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Topological Insulating Phase In Some Bulk And Low Dimensional Materials

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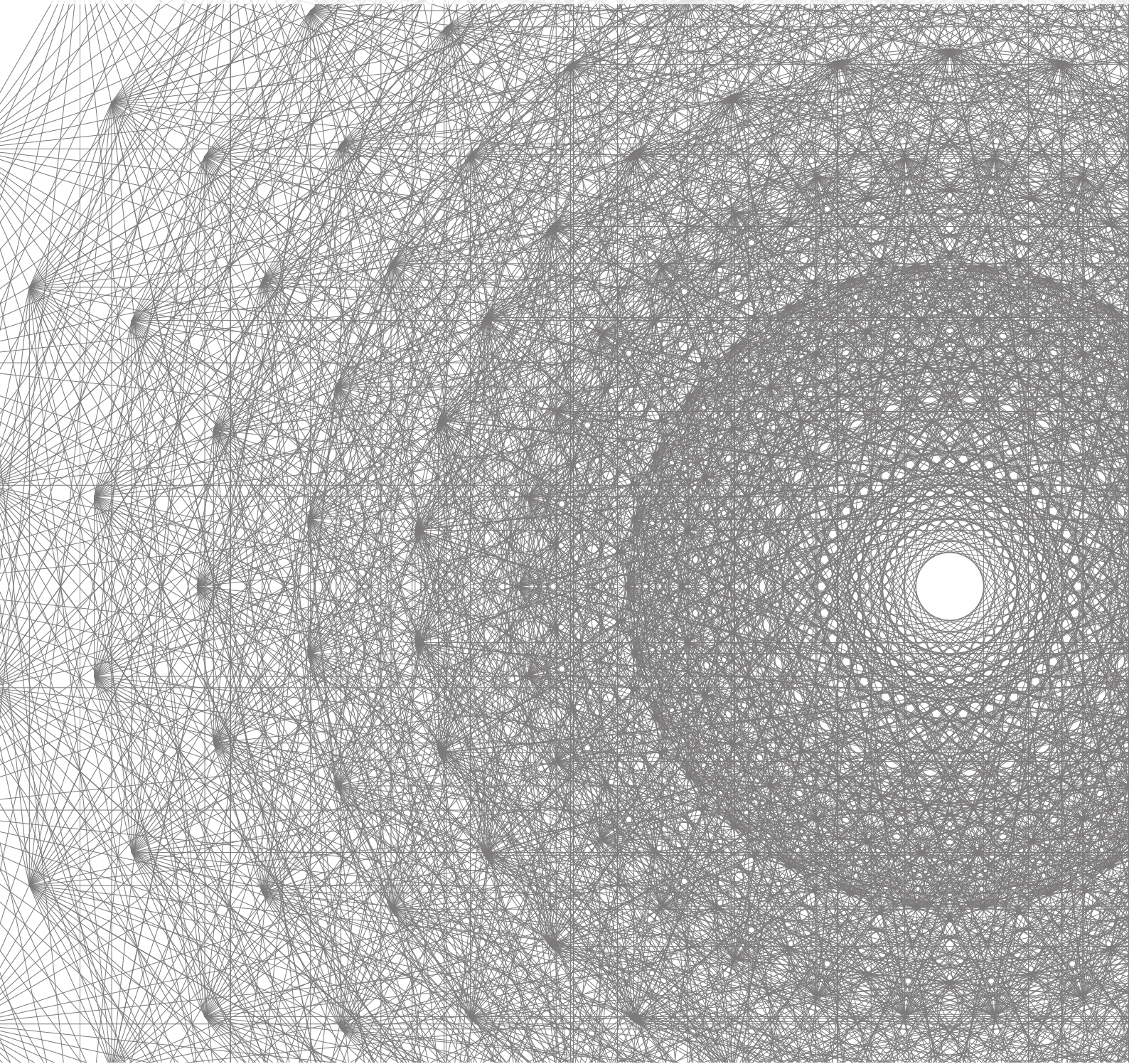
Executive Summary of the Doctoral Thesis, Submitted for PhD in Physics



