Extended Abstract

The emergence of quantum materials serves the field of condensed matter physics and material science enhancing the possibility to apply such materials in faster quantum computing, memory devices, information technology, and spintronics devices. By quantum materials we mean those, which are impossible to be described by the semiclassical particles and low-level quantum theory. However, these materials exhibit strong electron correlations with either some kind of electric or magnetic order or properties associated with non-generic quantum effects. In the present thesis, I will discuss the electric, magnetic and thermoelectric properties of some specific quantum materials which are basically associated with topological properties. Topological invariance originates with the concept of topology, which is a physical representation of the mathematical term genus. Under the application of an out-of-plane magnetic field, the two-dimensional quantum hall system exhibits insulating nature as bulk due to the localization of electrons, whereas contains conducting surface state as a result of the skipping orbital track of electrons. However, quantum materials with topological protection display a similar metallic surface state without the application of magnetic field and are termed quantum spin hall systems. These surface states are emerging from the band inversion and they are insensitive to nonmagnetic impurities and imperfections. Therefore, these surface states are robust against backscattering as the spins of conduction electrons are locked to their momentum as a consequence of strong spin-orbit coupling and preservation of time reversal symmetry. Due to the strong spin momentum locking and time reversal symmetry protected surface states, such materials have attracted great interest from the scientific community with anticipation of many fascinating phenomena like topological superconductivity, quantum anomalous Hall effect, and three-dimensional Weyl fermions. The Dirac-like dispersion of topological surface states and bulk band gap in three-dimensional topological insulators such as Bi_2Te_3 and Bi_2Se_3 and Sb_2Te_3 have been established theoretically and probed using Angle-resolved photoemission spectroscopy. Many interesting quantum phenomena such as Landau level

splitting, weak anti-antilocalization effect, Aharonov-Bohm oscillations and quantum conductance fluctuations are associated with these topological surface states. Moreover, magnetic doping in topological insulators furnishes another route to study the interconnection between topological surface state and magnetism. The time-reversal symmetry is expected to break with magnetic doping in topological insulators and it may devastate the Dirac-like dispersion revealing interesting properties. However, the creation of magnetic interfaces in confined topological systems like heterostructures of topological insulators and ferromagnetic materials provides a gateway to tune the topological and magnetic properties enhancing their feasibility from an application point of view. On the other hand, Weyl semimetals have also attracted considerable research interest in the research area of quantum condensed matter physics, due to their topological nature, ultra-high mobility of charge carriers and their possible applications in future electronic devices. These materials are recognized as an innovative topological phase of three-dimensional materials, which host conducting surface states along with sets of linear dispersive band crossing points in their bulk, called Weyl nodes. These band touching points are considered to be protected against small perturbations and disorder. However, some ferromagnetic Kagome type Weyl semimetals exhibit Skyrmion-like exotics magnetic order at a particular range of temperature under application of verry small magnetic field. Skyrmions are actually topologically protected spin configurations showing particle-like characteristics providing enormous stability even at nanoscale mostly driven by magnetic anisotropy, geometrical frustrations or exchange interactions. These magnetic nano whirls are demonstrated to be the potential carrier of information in future high-density data storage devices, ultrafast spintronics devices and microwave devices. This thesis is based on the investigation of magnetic and transport properties of different spin-modulated single crystalline topological insulators, magnetic/topological heterostructures and ferromagnetic Weyl semimetals displaying Skyrmion phase. In order to provide a systematic discussion, the present thesis is organized into seven different chapters. The contents of each chapter are summarized below.

In **Chapter 1**, the basic mechanisms of quantum materials have been articulated in detail. The key physical properties like time-reversal symmetry, spin momentum locking, absence of backscattering, quantum spin Hall effect, quantum anomalous Hall effect, band inversion, weak anti localization and the historical progress of topological insulators and Weyl semimetals are discussed. The chapter also deals with the development of two-dimensional and three-dimensional topological insulators and the effect of magnetic fields on them. Lastly, the development of Skyrmion-like magnetic order in ferromagnetic Weyl semimetal is explained. A brief bibliographic survey is covered in the chapter.

In **Chapter 2**, the synthesis processes that have been used to grow single crystalline topological insulators, Weyl semimetals and polycrystalline ferromagnetic materials are discussed along with the detailed thin film fabrication mechanism and optimization using pulsed laser deposition technique. Different experimental tools which have been adapted for the characterization of single crystal samples are addressed in detail. The cryogenic techniques incorporated for transport and magnetic properties measurement such as physical property measurement system and magnetic properties measurement system are discussed. The basic principles of Raman spectroscopy, X-ray photoemission spectroscopy, scanning electron microscopy, and atomic force microscopy is also considered in this chapter.

