Topological phases of 3D superlattices and 2D materials : theoretical modelling

The exotic physics of topological phases like topological insulators (TIs), topological crystalline insulators (TCIs), quantum spin Hall insulators (QSHIs), Dirac semimetals (DMs), Weyl semimetals (WSMs), and nodal-line semimetals (NDLSMs) have been the subject of extensive theoretical and experimental work over the past few decades. In most cases, symmetries play an important role in protecting the topological phases. One of the simplest and most fundamental of these is the time-reversal symmetry (TRS). The TRS symmetry is broken by inducing magnetism through magnetic doping and creating magnetic heterostructure. Topological materials lacking TRS may exhibit magnetic topological phases such as antiferromagnetic topological insulators, magnetic Weyl, Dirac, and nodal-line semimetals, and quantum anomalous Hall phases. However, it is challenging to find realistic materials that can support exotic topological states. The advancement of nanoscience and nanotechnology, as well as the commercialization of applications like quantum spintronics and quantum communication, demands the discovery of new candidate materials exhibiting exotic behaviors.

In search of new materials as candidates for exotic quantum phenomena, this thesis primarily focus on two different classes of materials-

(i) The topological phases in HgTe-based 3D superlattices: We use ab initio simulations to study the evolution of topological phases as a function of hydrostatic pressure and uniaxial strain in two types of superlattices: HgTe/CdTe and HgTe/HgSe, in our search for materials with three-dimensional flat band dispersions. Isoenergetic nodal lines have been discovered in short-period HgTe/CdTe superlattices, which could host strain-induced three-dimensional flat bands at the Fermi level without doping. There are a wide variety of topological phases in the phase diagram of short-period HgTe/HgSe superlattices. An perfect Weyl semimetal phase is realized in an unstrained HgTe/HgSe superlattice. The superlattice transforms into a small-gap topological insulator with many band inversions when subjected to compressive uniaxial strain.

(ii) The quantum phase of MSi_2Z_4, a new synthetic 2D material (M = Mo, W, and Z = N,P, As): Ultra-thin films of the 2D synthetic material MSi_2Z_4 (M = Mo or W and Z = N, P, and As) are studied for their spin-dependent electronic properties and topological exotic phases for quantum device applications using first-principles modeling. In the 2H phase, while MSi_2Z_4 (M=Mo,W and Z= N or As) monolayers are stacked to form bilayers or bulk, the electronic properties of the resulting material vary depending on its thickness. As a result of spin-orbit coupling (SOC), we observe that the monolayers are semiconductor having a 100 % spin polarization, with the spins locked in opposite directions along an out-of-plane direction at K and K_0, leading to spinvalley coupling. The spin polarization in the bilayer is zero due to the presence of the inversion symmetry. We show that, like in MoS_2 and WS_2 bilayers, an out-of-plane electric field can flip
the bilayers' spin polarization. Moreover, we predict a family of $1T^{'}$ structure MSi_2Z_4 (M = Mo or W and Z = P or As) materials with a switchable large bandgap QSH insulator. A band inversion between the metal (Mo/W) d and p states of P/As is introduced by a distortion in the 2H phase, leading to the creation of spinless Dirac cone states absent of spin-orbit interaction. By including the spin-orbit coupling, a 204 meV hybridization gap opens up at band crossing points, yielding spin-polarized conducting edge states with spin Hall conductivity. Through the application of a vertical electric field, we demonstrate that the inverted band gap can be manipulated, resulting in a topological phase transition from QSH to a trivial insulator with Rashba-like edge states. For the creation of various transistors, the electric field dependent features of 2H and $1T^{'}$ structures could turn out to be extremely useful.

This thesis is a collection of publications related to the topological phase of HgTe-based 3D superlattices and 2D materials MSi_2Z_4 (M= Mo,W and Z= N,P,As).

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