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Brief Background and Motivation

In the year 2016, David Thouless, Duncan Haldane, and Michael Kosterlitz shared the prestigious Nobel prize for their exceptional and seminal contributions to the field of condensed matter physics wherein they introduced and applied the concepts of topology to periodic systems.[1] They pioneered a different approach to acurately predict ordered phases and phase transitions in thin layered periodic systems.[2–6] This has had far reaching implications in research pertaining to topological insulators (TI), superconductors and other materials with applications in quantum computers, new generations of electronics and superconductors. This mechanism has attained the status of a fundamental theory in condensed matter physics with topological phases identified in chain of atoms (1D), thin layers of atoms (2D) and bulk (3D) periodic systems.[1] Eversince, several materials have been identified to exhibit topological behaviour wherein the material is insulating in D dimensions and conducting in $(D-1)$ dimensions.[7–10]

Initially, the topological properties were theoretically explored in graphene however, it was tough to realise such non-trivial phase at room temperature owing to the weak spin-orbit coupling (SOC) induced band-gap in graphene. Eventually, the first TI material with unconventional topological properties was identified in a system made up of quintuple layered arrangement of atoms, $Bi_{(1-x)}Sb_x$ (with the phase transitions governed by the concentration index 'x').[11] This was followed by observation of unconventional topologies in 2D material made of HgTe/CdTe quantum wells (with the phase transitions governed by the thickness of quantum well).[12] Inspired by these initial investigations, several materials were eventually explored and discovered to exhibit unconventional topological phases. This established a fact that, irrespective of the material class (i.e., 3D or 2D), non-trivial topologies can be realised intrinsically due strong SOC effects which can be expected from heavier elements of the periodic table.

Apart from strong SOC effects, several approaches were introduced to realise the non-trivial phase in 3D materials such as, application of strain/pressure, electric field, doping

etc.[13–15] These techniques were applied to a large number of 3D materials to realise the non-trivial phase/phase transitions. Off these, Half/Full-Heusler compounds stood out due to their multifunctional properties which involved; unconventional topologies, magnetic order, thermal transport properties, superconductivity etc. This is due to the unique valency (which is characteristic feature of Heusler compounds) which can be tuned by varying the chemical compositions under different permutations and combinations of elements from the s, p and d block of the periodic table.[16–19] With an emphasis on strong SOC effects, the search for unconventional topologies was also extended to Heusler compounds with elements from the f block of the periodic table.[20] Apart from ternary/quarternary Heusler compounds, binary compounds (which have inverted band order and are adiabatically connected to bulk HgTe) are also known to exhibit potential TI nature subject to quantum topological phase transitions under strain/pressure.[21]

From the perspective of 2D materials, TI nature is identified by the insulating bulk and conducting edges. Such unconventional behaviour of spin-charge accumulation along the edges is known as the quantum spin hall effect. However, instead of the strong magnetic field (as in quantum Hall effect) the SOC gives rise to quantum spin Hall effect. The magnetic field analogue governing 2D systems is the Berry curvature which indicates sharp changes in the Brillouin Zone (BZ) along the non-trivial bulk gap. 2D TI have promissing room temperature applications as spintronic/valleytronic material, ultra-fast switch etc. subject to existence of large non-trivial bandgap in the entire BZ while the edge is conducting. Systems which exhibit large non-trivial gap have been quite tough to be realised experimentally. However, several efforts have been carried out to realise such materials at room temperature such as, application of strain/pressure, electric field, hetero/homo-structures governed by interlayer van der Waals hybridizations, partial/complete functionalization etc.[22–25]