In **Chapter 3**, we have investigated the density functional theory calculation, temperature-dependent thermoelectric power and Raman spectroscopy of $Bi_{1.9}Dy_{0.1}Te_3$ topological insulator. In this system, discrepancy due to the rare earth ion Dy initiates a Red-shift in Raman active modes in the Bi_2Te_3 topological insulator. Here, the lattice thermal conductivity (κ_L) was evaluated in the Umklapp scattering limit using the temperature dependency of the vibrational phonon modes and was used to evaluate the Figure of merit (ZT) of the system. It has been demonstrated that the estimated Power factor and ZT are very large, confirming the efficiency of $Bi_{1.9}Dy_{0.1}Te_3$ for better thermoelectric and electronic applications. Such immense thermoelectric power value of the corresponding system was further supported by the density functional theory calculation.

In **Chapter 4**, Magnetic impurity induced Bi_2Se_3 single crystals and ferromagnetic/topological layered structures were prepared to compare the structural, electronic, physical and magnetic properties varying the dimensionality of the systems. For instance, the existence of the magnetic impurity potentially diminishes the time-reversal symmetry introducing a finite gap in the vicinity of the Dirac point. The aforesaid phenomenon modifies the topological surface state effectively. Reducing the dimensionality, the interfacial magnetic domains modify the electronic properties of the heterostructure at the layers and interfaces which were probed by in-depth X-ray photoemission spectroscopy analysis through the argon etching technique. Analyzing the depth profile investigation of the heterostructure, we succeed to draw a clear matrix of the layers and interfaces along the cross-sectional plane. Further, the physical and magnetic properties were investigated to enlighten the effect of strain over the confined system to clarify that the magnetic spin-induced inter-layer proximity effect enhances the edge state enormously developing the applicability of such heterostructures with new prospects.

In **Chapter 5**, we have introduced magnetic ordering into the nontrivial system of conventional Topological Insulators by creating magnetic interfaces. In this context, Antimony di-chalcogenide Sb_2Te_3 sandwiched between two thin layers of FeSe was prepared using the pulsed laser deposition technique. The prepared hetero-structure demonstrated good crystallinity along with homogeneous morphology displaying vivacious pyramid-shaped characteristic triangular islands. To comprehend the temperature and magnetic field modulated inter-layer properties of the prepared hetero-structure, transport, magneto-transport and magnetic properties were investigated. These properties establish the signature of the Kondo effect below 15 K, which has been attributed to the antiferromagnetic spin alignment at that temperature range. Around 150 K, longitudinal and transverse resistivity shows the metal-semiconductor transition, which was further elucidated through the anharmonic decay model in vibration phonon modes using Raman spectroscopy. Further, a significant local spin evolution was explored around 475 K by studying the magnetic properties of the system. The temperature dependency of the Raman modes confirmed a spin-phonon coupling initiated by local charge ordering at the proximity of the interface in the prepared hetero-structure.

In **Chapter 6**, the discovery of enormous properties associated with magnetic Skyrmions develops fundamental interests and technological relevancy due to the non-trivial real-space topology accompanying these spiral spin textures. $Co_3Sn_2S_2$ is a well-studied Kagome ferromagnet exhibiting a Skyrmion-like complex magnetic structure concerning a certain temperature and magnetic field. In our present study, we have introduced heavier and larger Selenium atoms by partially replacing Sulphur in $Co_3Sn_2S_2$ to induce chemical pressure on this specific complex spin structure. Most interestingly, it has been demonstrated that the application of chemical pressure enhances the Skyrmion phase range (ΔH-ΔT) as well as the Skyrmion stability in the present system. The temperature variation of anisotropy also suggests the presence of a mysterious magnetic phase just below the magnetic ordering transition. Additionally, the evidence of hidden double glassy states has also been demonstrated from ac-susceptibility data. Further, the existence of the Hopkinson effect associated with the slow spin relaxation near the global transition temperature is also observed in the present $Co_3Sn_2S_2$. However, the structural and magnetic properties of the present system, suggest that $Co_3Sn_2S_{2(1-x)}Se_{2x}$ is a potential candidate to be applied in spintronics devices and information technology.

Chapter 7 contains the summary of the present thesis with a brief glimpse of future studies.