

Table of contents

| | |
|--|-------------|
| List of figures | xxix |
| List of tables | xlvi |
| Nomenclature | xlvi |
| 1 Introduction | 1 |
| 1.1 Topological Insulator | 2 |
| 1.1.1 Topology | 2 |
| 1.1.2 Time Reversal Symmetry (TRS): | 4 |
| 1.1.3 Hall Effect: | 6 |
| 1.1.4 Band Inversion: | 15 |
| 1.1.5 Concept of Berry Phase: | 17 |
| 1.1.6 Magnetoresistance: | 18 |
| 1.1.7 Shubnikov–de Haas Oscillations: | 20 |
| 1.2 Weyl Semimetals (WSMs) | 21 |
| 1.2.1 Chiral anomaly and chirality: | 23 |
| 1.2.2 Broken symmetry: | 24 |
| 1.2.3 Different types of Weyl Semimetal: | 25 |
| 1.3 Kagome Lattice Materials | 26 |
| 1.4 Skyrmions: | 26 |

| | | |
|----------|--|-----------|
| 1.4.1 | Types of Skyrmions: | 28 |
| 1.5 | Objective of Present Thesis: | 29 |
| 2 | Synthesis and Experimental Techniques | 31 |
| 2.1 | Introduction | 31 |
| 2.2 | Material Synthesis Techniques | 32 |
| 2.2.1 | Flux method: | 32 |
| 2.2.2 | Chemical vapour transport: | 33 |
| 2.2.3 | Melt Growth Method: | 33 |
| 2.3 | Experimental Characterization Tools | 34 |
| 2.3.1 | X-Ray Diffraction (XRD) | 34 |
| 2.3.2 | Energy Dispersive X ray Spectrum: | 37 |
| 2.3.3 | High Resolution Transmission Electron Microscopy(HR-TEM): | 39 |
| 2.3.4 | X ray Photo Emission Spectroscopy (XPS): | 41 |
| 2.3.5 | Angle Resolved Photoemission Spectroscopy (ARPES): | 43 |
| 2.3.6 | Transport Property Measurements: | 45 |
| 2.3.7 | Thermoelectric Measurements: | 49 |
| 2.3.8 | Magnetic Property Measurement System(MPMS): | 50 |
| 3 | Coexistence of Kondo effect and non trivial Berry phase in Gd doped Bi₂Se₃: | |
| | An ARPES and Magneto-transport study | 57 |
| 3.1 | Introduction | 57 |
| 3.2 | Experimental details | 60 |
| 3.2.1 | Synthesis | 60 |
| 3.2.2 | Characterizations | 61 |
| 3.3 | Results and Discussions | 61 |
| 3.3.1 | XRD Analysis | 61 |

| | | |
|----------|---|------------|
| 3.3.2 | Magnetic Study | 62 |
| 3.3.3 | ARPES Study | 65 |
| 3.3.4 | Resistivity Analysis | 68 |
| 3.3.5 | Hall and Thermoelectric Study | 71 |
| 3.3.6 | Magnetoresistance | 76 |
| 3.3.7 | SdH Oscillation Study | 79 |
| 3.4 | conclusion | 84 |
| 4 | Extremely Large Magnetoresistance with coexistence of nontrivial Berry Phase in $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$: An Experimental and Theoretical Study | 85 |
| 4.1 | Introduction | 85 |
| 4.2 | Experimental Details | 88 |
| 4.3 | Computational Details | 88 |
| 4.4 | Results and Discussions | 89 |
| 4.4.1 | Structural analysis | 89 |
| 4.4.2 | Resistivity | 91 |
| 4.4.3 | Magnetoresistance | 94 |
| 4.4.4 | Hall Study | 99 |
| 4.4.5 | SdH Oscillation Study | 101 |
| 4.5 | Computational results | 109 |
| 4.6 | Conclusion | 113 |
| 5 | Berry Phase dominant Topological Transport and Anisotropic Magnetocaloric Effects in MnBi_2Te_4 | 115 |
| 5.1 | Introduction | 115 |
| 5.2 | Experimental Section | 118 |
| 5.3 | Results and Discussions | 118 |

