Abstract

The exploration of novel quantum materials has significantly advanced our understanding of fundamental physics while paving the way for next-generation electronic and spintronic applications. In our daily lives, we rely on efficient transportation systems, smart navigation, and well-balanced structures to optimize movement and energy use. Similarly, magnetic topological insulators (MTIs), Weyl semimetals, and kagome lattice materials offer groundbreaking solutions for modern electronics, quantum computing, and energy-efficient technologies by controlling how electrons behave at the quantum level. Magnetic topological insulators act like superhighways for electrons, allowing them to move without resistance along their edges while blocking bulk conduction. This is similar to cars traveling on an expressway without stopping, leading to low-power electronics and ultra-efficient quantum devices. On the other hand, Weyl semimetals function like a GPS navigation system for electrons, providing special "shortcuts" (Weyl nodes) that allow electrons to move faster and with minimal scattering. This unique property enables high-speed electronics, ultra-sensitive magnetic sensors, and next-generation data transfer technologies. Meanwhile, kagome lattice materials create an environment where electrons experience frustration, much like people balancing on a trampoline. This results in flat bands, unconventional superconductivity, and exotic magnetic states, which are crucial for lossless power grids, quantum encryption, and future quantum technologies. By studying and engineering these materials, we are unlocking the potential for smarter, faster, and more energy-efficient technologies. Just as highways, GPS, and balanced structures have transformed daily life, these quantum materials are paving the way for a future of revolutionary computing, ultra-efficient energy systems, and cutting-edge quantum applications. This thesis focuses on these three distinct yet interrelated classes of materials: magnetic topological insulators (MTIs), Weyl semimetals, and Kagome lattice systems. Each of

these material families exhibits unique electronic and magnetic properties, providing a rich platform for studying the interplay of topology, electron correlations, and magnetism. Magnetic topological insulators extend the physics of conventional topological insulators by incorporating magnetic interactions, leading to exotic quantum phenomena such as the quantum anomalous Hall effect and axion electrodynamics. The controlled manipulation of magnetism in these materials offer promising avenues for spintronic applications and topological quantum computing. Weyl semimetals, on the other hand, serve as condensed matter analogs of Weyl fermions, featuring gapless bulk states with nontrivial Berry curvature and robust Fermi arc surface states. These materials host unconventional transport properties, including large magnetoresistance, chiral anomaly-induced negative magnetoresistance, and anomalous Hall conductivity, making them an ideal platform for investigating topological responses in metallic systems. The Kagome lattice, a geometrically frustrated network of corner-sharing triangles, provides an intriguing playground for studying strongly correlated electron physics. In magnetic Kagome materials, the interplay between frustration, spin-orbit coupling, and topology gives rise to nontrivial band structures, flat bands, and quantum anomalous Hall states. These characteristics make Kagome systems highly relevant for understanding emergent quantum phases and novel magnetic excitations.

Throughout this thesis, a comprehensive experimental and theoretical investigation of these materials are presented, covering synthesis techniques, structural characterization, and transport measurements. By unifying these innovative concepts, this thesis aims to provide a comprehensive understanding of the intrinsic properties of these systems and their potential to transform technology. The findings presented here contribute to advancing the frontiers of quantum materials and their real-world applications. For a systematic discussion, this thesis has been organized into eight chapters.

In the ***first chapter***, we have discussed the fundamental properties of magnetic topological insulators (MTIs), Weyl semimetals, and kagome lattice materials, focusing on their structural, electronic, magnetic, and transport characteristics. MTI combine nontrivial band topology with magnetism, leading to exotic quantum effects such as the quantum anomalous Hall effect (QAHE), band inversion, and chiral edge modes that are essential for spintronics and quantum computing. Weyl semimetals, on the other hand, host massless Weyl fermions due to band crossings at Weyl nodes, resulting in unique transport signatures such as the chiral anomaly, extremely large magnetoresistance (XMR), and Fermi arc surface states, making them promising for next-generation electronics and sensing applications. Lastly, kagome lattice materials exhibit strong electron correlation effects due to their geometrically frustrated structure, leading to flat bands, anomalous Hall effect, topological Hall effect, skyrmions which are key to understanding strongly correlated quantum matter. The interplay of symmetry, topology, magnetism, and electron interactions in these materials will be explored to establish a foundation for their advanced quantum properties and technological applications.

In ***second chapter***, we provide a comprehensive overview of the synthesis processes used for growing topological insulators (TIs) and Weyl semimetals (WSMs) single crystals, along with the experimental techniques employed for their characterization. We detail the crystal growth methods, highlighting the precise control over stoichiometry and structural quality necessary to achieve high-purity single crystals. Additionally, we discuss the various characterization tools used to analyze the structural, electronic, and magnetic properties of these materials. This chapter also covers the cryogenic techniques integrated into transport and magnetic measurements, including the Physical Property Measurement System (PPMS) and Magnetic Property Measurement System (MPMS), which enable precise studies of electrical resistivity, magnetotransport, and magnetic susceptibility at low temperatures and high magnetic fields. Furthermore, we introduce the fundamental principles of photoemission spectroscopy, with a particular focus on Angle-Resolved Photoemission Spectroscopy (ARPES), which provides direct insights into the electronic band structure and topological nature of these materials. Through this discussion, we establish the key experimental methodologies essential for investigating the exotic quantum properties of TIs and WSMs.

