Preface

If I have seen further it is by standing on the shoulders of Giants.

Sir Issac Newton

The work presented in this thesis builds up on the seminal discoveries made by, Prof. David Thouless, Prof. Duncan Haldane and, Prof. Michael Kosterlitz in the field of condensed matter theory for which they were honoured with the prestigious Nobel Prize in Physics in the year 2016. It is based on their work that, the condensed matter physics community got deeper insights into the ordered phase and phase transitions of materials. Thus, pioneering a branch of Topological materials. For the first time, mathematical concept of Topology transcended into the quantum realm of periodic systems; unravelling unconventional physical properties.

The physical property unique to these class of materials is primarily, the insulating character in D dimensions and conducting character in $(D-1)$ dimensions. This translates into, ultra-high carrier mobilities, charge densities, dissipationless transport of Fermions etc. In this thesis, we embark on a journey wherein, we employ, state-of-the-art Density Functional Theory based *first-principles* calculations to investigate the Topological properties and phase transitions in bulk (3D) and low-dimensional (2D and 1D) materials followed by the investigation of their potential applications in the field of Thermoelectrics and Quantum Catalysis. We discover materials as potential candidates for, spintronic, valleytronic, quantum computation and energy applications.

Overall, the thesis is divided into six chapters with three working chapters. We begin by establishing the concept of Topological materials and discuss about the tools used in their investigations thereoff. We begin with investigations of Topological characters of half-heusler

compounds LiMgX (X = Bi, Sb, As) and binary compound AuI in their bulk phase. This is followed by investigation of the low-dimensional phase of the half-heusler and binary compound, alongwith functionalization techniques to realize unconventional physics. These are then followed by the investigations from applications point of view. Finally, the entire thesis is concluded by discussing some future prospects which would proliferate from the present work.