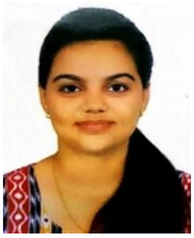
Letters to the Editor

Progress and Prospects of Novel Topological Phases of Materials



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The field of topological phases has captivated the condensed matter physics (CMP) community with its unique blend of theoretical elegance and practical relevance. The defining characteristic of the most celebrated topological insulator (TI) phase is their insulating bulk paired with a conductive surface; a property stemming from the non-trivial topology of their wavefunctions (Hasan et al 2023). In general, a *d*-dimensional system is classified as a TI if it has an insulating bulk and features boundary states that remain gapless, unaffected by local boundary perturbations unless the symmetry is broken. The TIs are characterized by the non-zero Z_2 invariant which signifies odd number of gapless spin-helical topological surface states (TSS) protected by time-reversal symmetry (TRS). Thus, this provides a solid framework that the scientific community continues to build upon for the potential applications of TIs in spintronics, quantum computing and nano-electronics. The adoption of topological classification in the last decade has unveiled various quantum materials, from insulators and superconductors to Dirac, Weyl semimetals, and fragile topological phases (Chen et al 2023). This letter to the editor outlines the recent advancements in TIs which pave the way for investigation of TIs and multifunctional quantum materials.

The non-trivial band topology is intricately embedded within the band structure of an insulator through band inversion. Intrinsic spin-orbit coupling (SOC) present in the system is a key factor in realizing the bulk band inversion or parity exchanges in most of the known TI genome. Numerous SOC induced TIs were theoretically and experimentally investigated ranging from HgTe/CdTe quantum wells, quintuple layered V_2VI_3 binary compounds, half-Heusler compounds, ternary non-centrosymmetric compounds etc (Patel et al 2024, Hsieh et al 2008, Dhori et al 2022, Dhori et al 2024, Sattigeri et al 2021). Despite theoretical predictions, the practical applications of TIs remain elusive largely due to the interference from the conduction contribution from the bulk in small bandgap semiconductor, precise control over material purity and challenging control over spin-momentum locking at elevated temperatures. Thus, in recent years, there has been a renewed interest in discovering materials that could bridge the gaps.

Topological insulators enable fault-tolerant quantum computing by hosting Majorana fermions with non-Abelian properties, facilitating robust qubits and gates. Their role in TI-superconductor heterostructures is pivotal for advancing quantum technologies. TIs are also predicted to be promising materials for enhancing thermoelectric performance and catalytic activity, further enriching their multifunctional characteristics (Dhori et al 2023, Sattigeri et al 2022). Furthermore, breaking the TRS through magnetic order leads to quantum anomalous Hall effect (QAHE). Intrinsic magnetic order induces quantized Hall conductance, eliminating the requirement for an external magnetic field in QAHE. Recent research focuses on investigating of moiré materials formed from graphene and transition-metal dichalcogenides, thin films with intrinsic magnetic TI and doped TIs for the theoretical prediction of QAHE in materials (Chang et al 2023).

Recently discovered obstructed atomic insulators (OAI) have ground-state charge center located at virtual-sites that are devoid of atoms. The cleavage through these virtual sites would lead to

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fractional occupied charges, subsequently giving rise to "obstructed surface states" (Liu et al 2023). The charge centers at these virtual sites, known as obstructed Wannier charge centers, can potentially facilitate ligand adsorption and electron transfer, positioning OAI as an excellent platform for surface catalysis. In 2023, Liu and coworkers observe obstructed surface states in $SrIn_2P_2$ using scanning tunnelling microscopy, angle-resolved photoemission spectroscopy and first principles calculations (Liu et al 2023).

After TIs, the classification of band character has been extended towards particle-hole symmetry, magnetic translation symmetry and crystal point group symmetry (such as mirror or rotational) which leads to topological superconductors (TS), magnetic insulators and topological crystalline insulators (TCIs), respectively. These TCIs serve as counterparts to TIs in materials that lack strong SOC (Fu et al). Recently, higher-order topological insulators (HOTIs) have been predicted. These materials are insulating in their interior and on their surfaces but have conducting channels at corners or along edges. HOTIs feature boundaries that, unlike traditional TIs, do not conduct through gapless states but act as TIs themselves. In an n^{th} order TI, gapless states appear on (d - n)-dimensional regions. For example, a 3D second-order TI has gapless states on 1D hinges, while a third order one has them on 0D corners. Similarly, a 2D second-order TI exhibits gapless states at its corners, introducing a unique family of topological phases (Parameswaran and Wan 2017). The bulk SnTe, surface modified Bi_2TeI, BiSe and BiTe predicted as helical HOTIs (Schindler et al 2018). This inspires further exploration into topological matter, aiming to uncover novel phases of matter along with their applications in modern day nano-electronics.

In the era of multifunctional materials, it is imperative to shed light on TIs coexisting with different physics phenomenon. Recently, intertwined topological states, Rashba effect and ferroelectricity in polar materials have gained considerable research interest owing to their promising applications in spintronics, current-induced switching in memory devices and enhanced spin-hall conductivity along with control over helicity and spin-texture of surface states by the polarization of bulk ferroelectricity (Mondal et al 2021, Gupta et al 2023, Narayan 2015). Ferroelectric TIs can also be used to augment conventional tunnel junctions or ferroelectric field effect transistors with complementary spin degrees of freedom. The hexagonal LiZnSb, KMgBi and XSnBi (X = K, Rb, Cs) are widely investigated for intertwined band topology, Rashba effect and ferroelectricity (Mondal et al 2021, Gupta et al 2023, Narayan 2015). The exploration of such multifunctional materials is scarcely observed making them a compelling focus for the research community. One can also speculate about the topological-multiferroic materials which further broadens the horizon for future studies.

Apart from TIs, its gapless cousins, topological semimetals (TSMs) revolutionized the frontiers of CMP. The TSMs are further classified as Dirac, Weyl, Nodal line and higher order fermion TSMs among others based on type of band degeneracies at crossing point in band structure. TSMs facilitate quantum transports which includes chiral anomaly, negative magnetoresistance etc. In general, materials exhibiting four- and two-fold band degeneracy for any crystal momentum at/near the Fermi level is known as Dirac and Weyl semimetals, respectively. Recently, Bradlyan et al. proposed higher order fermions with three-, six- and eight-fold degeneracy, respectively. The exploration of higher-order fermions is rarely addressed in the literature, paving the way for further design of such TSMs (Dhori et al 2024).

These areas represent some of the most promising and transformative research directions in condensed matter physics. This letter sparks further interest in exploration of TIs, OAIs, TCIs, HOTIs, TSMs and TIs with coexistence of different physics phenomenon is crucial for advancing both technological applications and our fundamental understanding of quantum phases. These novel phases of matter have potential applications in spintronics, quantum computing, low-power electronics and multiferroics among others.

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