

Contents

Acknowledgement	i
Abstract	ii
1 Introduction	1
1.1 Spin and Orbital Degrees of Freedom	1
1.2 Spin-orbit Coupling	2
1.2.1 Antisymmetric Spin-orbit Coupling	2
1.2.2 Site-dependent Antisymmetric Spin-orbit Coupling	3
1.3 Spontaneous Parity Breaking	6
1.4 Purpose of This Study	7
1.5 Organization of This Thesis	8
2 Model and Method	11
2.1 Model	11
2.2 Mean-field Approximation	11
2.3 Linear Response Theory	14
2.3.1 General Framework	14
2.3.2 Spectral Representation	15
2.3.3 Responses in Spin and Orbital Channels	17
2.3.4 Spin Hall Conductivity	17
3 Excitonic Multipole Order in a d-p Model on a Zigzag Chain	19
3.1 Introduction	19
3.2 Effective d - p Model on a Zigzag Chain	20
3.2.1 Reduction to Two Orbitals	20
3.2.2 Effects of Site-dependent Antisymmetric Spin-orbit Coupling	22
3.2.3 Electron-electron Interaction	24
3.3 Results and Discussion	25
3.3.1 Ground-state Phase Diagrams	25
3.3.2 Electronic Structure	27
3.3.3 Band Deformation by Magnetic Field	28
3.3.4 Magnetic and Orbital Responses to Electric Field	31
3.4 Summary of This Chapter	32

4	Emergent SOC Physics by Charge Ordering on a Triangular Lattice	36
4.1	Introduction	36
4.1.1	Charge Order on a Triangular Lattice in Transition Metal Compounds	36
4.1.2	Motivation of This Chapter	38
4.2	Two-orbital Model with LS coupling on a Triangular Lattice	39
4.3	Topological Insulators under Charge Ordering	40
4.3.1	Honeycomb-network Charge Order	41
4.3.2	Kagome-network Charge Order	43
4.4	Ground-state Phase Diagram	46
4.4.1	1/3 filling	46
4.4.2	3/8 filling	51
4.5	Effects of Bond Distortion	54
4.6	Summary of This Chapter	56
5	Summary	59