With this background, we were motivated to explore the non-trivial topological phases and quantum phase transitions in some bulk and low-dimensional materials. In this thesis, we present a thorough and extensive investigation of the TI nature in 3D and 2D

materials along with their applications as thermoelectrics and catalysis. We explored and predicted ternary Half-Heusler (HH) compounds such as, LiMgX (X = Bi,Sb,As) and binary compound such as zincblende AuI for their potential applications as strong 3D TI.[26–29] Their non-trivial TI nature are characterised in terms of band and orbital inversions leading to topological phase transitions followed by classification of the topological class in terms of the $\mathbb{Z}_2$ invariants and ARPES like surface state plots. 2D systems such as, LiMgAs (dimensionally engineered from bulk HH LiMgAs), partially functionalized Tellurium and Selenium and AuI monolayer were explored and predicted for the first time. We found these 2D systems to be large-gap TI systems with potential applications at room temperature.[30, 31] From multifunctional perspectives, we explored bulk AuI (for thermoelectric applications at room temperature) and 2D AuI (for catalytic activity) and LiMgAs (for topological quantum catalysis) for the first time.[29, 31, 32] The results presented in this thesis are quite exciting since we have predicted four large-gap 2D TI and three robust 3D TI materials.

Objectives:

1. To investigate HH compounds; LiMgX (X = Bi,Sb,As) for TI applications.
2. To dimensionally engineer 2D TI from bulk HH LiMgAs.
3. To investigate TI nature and thermoelectric properties of binary zincblende compound AuI.
4. To explore and investigate the effects of partial functionlization of 2D Tellurium and Selenium with respect to TI nature.
5. To investigate dimensionally engineered AuI monolayer for 2D TI nature and catalyic activity.
6. To investigate topological quantum catalysis in 2D TI LiMgAs.

Thesis Outline and Key Findings

Broadly, the thesis is divided into six chapters with the introduction, literature survey, objectives, motivation and methodology discussed in chapters I,II. This is followed by chapters III-V wherein the results of the research are presented in complete detail covering all the aspects in its length and breadth. The brief details of the chapter contents are provided in the following sub-sections.

Chapter I: Introduction

This chapter begins with the introduction to concept of topology and its link to periodic systems in condensed matter theory. This is followed by thorough discussions highlighting the development of the subject and its contemporary status in terms of research and development. This chapter will clearly establish the motivation and objectives (which govern chapters III-V of the thesis) with focus on the bulk and low dimensional materials, emphasising and identifying the existing caveats from the literature.

Chapter II: Methodology

This chapter discusses the origin and development of *first-principles* based density functional theory (DFT) which is the primary tool of investigation employed in this thesis. We begin with the fundamental formulations pertaining to the Kohn-Sham equations which are at the heart of DFT and employed in our computations using Quantum ESPRESSO code.[34] The ground state of a material is computed by employing a typical self-consistency loop presented in Fig. 0.1 below wherein,[33] we begin with an initial guess n(r) of the electronic density and then calculate the corresponding effective/Kohn-Sham potential ($V_{KS}[n]$) which is used in the reduced Schrödinger equation (also known as Kohn Sham equation) to calculate the actual electronic density. This loop continues until a reasonable accuracy is achieved known as self-consistency. We will also discuss in brief other methods such as, density functional perturbation theory (DFPT) (used to

