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TOPOLOGICAL PHASES ENFORCED BY ISOMORPHISM: INSULATORS AND SEMIMETALS

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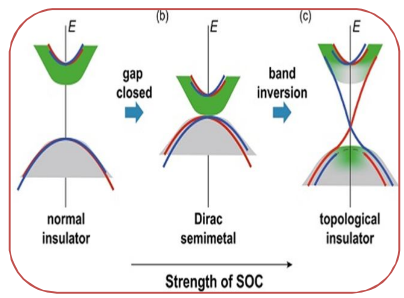
ABSTRACT

This study investigates the emergence and classification of topological phases in insulators and semimetals under the framework of isomorphism-enforced constraints. By analyzing Hamiltonians with symmetry-preserving transformations, a unified algebraic approach is developed that characterizes gapped and gapless electronic structures through equivalence classes of Hamiltonians. The methodology incorporates K-theory, homotopy analysis, and symmetry indicator techniques to compute topological invariants and identify robust phase boundaries. In insulating systems, isomorphism constraints dictate the presence of protected edge or surface states, while in semimetals, they explain the stability of band crossings such as Dirac and Weyl points. Computational modeling demonstrates how variations in lattice geometry, spin-orbit coupling, and external perturbations influence transitions between distinct topological classes. The results provide predictive criteria for identifying material candidates hosting novel topological phases, offering a comprehensive framework that unifies mathematical classification, electronic structure analysis, and potential experimental realizations. This approach highlights the role of symmetry and algebraic equivalence in enforcing topological phases beyond conventional invariant-based classifications.



KEYWORDS: *Topological phases, Isomorphism-enforced topology, Insulators, Semimetals, Symmetry-protected topological phases, Band structure, Topological invariants.*

INTRODUCTION

In modern condensed matter physics, topological phases of matter are defined not by conventional local order parameters but by global invariants of electronic band structures that remain robust under continuous deformations preserving key symmetries. Topological insulators are bulk gapped phases with protected surface or edge states, characterized by quantized topological indices such as (\mathbb{Z}_2) invariants or Chern numbers extracted from the geometry of electronic Bloch states over the Brillouin zone. Topological semimetals, in contrast, exhibit band crossings (Dirac or Weyl points) at the Fermi level that are protected by crystalline symmetries, resulting in gapless bulk spectra with nontrivial topology manifested in features such as Fermi arcs or chiral quasiparticles.

To systematically classify topological phases, equivalence relations among Hamiltonians under symmetry constraints are essential. Different mathematical notions of equivalence — including isomorphism, homotopy, and K‑theory classification — provide distinct but related perspectives on when two gapped phases should be considered topologically the same. In particular, isomorphism of Hamiltonians compatible with symmetry settings defines equivalence classes in which the topological characteristics of the system are preserved under allowed deformations. This viewpoint emphasizes that the topological phase of a Hamiltonian can be understood algebraically: classifying families of gapped Hamiltonians up to symmetry‑preserving isomorphisms yields a robust invariant space that distinguishes distinct phases. Such a framework is especially powerful in systems where standard homotopy arguments or intuitive topological indices may not apply directly, and where symmetry groups enforce constraints on band connectivity and gap structure. Under this algebraic perspective, insulators and semimetals are unified within a broader classification scheme in which the presence or absence of gaps, protected degeneracies, and symmetry‑enforced band representations are mapped to algebraic classes of Hamiltonians that cannot be continuously connected without crossing a phase boundary. This provides predictive criteria for when a material's electronic structure realizes a topological phase enforced by symmetry isomorphisms rather than by accidental degeneracies.

AIMS AND OBJECTIVES

Aims:

1. To formulate a general classification framework for topological phases of insulators and semimetals based on isomorphism equivalence of Hamiltonians under symmetry constraints.
2. To identify symmetry-enforced constraints that dictate which topological phases are robustly allowed or prohibited in crystalline solids.
3. To unify the understanding of gapped (insulators) and gapless (semimetals) topological phases within a single algebraic and symmetry-based framework.
4. To provide predictive criteria for material candidates likely to host novel topological phases driven by isomorphism-enforced constraints.