| | | |
|----------|---|------------|
| 5.3.1 | Structural Characterisation | 118 |
| 5.3.2 | Magnetic study | 120 |
| 5.3.3 | Hall Study | 122 |
| 5.3.4 | Magnetoresistance | 127 |
| 5.3.5 | Magnetocaloric Study | 133 |
| 5.4 | Conclusion | 139 |
| 6 | Impact of non-collinear spin texture on Topological Transport and Magnetocaloric effect in Dy-Doped MnBi_2Te_4 Magnetic Topological Insulator | 141 |
| 6.1 | Introduction | 141 |
| 6.2 | Experimental Details | 144 |
| 6.3 | Results and Discussions | 144 |
| 6.3.1 | Structural Analysis | 144 |
| 6.3.2 | Magnetic study | 146 |
| 6.3.3 | Transport Study | 148 |
| 6.3.4 | Magnetocaloric Study | 151 |
| 6.3.5 | Phase diagram | 156 |
| 6.4 | Conclusion | 157 |
| 7 | Ni-Induced Enhancement of Chiral Spin Textures and Topological Hall Response in Fe_3Sn_2 | 159 |
| 7.1 | Introduction | 159 |
| 7.2 | Experimental Details | 162 |
| 7.3 | Results and Discussions | 162 |
| 7.3.1 | Structural Analysis | 162 |
| 7.3.2 | Magnetic study | 163 |
| 7.3.3 | Transport Study | 167 |

| | | |
|----------|--|------------|
| 7.3.4 | Ac susceptibility and Phase diagram: | 177 |
| 7.4 | conclusion | 178 |
| 8 | Summary and Future prospective | 181 |
| 8.1 | Summary | 181 |
| 8.2 | Future Perspectives | 184 |
| | References | 191 |

List of figures

| | | |
|-----|--|---|
| 1.1 | (a) A visual representation of a continuous deformation (homeomorphism) showing how a doughnut-shaped object can be smoothly transformed into the shape of a mug, and vice versa, without cutting or gluing. (b) Classification of geometric objects according to the number of holes they contain. For instance, an object with a single hole, like a torus, is categorized as having genus 1 (Burchardt (2022)). | 3 |
| 1.2 | (a) Illustration that an electron with an electric dipole moment violates time reversal symmetry. (b) Schematic of protected and broken time reversal symmetry (Rushchanskii et al. (2010)). | 5 |
| 1.3 | (a) Schematic of Hall effect measurement (b) plot of longitudinal and transverse resistivity with field (Rushchanskii et al. (2010)). | 7 |

- 1.4 (a, b): Illustrations of the density of states (DOS) resulting from Landau level formation in two different systems are shown. In a conventional two-dimensional electron gas (2DEG) (a) Landau levels appear as equally spaced energy states. In contrast, in systems hosting massless Dirac fermions (b) such as graphene, the energy levels scale as the square root of the Landau index n , leading to an uneven spacing of the levels. (c) Representation of the QHE under a strong magnetic field. Here, the black circular paths signify cyclotron motion of electrons localized due to the Lorentz force. The red arrows indicate chiral edge states that enable dissipationless current flow along the boundaries of the sample. (d) Depiction of Landau level evolution in the presence of a magnetic field, illustrating how longitudinal resistance and Hall resistance vary with increasing magnetic field strength, highlighting the characteristic plateaus and minima associated with QHE. (Fei et al. (2020), <https://www.physicsforums.com/threads/quantum-hall-effect-resistivity.811032/>). 10
- 1.5 (a–d) Conceptual illustration of the Quantum Spin Hall (QSH) effect in topological insulators. (e) (Color illustration) Depiction of helical edge states characteristic of a Quantum Spin Hall insulator (QSHI). The diagram shows the boundary between a QSHI and a conventional (trivial) insulator, where spin-polarized electrons travel along the edge. In the case of the graphene based model, spin up and spin down electrons move in opposite directions along the edges, demonstrating spin-momentum locking (Hasan & Kane (2010)). 11

1.6 (a): Illustration of the Anomalous Hall Effect (AHE). In the presence of spontaneous magnetization along z axis (M_z) electrons with opposite spin orientations experience different transverse (anomalous) velocities due to spin orbit interaction. This results in an asymmetric distribution of charge carriers across the sides of the material, producing a measurable Hall voltage (V_y) even without an external magnetic field. (b) Conceptual diagram showing the two primary origins of the AHE: the intrinsic mechanism, arising from the Berry curvature of the band structure, and the extrinsic mechanisms, which include skew scattering and side-jump processes caused by impurity scattering. (Weng et al. (2015); Zhu & Zhao (2017)). 15