In ***third chapter*** we have discussed the structural, Magnetic, transport and thermoelectric properties of Gd rare earth doped Bi_2Se_3. The presence of magnetic impurities in topological insulators can disrupt their time reversal symmetry and lead to the emergence of an energy gap which has been confirmed by ARPES study. This study delves into the energy band structure and the Kondo effect through the introduction of Gadolinium (Gd) magnetic perturbations (at levels of x = 0.1, 0.16) into a pure Bi_2Se_3 single crystal. Thermoelectric properties are assessed across all prepared samples. The undoped sample displays the highest Seebeck coefficient and power factor values of 398.02 $\mu V K^{-1}$ and 6.83 $mW K^{-2} m^{-1}$, respectively, at room temperature. These values are notably high for thermoelectric applications at room temperature.

In ***fourth chapter*** we focused on Weyl semimetals NbP and TaP, known for their remarkable magnetoresistance (MR) at low temperatures due to charge carrier compensation. We synthesized an intermediate compound, $Nb_{0.5}Ta_{0.5}P$, which also exhibits extremely large magnetoresistance (XMR) at low temperatures. Although its MR% is one order of magnitude lower than that of the parent systems, $Nb_{0.5}Ta_{0.5}P$ demonstrates perfect charge carrier compensation up to 50 K. The magnetoresistance in this compound follows an B^2 dependence and mirrors the classical carrier mobility's temperature dependence. We noticed a deviation from Kohler's rule in both instances, demonstrating the existence of multiple kinds of charge carriers. We conducted an analysis of Shubnikov–de Haas (SdH) oscillations to investigate the Fermi surface evolution and the presence of a nontrivial Berry phase in all three compounds. In $Nb_{0.5}Ta_{0.5}P$, quantum oscillations revealed multiple

Fermi pockets. Additionally, density functional theory (DFT) calculations predicted bulk band structure features near the Fermi level, including band-crossing points. Changes in the density of states between the parent and doped systems were systematically observed, with the inclusion of spin–orbit coupling (SOC) revealing a band gap opening at Weyl node points. The significant enhancement in magnetoresistance observed in $Nb_{0.5}Ta_{0.5}P$ at room temperature suggests promising avenues for exploring similar systems with suitable substitutions to develop new high-performance materials for industrial and spintronic applications.

In ***fifth chapter*** we have discussed $MnBi_2Te_4$, a layered van der Waals magnetic topological insulator, exhibits a strong interplay between magnetism and topological transport phenomena. In its canted antiferromagnetic phase at 2 K, we observe a sizable anomalous Hall effect (AHE) with a maximum Hall resistivity of 14.7 $\mu\Omega.cm$, along with a possible topological Hall effect (THE) contribution of 7.9 $\mu\Omega.cm$. Scaling analysis confirms that the AHE is predominantly governed by the intrinsic Berry curvature mechanism. Magnetocaloric effect (MCE) measurements further reveal pronounced magnetic anisotropy, showing a field driven switch from inverse to conventional MCE along the c axis, while remaining conventional along the ab-plane with a maximum entropy change of 1.6 J/kg·K. These results highlight the strong correlation between spin texture, Berry phase effects, and thermal response, offering valuable insights into the topological and magnetic landscape of canted antiferromagnets.

In ***sixth chapter*** we have synthesized 5% Dy doped MBT (MBDT) and report the finding of a substantial anomalous Hall effect (AHE) and the topological origin of AHE is shown by the scaling study, which shows that the extrinsic skew scattering mechanism dominates. Furthermore, we describe a potential topological Hall effect (THE) contribution of $1.87\mu\Omega cm$ in a canted antiferromagnetic phase at 2 K. Magnetocaloric effect (MCE) data, which shows an unusual switching behaviour. The MCE changes from inverse to conventional along the c-axis as the magnetic field is adjusted, whereas the MCE remains conventional along the ab-plane, with a maximum entropy change of 2.23 J/kg.K along the c-axis which has enhanced by 85% due to Dy doping. The anisotropic MCE behaviour is consistent with the system's magnetic anisotropy and canted spin structure. The interaction of magnetic and transport properties indicates a strong link between spin structure and thermal response, providing insights into topological and magnetic processes in canted antiferromagnetic systems. Our findings open the door to studying magnetotransport characteristics and topological phases in materials with magnetic anisotropy and nontrivial spin patterns.

In ***seventh chapter*** We present a comprehensive study on the magnetic and transport properties of single-crystalline $Fe_{3-x}Ni_xSn_2$ (x = 0, 0.25), focusing on the effects of Ni substitution on magnetic ground states and topological transport behavior. Magnetization measurements reveal that Fe_3Sn_2 exhibits a spin-glass transition $T_{SG} \sim 85$ K, which shifts to ~ 95 K upon Ni doping, indicating enhanced magnetic frustration. High temperature magnetization data show a ferromagnetic transition temperature T_C at ~ 648 K for Fe_3Sn_2, which increases upto 674 K upon Ni doping, suggesting reinforced ferromagnetic exchange. Temperature and field dependent magnetoresistance (MR) studies reveal a crossover from positive MR at low temperatures to negative MR at higher temperatures, with features associated with skyrmion phases. Hall effect measurements display conventional and anomalous components, with a clear topological Hall effect (THE) evident at intermediate fields. Ni doping enhances the topological Hall resistivity by $\sim 19\%$, attributed to stronger Dzyaloshinskii–Moriya interactions and stabilized spin textures. In contrast to pristine, the Ni doped system not only retains the wide temperature stability of the skyrmion phase but also shows a enhanced range of the skyrmion phase from $H_2 \sim 0.5$ T to $H_3 \sim 1.06$ T magnetic fields, which is highly desirable for applications requiring stability against external field perturbations. This work highlights how chemical substitution in kagome magnets can tune magnetic frustration, electronic scattering, and topological transport, offering insight into emergent phenomena in frustrated magnetic systems.

In ***eighth chapter*** we have summarized the contains of the present thesis with a brief glimpse of future studies.