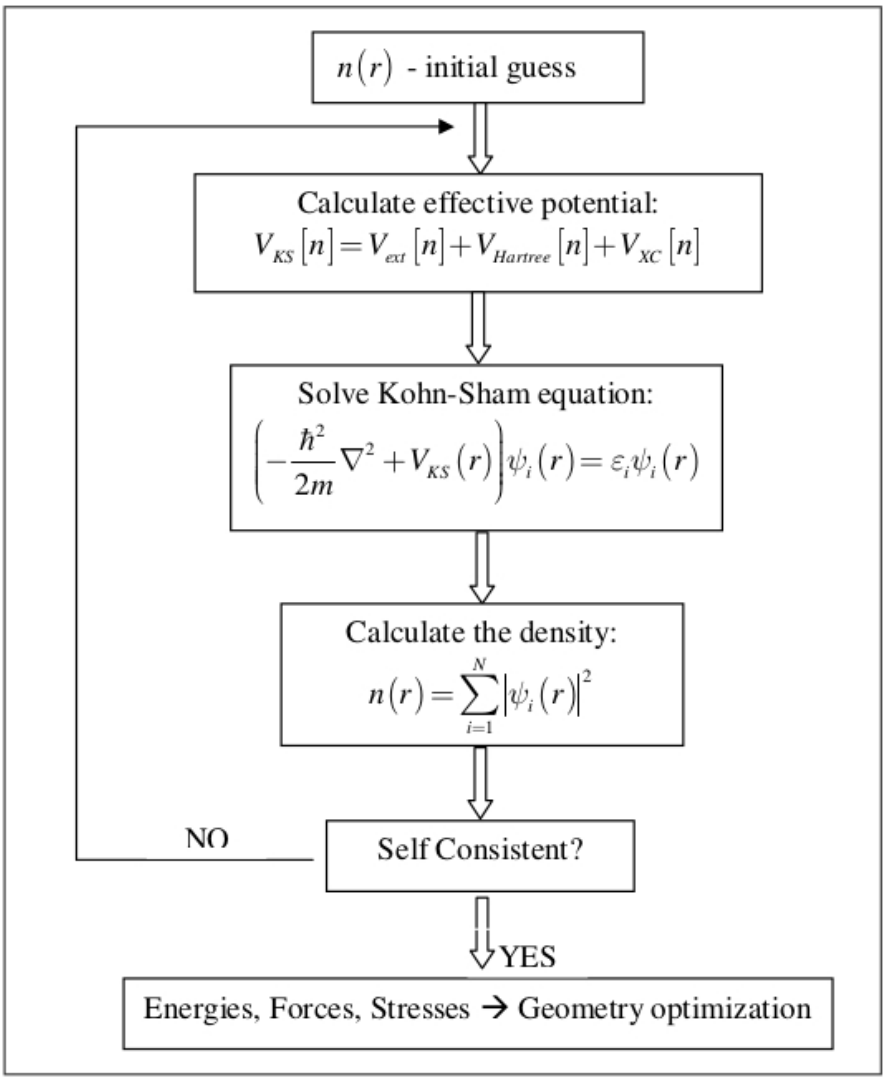

Figure 0.1: A typical self-consistency loop implemented in Quantum ESPRESSO code to compute the ground state of a material by solving the Kohn-Sham equations.[33]

compute and analyse the phonon dynamics), *ab-initio* molecular dynamics simulations (AIMD) (used to assess the structural stability of predicted materials at room temperature), ElaStic code (used to compute the elastic stress tensors to assess the mechanical stability of materials),[35] BoltzTrap code and the ShenBTE code (used to compute the thermoelctric properties of the predicted materials),[36,37] and, maximally localised wannier functions (MLWF) (used to create tight-binding model to investigate TI properties such as, $\mathbb{Z}_2$ invaraints (wherein, for systems without inversion symmetry, the invariants are calculated in terms of the Wanier Charge Centers in the vicinity of the Fermi level

along the two momentum planes in the BZ using Eq. 1 and 2), ARPES-like surface/edge spectra (using the imaginary part of the surface Green's functions (for a semi-infinite system and a dual surface presented in Eq. 3 and 4 respectively) which is calculated using the surface spectrum function $A(k_{||}, \omega)$ presented in Eq. 5), slab band structures etc.) using Wannier90 and WannierTools code.[38, 39]

$$\nu_0 = \Big[\big(\mathbb{Z}_2\big)_{(k_i=0)} + \big(\mathbb{Z}_2\big)_{(k_i=0.5)} \Big] \big(mod 2\big) \tag{1}$$

$$\nu_i = \big(\mathbb{Z}_2\big)_{(k_i=0.5)} \tag{2}$$

$$G_s(k_{||}, \omega) \simeq (\omega - \epsilon_n^s)^{-1} \tag{3}$$

$$\tilde{G}_s(k_{||}, \omega) \simeq (\omega - \tilde{\epsilon}_n^s)^{-1} \tag{4}$$

$$A(k_{||}, \omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} ImTrG_s(k_{||}, \omega + i\eta) \tag{5}$$