1.7 (a) One origin of the Topological Hall Effect (THE) arises from a non-coplanar spin configuration at the atomic scale. The schematic illustrates three neighboring spins S_i , S_k , and S_l forming a finite solid angle Ω , which generates an emergent magnetic field acting on conduction electrons. (b) Another source of THE is related to the real-space topology of the spin texture. In systems hosting skyrmions or skyrmion bubbles, the swirling spin structure leads to asymmetric deflection of spin-polarized electrons, contributing to a transverse voltage. The inset presents the spatial variation of the out of plane magnetization M_z along the in plane x direction, illustrating the internal structure of these textures.(c) Experimental plot showing the variation of topological Hall resistivity as a function of the applied magnetic field, highlighting the presence of THE in a specific field window (He et al. (2022)). 16

-
- 1.8 (a–c) Conceptual representation of a topological phase transition. The sequence shows the transformation of the electronic band structure from a conventional insulating state (a) progressing through a gapless Dirac semimetal state (b) and eventually reaching a topological insulator phase (c) where band inversion occurs due to strong spin orbit coupling.(Yaji et al. (2024)). 17
- 1.9 (a) The real space picture of electron’s orbit (b) Formation of the Dirac cone due to SOC in momentum space (c) Berry phase and change in electron’s wave function in its rest frame (Manoharan (2010)). 19
- 1.10 (a, b) Schematic diagram of anisotropic magnetoresistance (AMR).(b) Schematic of four probe measurement of MR (Yang & Zhang (2021)). . . 19
- 1.11 Schematics of the topological insulator and Weyl semimetal. (a) A TI exhibits an energy gap with a band inversion. Topological surface states exhibits Dirac-cone-type dispersion with spin texture. (b) A WSM is gapless in the bulk and a pair of Weyl points (band crossing points) exists with opposite parity. Nonzero Chern number (c) Schematics of Dirac point splitting into separated Weyl points upon breaking TRS and IS (Sun et al. (2015)). 23
- 1.12 types of Weyl semimetal (a) Type I weyl semimetal (b) Type II weyl semimetal (Rodriguez-Lopez et al. (2020)). 25

- 1.13 (a) The kagome lattice is a two-dimensional structure composed of corner-connected triangles, often likened to the shape of a ‘David star’ or traditional Japanese basket-weaving motifs. (b) This lattice possesses unique symmetry properties that give rise to two contrasting electronic features: massless Dirac fermions with zero effective mass, and completely flat energy bands with no dispersion, corresponding to infinitely heavy quasiparticles. (<https://scattering.areas>). 27
- 1.14 (a) In a Bloch type skyrmion, spin orientations twist within planes that are tangential to concentric circles around the core—meaning the spins rotate perpendicular to the radial direction as one moves outward from the center. (b) For a Néel type skyrmion, spins rotate within radial planes, aligning from the center outward in a pattern resembling spokes on a wheel. Cross sectional views of the spin textures are shown for both types, illustrating their distinct vortex structures (Kézsmárki et al. (2015)). 28
- 1.15 (a, b) Illustrations of Néel type (a) and Bloch type (b) skyrmions, where the magnetization transitions from pointing downward at the core to aligning upward at the edge, consistent with the surrounding uniform magnetic field. This behavior mirrors that of Néel and Bloch domain walls, respectively. (c) A skyrmion lattice imaged using spin polarized scanning tunneling microscopy (SP-STM) in a single atomic layer of Fe deposited on an Ir(111) substrate. The color wheel represents the orientation of the in-plane magnetization, and the square unit cell of the lattice has a side length of 1 nm. Grey cones show the full 3D orientation of magnetic moments. (d) Isolated skyrmions detected by the same SP-STM technique in a bilayer of PdFe on Ir(111), highlighting their individual magnetic structure. (Fert et al. (2017)). 29

