Contents

Acknowledgement i

Abstract ii

1 Introduction 1
- 1.1 Two-dimensional materials . . . 1
- 1.2 Graphene . . . 2
- 1.3 Post-graphene materials . . . 5
  - 1.3.1 Silicene, germanene, and stanene . . . 5
  - 1.3.2 Transition metal dichalcogenides . . . 6
  - 1.3.3 Transition metal trichalcogenides and trihalides . . . 10
- 1.4 Purpose of this thesis . . . 11
- 1.5 Organization of this thesis . . . 13

2 Model and method 14
- 2.1 *Ab initio* calculations . . . 14
  - 2.1.1 Density functional theory . . . 14
  - 2.1.2 Maximally localized Wannier function . . . 16
- 2.2 Multiorbital Hubbard model . . . 17
  - 2.2.1 t_{2g}-orbital system . . . 19
  - 2.2.2 e_g-orbital system . . . 21
- 2.3 Model analysis . . . 21
  - 2.3.1 Mean-field theory . . . 22
  - 2.3.2 Linear response theory . . . 22

3 Multiple Dirac nodes in transition metal trichalcogenides 25
- 3.1 Introduction to this chapter . . . 25
- 3.2 Details of *ab initio* calculations . . . 27
- 3.3 Multiple Dirac nodes . . . 28
  - 3.3.1 Representative example: $PdPS_3$ . . . 28
  - 3.3.2 Comparison with other group 10 TMTs . . . 31
- 3.4 Effect of spin-orbit coupling . . . 31
- 3.5 Tunable Dirac gap . . . 34
- 3.6 Effect of electron interactions . . . 35
  - 3.6.1 Mean-field analysis . . . 35

3.6.2 GGA calculations for magnetic solutions . . . 37
3.7 Effect of layer stacking . . . 38
3.7.1 Bilayer systems . . . 39
3.7.2 Bulk systems . . . 39
3.8 Summary of this chapter . . . 43

4 Engineering of e_g-band crossings in honeycomb-layered transition metal compounds 44
4.1 Introduction to this chapter . . . 44
4.2 Tight-binding model for the e_g manifold . . . 45
4.3 Phase diagram of e_g-band crossings . . . 46
4.4 Effect of spin-orbit coupling . . . 50
4.5 Comparison with previous *ab initio* calculations . . . 51
4.6 *Ab initio* calculations for Au trihalides . . . 52
4.7 Summary of this chapter . . . 53

5 Antiferromagnetic Kitaev-type interactions in polar spin-orbit Mott insulators 58
5.1 Introduction to this chapter . . . 58
5.2 Multiorbital Hubbard model on polar honeycomb structures . . . 59
5.3 Effective exchange interactions . . . 61
5.4 *Ab initio* estimate of exchange interactions for polar materials . . . 64
5.5 Summary of this chapter . . . 70

6 Summary 71

A Winding numbers of Dirac point nodes in e_g-orbital systems 74

B Effective Hamiltonian for quadratic band crossings in e_g-orbital systems 77

C Total energy comparison by GGA calculations for Au trihalides 78

D Kramers doublet in low-spin d^5-electron configuration 79