Chapter III: Topological Insulating Phase in Bulk Materials

We discuss the origin and background of the topological phases and phase transitions in 3D materials in this chapter. Specifically, we will discuss about HH compounds and present the results of our investigation on TI nature of HH's LiMgX (X=Bi,Sb,As) in the brackdrop of existing relevant literature. We will discuss the effects strain fields in realising non-trivial TI nature in HH. Also, we will discuss the different mechanisms by which TI nature can be realised in binary compound such as AuI. The topological phase transitions will also be qualitatively discussed in terms of the band order and orbital character inversions which are charactertistic to quantum transitions. This will be followed by the quantitative analysis in terms of the $\mathbb{Z}_2$ invariants ($= \nu_0, \nu_1\nu_2\nu_3$) and

ARPES-like surface spectra. Also, we will present and discuss about the stability of the proposed materials in terms of phonon dispersion curves etc.

Key Findings

We presented our investigations of topological quantum phase transitions in bulk materials. We began with Half-Heusler compounds LiMgX (X = Bi, Sb, As); governed by F$\bar{4}$3m space group with face centered cubic structures. LiMgBi was found to be dynamically stable with a direct global gap in the electronic band structure. On applying volume expansion pressure, we observed that at a critical pressure of 4.5% LiMgBi undergoes a topological quantum phase transition governed by *s-p* orbital band inversions with, spin-orbit coupling interactions induced gap of 1.10 meV. The closing and opening of the band gap was verified by using hybrid functional approach apart from the generalised gradient approach. The non-trivial character was verified by computing the surface state spectra which exhibit conducting nature. Also, we computed the $\mathbb{Z}_2$ invariants which were (ν_0, $\nu_1\nu_2\nu_3$) = (1, 0 0 0) which indicated that, LiMgBi is a strong topological insulator. We then presented similar phase transitions in LiMgSb, however, we observed that although LiMgSb presented band gap closing and reopening alongwith exchange of orbitals across Fermi level and conducting surface state spectra but, on computing the $\mathbb{Z}_2$ invariants we found it to be a trivial insulator. Similarly, LiMgAs which was another direct band gap semi-conductor was subjected to pressure. Similar to LiMgSb, this system also presented band gap closing and reopening with exchange of orbital characters across Fermi level and conducting surface state spectra, but on computing the $\mathbb{Z}_2$ invariants we found it to be a trivial insulator like LiMgSb. Although the site 'X' in LiMgX were replaced with members of pnictogen family but, we observed contradicting topological properties. With this we established the necessary and sufficient condition for realising a non-trivial topological insulator i.e., apart from band gap closing and reopening, orbital inversion across Fermi level and conducting surface state spectra, the system should *necessarily* exhibit non-trivial $\mathbb{Z}_2$ invariants. Further, since these systems (LiMgSb, and

LiMgAs) presented topological phase transitions at very high pressures we proposed that, dimensionally engineered monolayers can be realised using these bulk materials to realise non-trivial topological quantum phase transitions at relatively lower pressures.

Another problem in the topological insulator LiMgBi was that, the conduction bands crossed the Fermi level during the topological phase transitions. We addressed this issue by breaking the cubic symmetry and converting the material from a topological conductor to a topological insulator. We presented this phenomena in binary zincblende compound AuI. Although the stability of such a compound has been debated but, on computing phonon dispersion curves, formation energy and elastic tensors we found that, AuI is dynamically, energetically and mechanically stable. We followed two approaches to realise non-trivial topological properties in this binary compound, (i) application of isotropic ompression and (ii) application of uni-axial compressive pressure along [001] crystal direction. We observed semi-metal to topological conductor and topological insulator transitions respectively under the said approaches. We observed that, due to the bulk inversion asymmetry, AuI exhibits Dresselhaus-like band-spin splittings characterized by unconventional s, p-d orbital band inversions. The non-trivial nature was confirmed by computing the conducting surface state spectra and the principle $\mathbb{Z}_2$ invariant which was $\nu_0 = 1$ (when cubic symmetry was retained and broken).

