
Contents

Preface	i
Acknowledgements	iii
Contents	v
List of Figures	viii
List of Tables	xiii
1 Introduction	1
1.1 Concepts of Topology	1
1.2 Topology in Condensed Matter	2
1.3 Topology and Quantum Hall Effect	4
1.4 Topological Invariant	6
1.5 Quantum Spin Hall Effect and Beyond	8
1.6 Topological Phenomena in Bulk Regime	10
1.7 Current Status	13
1.8 Scope of the Thesis	14
1.9 Objectives and Thesis Outline	15
Bibliography	19
2 Methods and Formalisms	24
2.1 Many-body Problem	24
2.2 Eigen Function Based Approximations	26
Born-Oppenheimer Approach	26
Hartree Approach	27
Hartree-Fock Approach	28
2.3 Density Based Approximations	29
Thomas-Fermi Approach	29
Hohenberg-Kohn Approach	30
Kohn-Sham Approach	32
2.4 Exchange and Correlation Functionals	34
Local Density Approximation	34
Generalized Gradient Approximation	34

	Hybrid Approximation	35
2.5	Electronic Approximations	36
	Pseudopotentials	36
	van der Waals Corrections	37
2.6	Lattice Dynamics, Elastic Constants and AIMD	38
	Density Functional Perturbation Theory	38
	Elastic Properties	40
	ab-initio Molecular Dynamics	42
2.7	Boltzmann Transport Theory	43
2.8	Topological Properties	45
	Maximally Localised Wannier Functions	45
	Berry Connection and Curvature	47
	Spin Hall Conductivity	47
	Tight-Binding Model	48
	Topological Invariants	49
	Surface States	50
2.9	Computational Packages	51
	Bibliography	54
3	Topological Insulating Phase in Some Bulk Materials	60
3.1	The Case of Half-Heusler' LiMgX (X = Bi, Sb, As)	60
	LiMgBi: Structure and Lattice Dynamics	63
	LiMgBi: Electronic Properties	64
	LiMgBi: Topological Properties	69
	LiMgSb and LiMgAs: Structure and Lattice Dynamics	70
	LiMgSb and LiMgAs: Electronic Properties	71
	LiMgSb and LiMgAs: Topological Properties	74
3.2	The Case of Binary Compound AuI	75
	AuI: Structure, Lattice Dynamics and Stability	76
	AuI: Electronic Properties	79
	AuI: Topological Properties	83
3.3	Conclusion	84
	Bibliography	86
4	Topological Insulating Phase in Some Low Dimensional Materials	92
4.1	Dimensionally Engineered Topological Insulator: LiMgAs	92
	Structure and Lattice Dynamics	94
	Electronic Properties	95
	Topological Properties	98
4.2	Functionalization; a Tool for Large-gap Topological Insulator	99
	Structure and Lattice Dynamics	101
	Electronic Properties	103
	Substrate Effects	105
	Topological Properties	107
4.3	Strain Induced Topological Insulator: AuI	110
	Structure, Lattice Dynamics and AIMD	111
	Electronic Properties	113

Topological Properties	115
4.4 Conclusion	116
Bibliography	119
5 Energy Applications of Bulk and Low Dimensional Topological Materials	124
5.1 Thermoelectric Applications of Bulk Topological Insulator: AuI	124
Structure and Lattice Dynamics	126
Thermoelectric Transport Properties: Lattice Contribution	128
Thermoelectric Transport Properties: Electronic Contribution	130
Thermoelectric Transport Properties: Figure of Merit	131
5.2 Catalytic Activity of Two Dimensional Topological Insulator: AuI	133
Catalysis Mechanism	134
5.3 Topological Quantum Catalysis in LiMgAs	137
Structure and Lattice Dynamics	139
A Revisit to Topological Properties	140
Basal Catalytic Activity	141
Topological Catalysis	142
5.4 Conclusion	146
Bibliography	149
6 Summary and Future Prospects	157
A Computational Details	164
A.1 Bulk Materials	164
LiMgBi	164
LiMgSb	165
LiMgAs	165
AuI	166
A.2 Low Dimensional Materials	168
LiMgAs Monolayer	168
Functionalized Tellurene and Selenene	169
AuI Monolayer	169
Topological Quantum Catalyst LiMgAs	170
Bibliography	172
B List of Publications	174
B.1 Related to Thesis	174
B.2 Other than Thesis	175