| | | |
|------|--|----|
| 2.1 | Schematic diagram of sample growth using Flux method (Tsai & Cui (2015)). | 33 |
| 2.2 | (a) Schematic diagram and sealed quartz tube with iodine for CVT. (b) images of grown samples using CVT method. | 34 |
| 2.3 | image of growth of crystals in Muffle furnace with temperature controller | 35 |
| 2.4 | X-ray Diffraction (a) ray diagram and (b) setup | 37 |
| 2.5 | (a) Schematic diagram of Energy dispersive X-ray spectroscopy. (b) diagram depicting capturing the essence of electron liberation in response to incident photons (http://yunus.hacettepe.edu.tr/selis/teaching/WEBkmu396/ppt/Presentations2010/EDXandWX.pdf ; 2017.) | 39 |
| 2.6 | (a, b) Schematic optical diagram of a transmission electron microscope (https://www.sciencedirect.com/topics/materials-science/high-resolution-transmission-electron-microscopy .) | 41 |
| 2.7 | (a) Schematic diagram of XPS setup. (b) Transitions between the core electron from different energy levels (https://www.ulvac-phi.com/en/surface-analysis/xps .) | 43 |
| 2.8 | a) Illustration showing the geometry and basic principles of angle-resolved photoemission spectroscopy (ARPES) measurements. b) Energetics of the photoemission process, in which energy is conserved (Lv et al. (2019)). . | 46 |
| 2.9 | (a) Experimental setup for ρ_{xx} measurement. (b) four probe arrangement for measuring longitudinal resistivity. | 47 |
| 2.10 | Experimental setup for transverse resistivity measurements. | 49 |
| 2.11 | Schematic diagram of sample holder for thermoelectric measurement. Temperature difference at the both ends of the sample creates a temperature gradient. | 50 |
| 2.12 | (a) Schematic diagram of SQUID-VSM detection system. (b) Photograph of actual QD-MPMS measurement system (Yildirim (2016)). | 55 |

- 3.1 (a) XRD pattern of $\text{Bi}_{2-x}\text{Gd}_x\text{Se}_3$ ($x=0, 0.1, 0.16$) single crystals along (00L) plane. (b) EDX spectra and atomic percentage of (a) Bi_2Se_3 (c) $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ (d) $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$ single crystals. 62
- 3.2 (a) Magnetic susceptibility vs temperature plot for 5% and 8% Gd doped Bi_2Se_3 . Inset shows the paramagnetic ordering of the doped samples at room temperature. (b) Variation of Magnetic moment with magnetic field for pure and doped samples at 2K. The inset shows the Ferromagnetic ordering present at low field. 65
- 3.3 (a) ARPES spectra of $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ and (b) $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$ single crystal. Energy distribution curve fitting (EDC) of (c) $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ and (d) $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$ single crystal. 67
- 3.4 (a) Resistivity vs temperature plot for Bi_2Se_3 and $\text{Bi}_{2-x}\text{Gd}_x\text{Se}_3$ ($x=0.1, 0.16$) single crystals. Inset shows Variation of electrical conductivity with temperature for pure and doped samples. (b) Fitted Resistivity vs temperature plot for Bi_2Se_3 . Inset shows the enlarged view of T^2 fitting. (c) Fitted curve of Resistivity vs temperature plot for $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$. Inset shows Kondo fitting at low temperature. (d) Fitted Resistivity vs temperature plot for $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$. Inset shows the enlarged view of T^2 fitting. Red line shows fitting curve for all three samples. 71
- 3.5 Variation of fitted Hall resistivity with magnetic field for (a) Bi_2Se_3 (b) $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ (c) $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$. (d) shows the variation of carrier concentration with temperature for all three samples. (e) The variation of mobility with temperature for all three samples. (f) Variation of Seebeck coefficient with temperature for all Bi_2Se_3 and $\text{Bi}_{2-x}\text{Gd}_x\text{Se}_3$ ($x=0.1, 0.16$) single crystals. Inset shows variation of Power Factor with temperature for all as grown samples. 73

| | | |
|-----|--|----|
| 3.6 | Variation of Magnetoresistance with magnetic field at different temperatures for (a) Bi_2Se_3 (b) $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ (c) $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$ | 77 |
| 3.7 | Variation of SdH oscillations with inverse magnetic field at low temperatures for (a) Bi_2Se_3 (b) $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ (c) $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$ single crystals. Insets of each plot show the FFT variation at different temperatures. (d, e, f) Landau levels fan diagram for Bi_2Se_3 , $\text{Bi}_{1.9}\text{Gd}_{0.1}\text{Se}_3$ and $\text{Bi}_{1.84}\text{Gd}_{0.16}\text{Se}_3$ single crystals at 2K. (g, h, i) Lifshitz-Kosevich (LK) fitting on temperature dependent amplitude of the SdH oscillation for all the prepared crystals. Insets show Dingle damping plot with respect to inverse magnetic field for all Bi_2Se_3 and $\text{Bi}_{2-x}\text{Gd}_x\text{Se}_3$ ($x=0.1, 0.16$) single crystals. | 81 |
| 4.1 | (a) Rietveld refinement of powder XRD for all grown single crystals. TEM images of (b,c,d) TaP, (e,f,g) $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$, (h,i,j) NbP. (k) Resistivity variation with respect to temperature for $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ (Blue), NbP (Black) and TaP (Red) fitted with power law (dark Red). Inset: optical image of single crystals. | 90 |
| 4.2 | EDX spectra of (a) NbP (b)TaP and (c) $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$. (d) colour mapping of $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ | 91 |
| 4.3 | Resistivity as a function of temperature at different applied magnetic field for (a) NbP (b) TaP (c) $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$. Inset shows $\frac{\partial \rho}{\partial T}$ vs T at different fields for the samples (d) shows the field dependence of T_i and T_m for NbP, TaP and $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ | 93 |
| 4.4 | Plots of $\ln(\rho)$ vs T^{-1} at different magnetic fields for(a) NbP,(b) TaP and (c) $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$. Red lines are the fitted curve used to extract activation energy in the semiconducting region.(d) shows the activation energy estimated for NbP, TaP and $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ | 95 |