Chapter IV: Topological Insulating Phase in Low-Dimensional Materials

In this chapter we will discuss the origin of TI nature in 2D quantum materials. We will emphasise and discuss effects arising in 2D TI materials in terms of the Berry and spin-Berry curvatures alongside their relevance as an analogue to the magnetic field in quantum spin hall effect. We will discuss in brief; different methods from literature by which non-trivial TI nature can be explored in 2D materials. With this background we will discuss three methods (such as, dimensional engineering, application of stress/strain and partial functionalization) by which non-trivial TI nature is realised in 2D materials LiMgAs, AuI, Tellurene and Selenene. We will discuss the TI nature in terms of the qualitative

and quantitative analysis (similar to that in chapter III) wherein we will present the non-trivial band and orbital inversions, unconventinaly Berry and spin-Berry curvature behaviour (at specific points in the BZ), quantum conductivity, $\mathbb{Z}_2$ invariant (ν), ARPES-like egde state spectra and slab band structures. Apart from this, we will also discuss in short various routes to synthesize the proposed 2D materials. Also, we will present and discuss about the stability of the proposed materials in terms of phonon dispersion curves, AIMD etc.

Key Findings

We presented our investigations on the dimensional engineering of non-trivial two dimensional topological insulator LiMgAs from trivial bulk parent. As expected, this system presented non-trivial topological quantum phase transitions at low pressure due to quantum confinement effects and large surface-volume ratio. The proposed monolayer of LiMgAs was found to be dynamically stable with absence of negative phonon frequencies in the entire brillouin zone. Also, the non-trivial phase of LiMgAs monolayer exhibits unconventional Fermion velocities along different directions of the brillouin zone. The non-trivial topological phase transition in this system is characterised by s-p orbital inversions across the Fermi level accompanying the inversion in band dispersions. This system is proposed to exhibit room temperature applications owing to large-gap induced by spin-orbit interactions. Also, we compared the band inversion strength which is stronger as compared to the bulk parent, indicating towards the underlying quantum confinement effects. We finally confirmed the non-trivial nature by computing the $\mathbb{Z}_2$ invariant which was $\nu = 1$ and edge state spectra indicating a conducting Dirac dispersion along the edge brillouin zone path.

To further increase the non-trivial gap solely due to spin-orbit interactions i.e., without applying strain, we explored functionalization technique. We presented, elemental monolayers of Tellurium and Selenium for the first time. According to previous reports in literature, we too observed that, the free-standing elemental monolayers are dynamically

unstable. However, on partially functionalizing these monolayers with oxygen and sulphur (since, they would form bonds due to mutually favourable electronic configurations) we observed that TeO, SeS and SeS were dynamically stable except TeS. These stable monolayers were then explored for their electronic properties and we found that both, TeO and SeS present are large-gap systems under the influence of spin-orbit interactions. On inclusion of spin-orbit interactions we observed s-p orbital inversions across the Fermi indicating towards potential non-trivial character of TeO and SeS. The effect was attributed to orbital filtering effects which saturate the dangle bonds (originating from the pz-orbitals) in z-direction giving rise to extra degrees of freedom to the electrons. This was confirmed by plotting the π and σ orbital projected band structures. We performed in depth analysis of TeO since it exhibited highest non-trivial gap under spin-orbit interactions of 0.365 eV. We presented the Berry curvature and spin-Berry curvature analysis of TeO in the non-trivial regime under the influence of spin-orbit interactions. From the analysis we observed that, TeO can be used for spintronic and valleytronic applications, due to the opposite Lorentz forces acting on the electrons which leads to the spin-charge accumulation along the edges. This was presented in terms of the spin-projected electronic band structure along the two valleys points in the brillouin zone. The large-gap induced due to spin-orbit interactions also leads to unconventionally high spin Hall conductivity in the global gap (which was observed to be superior to several other materials). From experimental perspective, we also presented the investigations of quantum well hBN/TeO/hBN which was found to retain the large-gap due to spin-orbit interactions under a tensile strain of 14%. These computations were followed by computing the edge state spectra of TeO and SeS. Clearly, TeO and SeS presented Dirac dispersions along the edge brillouin zone path. Also, we presented that the spin channels along the edges of SeS traverse in opposite directions by plotting the edge spectra along the [100] and [010] crystal directions. Ultimately, we presented the $\mathbb{Z}_2$ invariant which was found to be $\nu = 1$ indicating that, the non-trivial characters are indeed topological in nature and that, TeO and SeS are two dimensional topological insulators.