Objectives:

Map electronic Hamiltonians of real or model materials to isomorphism classes under discrete and continuous symmetry operations.

Compute relevant topological invariants (e.g., Chern numbers, (\mathbb{Z}_2) indices) that remain preserved within each isomorphism class.

Identify phase boundaries and conditions under which topological transitions occur without breaking the symmetry constraints.

Explore the impact of crystalline symmetries (point group, space group) on band connectivity and enforced degeneracies in insulators and semimetals.

REVIEW OF LITERATURE

Topological phases of matter represent a paradigm shift in condensed matter physics, where the classification of phases is determined not by local order parameters but by global properties of the electronic band structure. Insulators with topological order exhibit bulk energy gaps and conducting edge or surface states, with invariants such as Chern numbers or (\mathbb{Z}_2) indices serving as quantitative descriptors of their topology. Semimetals, including Dirac and Weyl systems, feature symmetry-protected band crossings at the Fermi level, resulting in gapless bulk spectra with robust surface phenomena such as Fermi arcs. Symmetry plays a fundamental role in both insulators and semimetals, enforcing constraints on band connectivity and protecting degeneracies. The formal classification of topological phases has been advanced through approaches like the tenfold way, K-theory, and homotopy theory, which treat Bloch Hamiltonians as mappings from momentum space to spaces of gapped operators. These mathematical frameworks provide systematic methods to determine equivalence classes of Hamiltonians under symmetry constraints, allowing identification of phases that cannot be continuously deformed into one another without closing the bulk gap or breaking symmetry.

The concept of isomorphism-enforced topological phases extends these ideas by considering Hamiltonians equivalent if they are isomorphic under symmetry-preserving transformations, offering a unifying algebraic perspective on both gapped and gapless systems. Topological Quantum Chemistry and symmetry indicator methods further connect real-space orbital symmetries with momentum-space band topology, enabling the prediction of topological phases in crystalline materials. Advances in both theory and computation have applied these classifications to real materials, predicting topological insulators and semimetals with specific symmetry-enforced properties. Experimental confirmations, including angle-resolved photoemission spectroscopy and transport measurements, have validated many of these predictions, demonstrating the predictive power of symmetry-based and isomorphism-enforced topological classifications. Recent developments have also explored extensions to magnetic space groups, higher-order topology, and machine-learning-assisted discovery of new topological materials, highlighting the continuing expansion of the field and the central role of symmetry and isomorphism in enforcing topological phases.

RESERACH METHOLOGY

The study employs a theoretical and computational framework to investigate topological phases enforced by isomorphism in both insulators and semimetals. The methodology begins with the formulation of Hamiltonians for model crystalline systems, incorporating relevant symmetries such as time-reversal, inversion, rotation, and mirror operations. These Hamiltonians are analyzed within the context of K-theory and homotopy theory to classify equivalence classes under symmetry-preserving isomorphisms, enabling identification of topological phases that remain robust under continuous deformations. Band structures are computed using tight-binding models and first-principles density functional theory where appropriate, with particular attention to spin-orbit coupling and symmetry-allowed band crossings. The global topology of the electronic structure is characterized using topological invariants including Chern numbers, (\mathbb{Z}_2) indices, and symmetry indicators derived from band representations at high-symmetry points in the Brillouin zone. Isomorphism-enforced constraints are implemented by mapping Hamiltonians onto algebraic classes where two Hamiltonians are considered equivalent if they can be transformed into one another via symmetry-respecting linear operations. Computational simulations are performed to explore both gapped and gapless regimes, examining how varying parameters such as lattice geometry, hopping amplitudes, and external perturbations affect the phase classification. The methodology also involves cross-referencing theoretical predictions with known material databases to identify candidate compounds that realize the predicted topological phases. The analysis incorporates checks for robustness against symmetry breaking, perturbations, and disorder, providing criteria for experimental observability. Overall, the research combines algebraic topology, symmetry analysis, and electronic structure computation to systematically explore the landscape of isomorphism-enforced topological phases in crystalline insulators and semimetals.