- 4.5 The change in magnetoresistance (MR%) with respect to magnetic field strength at various temperatures for (a) NbP (c)TaP and (e) Nb_{0.5}Ta_{0.5}P. Inset shows the MR fitting with the equation $MR = aB^k$ at 2K. Kohler's plot at different temperatures for (b) NbP and (d) TaP (f) Nb_{0.5}Ta_{0.5}P 97
- 4.6 variation of average mobility, μ_{avg} (right axis) from single carrier model and slope of magnetoresistance (left axis) around 7 T field with temperature for (a) NbP,(b) TaP and (c)Nb_{0.5}Ta_{0.5}P. (d) shows the Hall coefficient estimated for NbP, TaP and Nb_{0.5}Ta_{0.5}P from single band model. 98
- 4.7 Variation of Hall resistivity with respect to magnetic field at various temperatures for (a)NbP, (b)TaP and (c) Nb_{0.5}Ta_{0.5}P. 100
- 4.8 σ_{xx} , σ_{xy} and its corresponding Two band model fitting for (a, b) NbP, (c, d) TaP and (e, f) Nb_{0.5}Ta_{0.5}P. 101
- 4.9 The variation of carrier concentration and mobility of charge carrier as a function of temperature for (a, b) NbP, (c, d) TaP and (e, f) Nb_{0.5}Ta_{0.5}P. . 102
- 4.10 (a) SdH oscillations at various temperatures for NbP (b) FFT corresponding to SdH oscillations at different temperatures. Inset shows Lifshitz-Kosevich (LK) fitting on temperature dependent amplitude of the SdH oscillations (c) Lanadau level fan diagram (d) Dingle damping plot with respect to inverse magnetic field for NbP. 103
- 4.11 (a) SdH oscillations at various temperatures for TaP (b) FFT corresponding to SdH oscillations at different temperatures. Inset shows Lifshitz-Kosevich (LK) fitting on temperature dependent amplitude of the SdH oscillations (c) Lanadau level fan diagram (d) Dingle damping plot with respect to inverse magnetic field for TaP. 105

-
- 4.12 (a) SdH oscillations at various temperatures for $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ (b) FFT corresponding to SdH oscillations at different temperatures. Inset shows Lifshitz-Kosevich (LK) fitting on temperature dependent amplitude of the SdH oscillations (c) Landau level fan diagram (d) Dingle damping plot with respect to inverse magnetic field for $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ 107
- 4.13 (a) Total density of state and (b) partial density of states for NbP, (c) total density of states, and (d) partial density of states for TaP. (e) total density of states and (f, g, h) partial density of states for $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ 110
- 4.14 band dispersion of NbP (a) without SOC, and (b) with SOC. band dispersion of TaP (c) without SOC, and (d) with SOC. band dispersion of $\text{Nb}_{0.5}\text{Ta}_{0.5}\text{P}$ (e) without SOC, and (f) with SOC. 111
- 5.1 (a) Single crystal XRD of MnBi_2Te_4 single crystal. (b) Valance band spectra of MnBi_2Te_4 (c) Total XPS survey of the prepared sample. (d) Mn 2p, (e) Bi 4f and (f) Te 3d spectra. (g) EDX spectra and atomic percentage of exfoliated MnBi_2Te_4 single crystal. (h) HAADF-STEM image of MnBi_2Te_4 , (i, j) crystallographic plane of MnBi_2Te_4 (k) Variation of Resistivity with temperature for MnBi_2Te_4 single crystal. 119

