon scattering, and understanding this limitation is essential for topological semimetal device

applications.

Finally, the coupling of surface-state GNNs with quantum transport simulation—feeding GNN-generated tight-binding Hamiltonians into non-equilibrium Green's function or Landauer-Büttiker transport codes—will create end-to-end predictive pipelines from crystal structure to device-level spin transport characteristics, fully realizing the potential of AI-driven topological materials design.

8. Conclusion

Graph neural networks have matured to the point where they can predict surface states in topological semimetals with accuracy approaching—and in some cases exceeding—conventional DFT methods, at a computational cost reduced by three to four orders of magnitude. The key architectural advance enabling this progress is equivariance: by building in the physical symmetries that surface states must respect, GNNs avoid the symmetry-breaking artifacts that afflict earlier machine learning approaches and achieve reliable predictions of spin textures, arc morphologies, and topological invariants. The direct connection between these predictions and experimentally measurable quantities—ARPES spectra, anomalous Hall conductivity, spin transport in ferromagnet/semimetal heterostructures—positions GNNs as an indispensable tool in the rational design of next-generation topological quantum devices.

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