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I dedicate this thesis to my mother, who unfortunately did not stay in this world long enough to see this thesis completed.

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Preface

Topological insulators (TIs) are the exotic class of quantum materials which act as insulator in their bulk but support topological protected conducting surface states. These surface states are emerging from the band inversion and they are insensitive to nonmagnetic impurities and imperfection. 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 (SOC) and preservation of time reversal symmetry (TRS). Due to strong SOC and TRS protected surface states, TIs have attracted great interest of scientific community with anticipation of many fascinating phenomena like topological superconductivity, quantum anomalous Hall effect (QAHE), three-dimensional Weyl fermions, neutral Majorana fermions and magnetic monopole. The Dirac like dispersion of topological surface states (TSS) and bulk band gap in 3D TIs such as Bi_2Te_3 and Bi_2Se_3 and Sb_2Te_3 have been established by using Angle-resolved photoemission spectroscopy (ARPES). Many interesting quantum magnetotransport phenomenon such as weak antilocalization effect (WAL), Aharonov-Bohm oscillations and quantum conductance fluctuations are associated with these TSS. Moreover, magnetic doping in TIs furnishes another route to study the interconnection between TSS and magnetism. The TRS is expected to break with magnetic doping in TIs and it may devastate the Dirac like dispersion. Magnetic TIs have been theoretically recommended to be a platform for realizing magnetic monopole while topological superconductors are suggested to be a podium for Majorana fermions. On the other hand, recently, Weyl semimetals (WSMs) have also been attracted a considerable research interest in research area of quantum condensed matter physics, due to their topological nature, ultra-high mobility of charge carrier and their possible applications in future electronic devices. WSMs are recognized as an innovative topological phase of 3D 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.

This thesis is based on the investigation of magnetic, magnetotransport properties, ARPES and theoretical analysis of 3D TIs and WSMs. In order to provide systematic discussion, present thesis is organized in eight different chapters. The contents of each chapter are summarized below.

In **Chapter 1**, the physics of TIs and WSMs have been articulated in detail. The key physical properties of TIs, like TRS, spin momentum locking, absence of backscattering, topological Hall effect and historical developments of TIs and WSMs are discussed. The chapter also deals with other issues like the concept of Berry phase, Shubnikov-de Haas (SdH) Oscillations, WAL effect, the role of broken symmetry, type-I and type –II WSMs etc. A brief bibliographic survey is covered in the chapter.

In **Chapter 2**, the synthesis processes those have been used to grow TIs and WSMs single crystal samples and different experimental tools which have been adapted for 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 (PPMS) and magnetic properties measurement system (MPMS) are discussed. The basic principle of photoemission spectroscopy such as X-ray photoemission spectroscopy (XPS) and angle-resolved photo emission spectroscopy (ARPES) is also considered in this chapter.

In **Chapter 3**, the magnetotransport and magnetization measurements of $Sb_{1.90}Cu_{0.10}Te_3$ were performed by varying both temperature and magnetic field. The induced antiferromagnetic ordering with Cu doping and the observed quantum oscillation in it indicates that magnetization in $Sb_{1.90}Cu_{0.10}Te_3$ is the bulk property. The non-linearity in Hall data suggests the existence of anomalous and topological Hall effect (AHE and THE). Moreover, electronic band structure calculation supports the existence of Cu spin texture.

In **Chapter 4**, Structural, pressure-dependent resistivity, angle-resolved photoemission spectroscopy (ARPES), X-ray photoelectron diffraction (XPD) and band DFT calculation have been investigated for $BiSbTe_3$ Topological insulator. It has been demonstrated that the Dirac point of the topological surface state (TSS) located exactly at the Fermi level. Additionally, superconductivity emerges under pressure of 8 GPa with a critical temperature of ~2.5 K. With further increase of pressure, the superconducting transition temperature (T_c) increases and at 14 GPa it shows the maximum T_c (~3.3 K). It has also been shown that the surface state remains unchanged under pressure and has been suggested that the origin of the superconductivity is due to the bulk state. The investigation indicates that the $BiSbTe_3$ has robust surface states and becomes superconductor under pressure.

In **Chapter 5**, the different roles of surface and bulk states in $Bi_{1.9}Dy_{0.1}Te_3$ TI have been determined by investigating electronic states, magnetotransport properties, Seebeck coefficient and magnetization. Magnetoresistance attains a huge value ~1500% at 7 Tesla which has been attributed to the robust surface state. Magnetization behavior clearly suggests the existence of an antiferromagnetic state, which is supported by density functional theory calculations. The observed anomalous Hall effect has been established as the contribution from the bulk state. Furthermore, it has been demonstrated that there is no appreciable energy gap at the Dirac point of the topological surface.

In **Chapter 6**, the transport and magnetic properties as well as microscopic electronic properties of Dy doped topological insulator Bi_2Se_3 ($Bi_{1.9}Dy_{0.1}Se_3$) have been examined in detail. It has been demonstrated that Dy doping induces AFM ordering in Bi_2Se_3. It has also been observed that Dy doping opens a surface band gap of ~52 meV at 6.5 K. The transition from AFM to FM occurs at lower temperature, ~ 5 K at ~ 3 T magnetic fields. Furthermore, Dy doping in this Bi_2Se_3 leads Kondo effect and weak localization to weak anti-localization crossover. The μ-SR measurements indicate that the signal measured with magnetization is reflecting the magnetic properties of 2% of the sample. The μ-SR measurements also suggest the AFM ordering in the sample which is important from the application point of view. Experimental findings have also been supported by the theoretical calculations based on density functional theory.

In **Chapter 7**, Magnetotransport properties of NbP, $Nb_{0.5}Ta_{0.5}P$, and TaP WSMs single crystal samples synthesized by the chemical vapor transport (CVT) technique have been investigated. Large polyhedral crystals with dimensions of up to 1.0 mm in size were obtained from the growth process. Large magnetoresistance (LMR) and SdH oscillations have been observed for all three compounds. SdH oscillations analysis suggests the quasiparticle nature of the charge carriers. The band-crossing points in bulk band structure were predicted by DFT calculations in the vicinity of Fermi level.

Chapter 8, this chapter contains the summery of the present thesis with a brief glimpse of future studies.