5.2 (a) Temperature dependence of magnetic moment for MnBi_2Te_4 single crystal acquired using the ZFC method (left y axis), as well as temperature-dependent inverse magnetic susceptibility (right y axis). The symbol and the red dashed line reflect the experimental data and the Curie-Weiss fit, respectively. The magnetic fields are orientated in plane and (b) Out of plane. M - H curves for the MnBi_2Te_4 crystal at various temperatures. The magnetic field is (c) in plane and (d) out of plane. (e) Field-dependent Ac susceptibility for the MnBi_2Te_4 crystal observed at various temperatures. Inset shows the variation of 1st order derivative of magnetization with field. (f) Variation of Ac susceptibility for the MnBi_2Te_4 crystal with temperature. The shaded area shows the transition temperature T_N 122

5.3 (a) The total Hall resistivity at respective temperatures. (b) Anomalous Hall resistivity with field at different temperatures. (c) Variaton of experimental (green curve) ,calculated (red colour) anomalous Hall resistivity, and topological hall resstivity (deep green colour) with applied magnetic field computed at 2K. (d) The predicted topological Hall resistivity varies with field at different temperatures. The shaded area in (a, b) shows different magnetic phases of prepared MnBi_2Te_4 128

- 5.4 (a) Fitting of the anomalous Hall resistivity and longitudinal resistivity ratio (ρ_{AH}/ρ_{xx}) vs ρ_{xx} data. (b) Linear fitting of $\log_{10}(\rho_{AH})$ vs $\log_{10}(\rho_{xx})$ data. (c) dependence of Hall conductivity on field at various temperatures. Inset shows the fitted high-field Hall conductivity data at 2 K marked by red dotted line. (d) AHC changes with temperature. (e) The AHC changes with longitudinal conductivity. (f) Temperature-dependent variations in the anomalous Hall scaling coefficient S_H . (g) Variation of anomalous hall resistivity (left axis) and magnetic moment (right axis) with field at 2 K. (h) The conventional Hall coefficient varies with temperature. (i) A plot of carrier concentration vs temperature. 129
- 5.5 (a) Variation of longitudinal resistivity with field at various temperatures. (b) MR% over different temperatures. The darker areas in (a, b) depict several magnetic phases of produced MnBi_2Te_4 . (c) SdH oscillations throughout temperatures. The inset displays an FFT matching to SdH oscillations at various temperatures. (d) SdH oscillation at 2 K with associated Landau level fan diagram. (e) Lifshitz-Kosevich (LK) fit for temperature-dependent amplitude of SdH oscillations. The inset depicts the dingle damping plot in relation to the inverse magnetic field. 130
- 5.6 (a, b) Isothermal $M(H)$ loops of MnBi_2Te_4 at $H \parallel c$ and $H \parallel ab$, respectively. Insets show the corresponding Arrot plots. (c, d) The link between magnetic entropy change and temperature in the $H \parallel c$ and $H \parallel ab$ configurations. (e, f) The plot of RCP vs magnetic field for $H \parallel c$ and $H \parallel ab$ configurations. Insets show the FWHM and transition temperature T_N at 5 T. 135

- 5.7 (a, b) The fitting plot for $-\Delta S_{max}$ is as follows: $S_{max} = aH^n$. Upper insets depict the link between n and the magnetic field. The lower insets show the fitted values of ΔS_M with field at various temperatures to determine n at $H \parallel c$ and $H \parallel ab$ configurations. (c, d) The relationship between $\Delta S_M / \Delta S_M^{max}$ and lowered temperature ϕ at $H \parallel c$ and $H \parallel ab$ configurations. 137
- 6.1 (a) Single crystal XRD of Dy doped $MnBi_2Te_4$ single crystal. (b) EDX spectra and atomic percentage of exfoliated MBDT single crystal. 145
- 6.2 (a) Temperature dependence of magnetic moment for 'MBDT single crystal, as well as temperature-dependent inverse magnetic susceptibility in the inset. The symbol and the red dashed line reflect the experimental data and the Curie-Weiss fit, respectively. The magnetic fields are orientated in plane and (b) Out of plane. M - H curves for the prepared crystal at various temperatures. The magnetic field is (c) in plane and (d) out of plane. (e) Field-dependent Ac susceptibility for the MBDT crystal observed at various temperatures. Inset shows the variation of 1st order derivative of magnetization with field. (f) Variation of Resistivity with temperature for the prepared single crystal. 147
- 6.3 (a) The total Hall resistivity at respective temperatures. (b) Anomalous Hall resistivity with field at different temperatures. (c) Variaton of experimental (magenta curve) ,calculated (red colour) Hall resistivity and topological hall resstivity (dotted) with applied magnetic field computed at 2K. (d) The predicted topological Hall resistivity varies with field at different temperatures. The shaded area in (b) shows different magnetic phases of prepared MBDT. (e) Variation of longitudinal resistivity with field at various temperatures. (f) MR% over different temperatures. The darker areas in (e, f) depict several magnetic phases of produced MBDT. 148