Similar to the dimensional engineering of LiMgAs from bulk parent, we presented the dimensionally engineered AuI monolayer. We saw that, due to quantum confinement effects, the low dimensional phase exhibits a narrow gap as compared to the bulk parent which exhibits semi-metallic character. The ground state of this system was found to exhibit buckled structure governed by the P3m1 space group rather than $P6_3mmc$ space group. However, in the P3m1 phase, AuI monolayer presented a gap of 14.4 meV, from here we subjected the system to compressive and tensile pressures to mark the topological quantum phase transition boundaries. We found that, the lower boundary was at -2% and the upper boundary was at 4%, within this region, AuI presented non-trivial topological insulating phase in two different structural phases of P3m1 and $P6_3mmc$ with the non-trivial gap as high as 0.113 eV under spin-orbit interactions. The underlying mechanism was found to be unconventional *s*, *p*-*d* orbital inversion mechanism alongwith the inverted band disperions. Also, we presented the inversion mechanism in terms of the exchange of charge densities or electron localisation functions across the Fermi level. To ascertain that, the non-trivial nature persists at the pressure of 3% (where the spin-orbit interactions induced gap is 0.113 eV) we computed the slab band structures and the edge state spectra both of which clearly host the non-trivial Dirac like edge dispersion in the edge brillouin zone. Finally we present the $\mathbb{Z}_2$ invariant and find that it is $\nu = 1$ in the region of -2% to 4% strain.

Chapter V: Energy Applications of Topological Materials

This chapter will focus on multifunctional applications of the 3D and 2D materials proposed in chapters III and IV. We will begin with brief dicussions on the background of the thermoelectric applications of 3D TI materials (specifically in terms of ternary HH compounds) and the implications of their non-trivial topologies on the thermoelectric transport properties. Followed by this, we will discuss the results of the investigation of thermoelectric properties of binary zincblende compound AuI. We will next discuss in brief the catalytic activity of quantum materials towards Hydrogen evolution reac-

tions (HER) in terms of different mechanisms of HER such as Volmer, Volmer-Tafel and Volmer-Heyrovsky. This will be followed by the qualitative and quantitative anaylsis of the catalytic activity of AuI towards HER. We will then establish the relation between the non-trivial topologies and catalysis. The relevant results will be discussed in terms of the qualitative and quantitative analysis of the topological quantum catalysis in 2D LiMgAs.

Key Findings

We presented our computational results wherein, topological insulators were explored for potential energy applications such as, thermoelectrics and catalysis. We presented our computations of thermoelectric transport properties for bulk AuI due to the dense states across the Fermi level and the semi-metallic band dispersion. Due to semi-metallic nature, the electronic mobility was found to be high resulting in a high power factor. Also, we observed strong phonon-phonon scattering which lead to smaller lattice thermal conductivity. We employed the semi-classical Botlzmann transport equations to compute the thermoelectric transport coefficients. We explored the thermoelectric parameters at various temperatures and carrier concentrations. We found that, contrary to several thermoelectric materials which exhibit high figure of merit at higher temperatures, AuI exhibits excellent figure of merit of 0.55 at room temperature which is more useful from practical purposes.