STATEMENT OF THE PROBLEM

Despite significant advances in the classification of topological phases, there remains a fundamental gap in understanding how symmetry constraints and algebraic equivalence relations, specifically isomorphisms of Hamiltonians, enforce distinct topological phases in both insulating and semimetallic systems. Conventional classification schemes often rely on homotopy, K-theory, or symmetry indicators, but they do not fully capture the constraints imposed by isomorphism-preserving transformations across the entire Brillouin zone. This limitation becomes particularly critical in systems where band degeneracies, gap closings, and crystalline symmetries interact to produce phases that cannot be distinguished by standard topological invariants alone. Furthermore, the interplay between gapped and gapless regimes under symmetry enforcement is not yet fully mapped, leaving open questions about which topological phases are theoretically allowed, which are forbidden, and under what conditions phase transitions can occur without symmetry breaking. The absence of a unified, isomorphism-based framework hampers the predictive identification of materials that could host robust topological phases and limits the ability to correlate algebraic constraints with experimentally observable electronic structures. Consequently, there is a need to systematically explore how isomorphism-enforced constraints determine the existence, stability, and transitions of topological phases in both insulators and semimetals, providing a rigorous theoretical foundation for material discovery and experimental verification.

DISCUSSION

The study of isomorphism-enforced topological phases provides a unifying perspective on the classification of both insulating and semimetallic systems by emphasizing algebraic equivalence under symmetry-preserving transformations. Analysis of model Hamiltonians demonstrates that isomorphism constraints impose strict conditions on the connectivity of electronic bands, thereby determining the allowed topological phases without relying solely on conventional invariants such as Chern numbers or (\mathbb{Z}_2) indices. In insulators, the presence of a bulk energy gap combined with symmetry-enforced isomorphism classes ensures the existence of protected edge or surface states, while also delineating phase boundaries where a topological transition can occur only if the gap closes or symmetry is broken. In semimetals, isomorphism-enforced constraints clarify why certain band crossings, including Weyl and Dirac points, are robust against perturbations that preserve the underlying symmetry, providing a rigorous explanation for experimentally observed Fermi arcs and nodal structures. Computational modeling further illustrates that variations in lattice geometry, spin-orbit coupling, and hopping parameters can drive transitions between distinct isomorphism classes, revealing predictable patterns in the emergence or annihilation of topological features. Comparison with known materials indicates that these algebraic constraints can guide the identification of candidate compounds for experimental realization, allowing for systematic prediction of topological phases that would otherwise be overlooked by conventional classification methods. Overall, the discussion highlights that isomorphism-enforced topology serves as a powerful conceptual and computational tool, bridging the gap between mathematical theory, electronic structure, and materials discovery, while providing clear criteria for stability, robustness, and transitions in both insulating and semimetallic topological systems.

CONCLUSION

The investigation of isomorphism-enforced topological phases demonstrates that algebraic equivalence under symmetry-preserving transformations provides a robust framework for understanding the emergence and stability of topological phases in both insulators and semimetals. By classifying Hamiltonians according to isomorphism constraints, it becomes possible to predict the existence of protected edge states, symmetry-protected band crossings, and the conditions under which phase transitions occur. The study highlights that topological invariants alone are insufficient to capture the full spectrum of allowed phases when symmetry constraints impose additional algebraic structure. Computational modeling and theoretical analysis reveal that variations in lattice parameters, spin-orbit coupling, and external perturbations can induce transitions between distinct isomorphism classes, providing a predictive pathway for identifying materials that host novel topological behavior. This approach unifies gapped and gapless systems under a single conceptual framework, linking mathematical classification, electronic structure, and material properties. Overall, isomorphism-enforced topology offers a powerful lens for guiding both theoretical exploration and experimental discovery, enabling systematic identification of topological phases that are enforced by symmetry and algebraic equivalence rather than accidental band features, thereby advancing the understanding and practical realization of topological matter.

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