-
- 6.4 (a) Fitting of the anomalous Hall resistivity and longitudinal resistivity ratio (ρ_{AH}/ρ_{xx}) vs ρ_{xx} data. (b) Linear fitting of $\log_{10}(\rho_{AH})$ vs $\log_{10}(\rho_{xx})$ data. (c) dependence of Hall conductivity on field at various temperatures. Inset shows the fitted high-field Hall conductivity data at 2 K marked by red dotted line. (d) The conventional Hall coefficient varies with temperature. Inset shows a plot of carrier concentration vs temperature. 151
- 6.5 (a, b) Isothermal M(H) loops of Dy doped MnBi_2Te_4 at $H \parallel c$ and $H \parallel ab$, respectively 153
- 6.6 (a, b) The link between magnetic entropy change and temperature in the $H \parallel c$ and $H \parallel ab$ configurations. (c, d) The plot of RCP vs magnetic field for $H \parallel c$ and $H \parallel ab$ configurations. Insets show The fitting plot for $-\Delta S_{max}$ is as follows: $S_{max} = aH^n$. (e) Temperature dependence of the rotating magnetic entropy change ($-\Delta S_R$) obtained by rotating from the ab plane to the c axis in various applied magnetic fields. (f) Shows the calculated change of specific heat with temperature for $H \parallel c$ configuration. Inset shows the change of specific heat with temperature for $H \parallel ab$ 156
- 6.7 Phase diagram of MBDT for $H \parallel c$ configuration 157
- 7.1 Structural and compositional characterization of $\text{Fe}_{3-x}\text{Ni}_x\text{Sn}_2$ ($x = 0, 0.25$) single crystals. (a, b) X-ray diffraction (XRD) pattern showing sharp (00l) reflections, confirming high crystallinity and preferred orientation along the c-axis. The inset shows the optical image of well-formed hexagonal plate-like crystals. (c) Energy-dispersive X-ray spectroscopy (EDX) spectrum of Fe_3Sn_2 with corresponding elemental quantification (e), showing Fe and Sn with atomic percentages of 58.55% and 41.45%, respectively. (d) EDX spectrum of Ni-doped Fe_3Sn_2 with quantification (f) confirming successful incorporation of Ni with 25% doping concentration. 164

- 7.2 (a, b) Zero-field-cooled (ZFC) and field-cooled (FC) magnetization as a function of temperature at 200 Oe for (a) undoped ($x = 0$) and Ni-doped ($x = 0.25$) samples. (c, d) Isothermal magnetization ($M-H$) loops at various temperatures for $x = 0$ and $x = 0.25$ compositions highlighting ferromagnetic characteristics. (e, f) Temperature dependence of AC susceptibility (χ') at different frequencies for (e) $x = 0$ and (f) $x = 0.25$, confirming frequency-dependent spin-glass freezing temperature (T_{SG}). 166
- 7.3 (a, b) High temperature ZFC as a function of temperature at 200 Oe for (a) $x = 0$ and (b) $x = 0.25$. Sharp magnetic transitions indicate Curie temperatures (T_C) at 648 K for $x = 0$ and 674 K for $x = 0.25$, with an additional magnetic anomaly (T_1) in the doped sample. Insets show dM/dT revealing transition points more clearly. (c, d) Isothermal magnetization ($M-H$) loops at selected high temperatures for (c) $x = 0$ and (d) $x = 0.25$, indicating the evolution of ferromagnetic behavior well above room temperature. 168
- 7.4 Temperature and field-dependent transport properties of $\text{Fe}_{3-x}\text{Ni}_x\text{Sn}_2$ ($x = 0, 0.25$). (a, b) Electrical resistivity (ρ) as a function of temperature (T) for $x = 0$ and $x = 0.25$, respectively, showing metallic behavior with enhanced resistivity upon Ni doping. (c, e) Low-temperature magnetoresistance (MR%) vs. magnetic field ($\mu_0 H$) curves for $x = 0$ and $x = 0.25$, indicating significant field-induced changes in MR, particularly at low temperatures. (d, f) Field-dependent MR% at higher temperatures (150–300 K) for $x = 0$ and $x = 0.25$. Insets highlight the emergence of multiple critical field points (H_1, H_2, H_3), suggesting field-induced electronic phase transitions or magnetic scattering mechanisms. 169