We also presented our investigations on the catalytic activity of AuI monolayer towards hydrogen evolution reaction. The dimensionally engieered AuI monolayer exposes the basal plane containing Au which is a transition metal known for superior catalytic activities. We therefore presented the hydrogen evolution reactions along the basal plane of the two dimensional topological insulator AuI. The basal plane was preferred over the edge sites because, under pristine conditions (i.e., without any strain) the non-trivial gap was found to be 14.4 meV which is far less than the thermal energy at room temperature. Hence, the edge conducting states won't be prominent which implied that, there won't

be significant difference in the catalytic response of the basal plane as compared to the edge plane. We presented various mechanisms by which a hydrogen evolution reaction could occur on the basal plane of two dimensional topological insulator AuI. Based on the adsorption energy and Gibb's free energy values, we conclude that, the basal plane of AuI favours Volmer-Heyrovsky over Volmer-Tafel reaction. Also, the preferred site of interaction would be over Au rather than I since at I the hydrogen atom interacts too strongly. We confirm the evolution of hydrogen molecule by plotting the charge density profiles in 3D.

Similarly, inspired by the latest developments in the field of topological quantum catalysis, we explored two dimensional LiMgAs for topological catalysis favouring hydrogen evolution reaction. We presented the transformation of the hexagonal unit cell into an orthorhombic unit cell by using a rotation transformation matrix. The stability of the proposed system was confirmed by computing ab-initio molecular dynamics simulations. We reiterated the, non-trivial topological quantum phase transitions by presenting the exchange of charge density profiles of bands near the Fermi level. Also, we presented the electronic slab band structure which indicated the edge Dirac semi-metallic nature. This was confirmed by plotting the edge charge densities in for the zig-zag and planar-like nanoribbon configurations wherein, we observed distinct egde charge accumulations. We begin with the computation of catalytic activity on the basal plane of LiMgAs monolayer and found that the system would be ineffecient due to large adsorption energies and Gibb's free energy. Hoever, we observed that, the catalytic activity along the edges was excellent with Gibb's free energy as low as -0.02 eV. This places two dimensional topological insulator LiMgAs into the Sabartiers optimum i.e., near the top of the volcano plot with high exchange current densities. Also, we explored various mechanisms of hydrogen evolution reactions such as, Volmer, Volmer-Tafel and Volmer-Heyrovsky. Off the planar and zig-zag nanoribbon terminations, we found that, the zig-zag nanoribbon configuration facilitated both the mechanisms of hydrogen evolution reaction (i.e., Volmer-Tafel and Volmer-Heyrovsky) whereas, the planar-like nanoribbon configuration facilitates only

Volmer-Heyrovsky reaction. In order to confirm that, such superior catalytic activity is originating from the conducting edge states (due to the topological insulating nature of LiMgAs), we investigated the catalytic activity along the middle regions of the nanoribbon. We found that, the superior catalytic activity is indeed originating due to the conducting edge states and that the results are not a numerical artifact.

Chapter VI: Conclusion and Future Prospects

This chapter will summarise and culminate the results and discussions done in previous chapters in backdrop of the motivation and objectives presented at the onset of this thesis in chapter I. We will metion in brief the key and outstanding features of this thesis accompanied with emphasis and reiteration of the unconventional/exceptional results obtained from our *first-principles* investigations. This summary will be succeeded with discussions on the future prospects and scope for further explorations which might branch-out from the results presented and discussed in this thesis along-side my plans to further explore and investigate topological materials.

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2. "A first-principles Investigation Of Topological Phase Transition In Half-Heusler LiMgSb Driven By Volume Expansive Pressure", **Sattigeri, R. M.** et.al., *AIP Conf. Proc.*, **2265**(1), 030020 (2020)

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