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It is certified that the work contained in the thesis titled ***"Study of Magnetic and Transport Properties of Some Topological materials"*** by ***Mahima Singh*** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

It is further certified that the student has fulfilled all the requirements of comprehensive examination, candidacy and SOTA for the award of Ph.D. Degree.

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DECLARATION BY THE CANDIDATE

I, ***"Mahima Singh"***, certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of ***"Prof. Sandip Chatterjee"*** from ***"July 2016"*** to ***"December 2021"***, at the ***"Department of Physics"***, Indian Institute of Technology (BHU), Varanasi. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc*., reported in journals, books, magazines, reports dissertations, theses, *etc*., or available at websites and have not included them in this thesis and have not cited as my own work.

Mahima Singh

Date: 31-12-2021
Place: IIT (BHU), Varanasi

Signature of the student
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CERTIFICATE BY THE SUPERVISOR

It is certified that the above statement made by the student is correct to the best of my/our knowledge.

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(Mahima Singh)

I dedicate this thesis to my Brother (Kanishk) and mother (Geeta) for their selfless love.

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Preface

Three-dimensional (3D) topological insulators are a new state of quantum matter characterized by nontrivial bulk band topology. The nontrivial state originates from band inversion. In the Brillouin zone, there are some time-reversal invariant points at which band inversion occurs due to spin-orbit coupling. Topological insulators have insulating bulk and conducting surface states with a Dirac-cone-like dispersion. In 3D topological insulator surface state possess an odd number of massless Dirac cone. The Dirac crossing point is protected against small perturbations by time-reversal symmetry, which leads to a variety of effects. The gapless surface state of TI gives novel phenomena such as the Quantum spin hall effect, a large value of Magneto-resistance, and another interesting quantum phenomenon such as weak antilocalization (WAL). Such exotic properties of TIs make them the future of next-generation spintronic devices.

The surface state of a topological insulator remains unaffected from nonmagnetic dopants or defects but can be modified by breaking time-reversal symmetry (TRS). On introducing magnetism in a topological insulator, Time reversal symmetry can be broken, which leads to the new path of magnetic monopoles, quantum anomalous Hall effect, and novel magnetoelectric quantum states. The possibility of topological superconductivity, Majorana fermions, and exciton condensation in TIs are fascinating. The Dirac cone-like dispersion of topological surface state (TSS) in Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 have been studied using Angle-resolved photoemission spectroscopy (ARPES). Quantum magnetotransport phenomena such as WAL, Shubnikov-de Hass (SdH) oscillations, Aharonov-Bhom oscillations are associated with the surface states. However, it is very difficult to differentiate between the bulk and surface state. Besides the TSS, the bulk states in Bi2Se3 are of great

interest as their spin splitting is found to be twice the cyclotron energy observed in quantum oscillation.

The present thesis is focused on the magnetotransport, ARPES, the thermoelectric study of pure and doped Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 TIs. This thesis contains the study of $Bi_{2-x}M_x(SeS)_3$ indicates that surface magnetic ordering may or may not break the time-reversal symmetry (TRS). In contrast, bulk magnetic ordering breaks the TRS suggesting the potentiality of these materials for spintronic application. The angle resolved photo-emission spectroscopy (ARPES) study and magneto-transport properties of $Bi_2Cu_xTe_{3-x}$ have been investigated. In $Bi_{1.5}Sb_{0.5}Te_{1.3}Se_{1.7}$ system, Both the positive magnetoresistance (p-MR) and negative magnetoresistance (n-MR) under perpendicular magnetic field as well as a change-over from Weak Anti Localization (WAL) to Weak Localization (WL) are observed. For a systematic discussion, this thesis has been organized into six chapters.

In **Chapter 1,** 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 etc. A brief bibliographic survey is covered in the chapter.

In **Chapter 2**, the synthesis processes that have been used to grow TIs and WSMs single crystal samples and 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 (PPMS) and magnetic properties measurement system (MPMS) are

discussed. The basic principle of photoemission spectroscopy, such as angle-resolved photoemission spectroscopy (ARPES) is also considered in this chapter.

In **chapter 3,** The Hall effect, angle-resolved photoemission spectroscopy (ARPES) and magnetization of $Bi_{2-x}M_x(SeS)_3$ (with M=Fe, Mn) have been investigated. In Fe doped $Bi_2(SeS)_3$, the presence of both the electron-mediated RKKY coupling and carrier-independent van Vleck magnetism have been demonstrated. On the other hand, in Mn-doped sample, hole-mediated RKKY coupling is observed. The result from the DFT calculation also supports this experimental interpretation. Furthermore, both ARPES and magnetic studies indicate that surface magnetic ordering may or may not break the time-reversal symmetry (TRS), whereas bulk magnetic ordering breaks the TRS. This observation suggests the usefulness of TI-based devices for spintronics.

In **Chapter 4**, the ARPES and magneto-transport properties of $Bi_2Cu_xTe_{3-x}$ single crystals have been investigated. ARPES study indicates the clear existence of surface states in the as-prepared samples. The band gap for x=0.03 is ~5 meV, and that for the x=0.15 sample, the value is ~16 meV. The presence of Cu introduces magnetic ordering in Bi_2Te_3which is clear from magnetic measurement. The occurrence of anomalous Hall effect is not due to the magnetic ordering but due to the 2D transport as is clear from SdH oscillation and from ARPES result.

In **Chapter 5**, the Single-phase and single-crystalline nature of the samples were established from XRD and Laue's diffraction patterns. The insulating character has been confirmed from resistivity analysis which is a consequence of the reduction in anti-site defects with sulphur doping. Furthermore, both p-MR and n-MR have been found on account of crossover from WAL to WL. From the ARPES measurement, it has been observed that on

increasing the doping concentration of sulphur, the gap is closed at the DP and DP lifts upwards. Overall, the role of sulphur doping is becoming very interesting.

In **Chapter 6**, the electron-phonon interaction plays a vital role in the transport properties of Fe and S doped Bi_2Se_3. After doping magnetic elements, the surface state still exists and provides unsaturated linear Magneto-resistance from which we calculated SdH oscillation. Resistivity, Thermoelectric study and Raman study of these samples supports the role of electron-phonon interaction in the transport properties.

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