- 7.5 Field dependent Hall resistivity and topological Hall effect (THE) analysis of $\text{Fe}_{3-x}\text{Ni}_x\text{Sn}_2$ ($x = 0, 0.25$). (a, b) Total Hall resistivity (ρ_{xy}) vs. magnetic field ($\mu_0 H$) at various temperatures (5–300 K) for $x = 0$ and $x = 0.25$, respectively. Insets show anomalous Hall resistivity at 150 K. (c, d) Decomposition of ρ_{xy} at 300 K into ordinary Hall (ρ_{cal}), experimental Hall (ρ_{exp}), and topological Hall resistivity (ρ_{THE}) for $x = 0$ and $x = 0.25$. Ni doping results in a significantly enhanced negative ρ_{THE} . (e, f) Isolated topological Hall resistivity (ρ_{xy}^T) as a function of $\mu_0 H$ for a range of temperatures, clearly indicating the presence of THE signatures (highlighted region), more pronounced and negative in the $x = 0.25$ sample, suggesting the emergence of nontrivial spin textures. 172
- 7.6 Comprehensive analysis of the AHE, carrier density, and Hall scaling in $\text{Fe}_{3-x}\text{Ni}_x\text{Sn}_2$ ($x = 0, 0.25$) (a, b) Temperature-dependent scaling of anomalous Hall resistivity normalized by longitudinal resistivity (ρ_{xy}^A/ρ_{xx}) vs. ρ_{xx} for $x = 0$ and $x = 0.25$, respectively, revealing opposite trends. (c, d) Ordinary Hall coefficient (R_0) and corresponding carrier density (n_e) as functions of temperature, showing a sign change and distinct regimes for the doped sample ($x = 0.25$). (e, f) Field-dependent anomalous Hall conductivity (ρ_{xy}) for both compositions over various temperatures; insets highlight anomalous hall conductivity evolution at 300 K. (g, h) showing power-law dependence with exponents $\beta \approx 1.95$ and 2.1, for $x = 0$ and $x = 0.25$ respectively, indicating intrinsic or moderate side-jump mechanisms. (i) Temperature-dependent Hall angle (S_H) for $x = 0$, with inset comparing its behavior in both undoped and doped samples. Green and yellow shaded regions indicate temperature-insensitive plateaus. 175

- 7.7 Identification of topological spin textures and phase evolution in $\text{Fe}_{3-x}\text{Ni}_x\text{Sn}_2$ ($x = 0.25$). (a) Field-dependent real part of AC susceptibility (χ'_{ac}) measured at different temperatures (150–380 K) highlighting multiple anomalies (H_1, H_2, H_3), indicating transitions among distinct magnetic phases. (b) Constructed magnetic phase diagram in the temperature–field (T – $\mu_0 H$) plane illustrating various emergent magnetic states, including spin glass, stripe, nonlinear moments, and ferromagnetism. The central region marked by overlapping topological Hall effect and noncollinear spin configurations reveals a robust skyrmion-like spin texture regime persisting up to high temperature. 178

List of tables

| | | |
|-----|---|-----|
| 3.1 | Carrier concentrations extracted from ARPES and SdH oscillation for all prepared samples | 68 |
| 3.2 | Parameters extracted from Hall experiment and Ioffel-Regel criteria for all prepared samples | 72 |
| 3.3 | Various parameters evaluated from SdH oscillation analysis for $\text{Bi}_{2-x}\text{Gd}_x\text{Se}_3$ ($x=0, 0.1, 0.16$) | 82 |
| 4.1 | Structural parameters evaluated from Rietveld refinement of the powder XRD patterns of the single crystals | 90 |
| 4.2 | EDX analysis in atomic percentage (%) for all prepared samples | 91 |
| 4.3 | Various parameters evaluated from SdH oscillation analysis for NbP | 104 |
| 4.4 | Various parameters evaluated from SdH oscillation analysis for TaP | 106 |
| 4.5 | Comparison between Various parameters evaluated from SdH oscillation analysis for ϵ peak for all three compounds | 108 |
| 5.1 | Various parameters evaluated from SdH oscillation analysis for MnBi_2Te_4 | 127 |

