

CONTENTS

PREFACE	xi
INTRODUCTION	xv
CHAPTER 1	
<i>Part I: Electronic Band Structure of $\text{AgCd}_2\text{GaS}_4$: Theory and Experiment</i>	1
1.1 Historical Review	2
1.2 Experimental Details	3
1.3 Theoretical Calculations	4
1.4 Results and Discussion	5
1.4.1 Band Structure and Density of States	6
1.5 Conclusions	10
<i>Part II: First and Second Harmonic Generation of the Optical Susceptibilities for the Non-Centro-Symmetric Orthorhombic $\text{AgCd}_2\text{GaS}_4$</i>	13
1.1 Historical Review	14
1.2 Theoretical Calculation	15
1.3 Results and Discussion	16
1.3.1 Linear Optical Susceptibilities	16
1.3.2 Refraction Index and Birefringence	18
1.3.3 Second Order Susceptibilities	20
1.4 Conclusions	23

CHAPTER 2

Part I: Bismuth in Gallium Arsenide: Structural and Electronic Properties of GaAs_{1-x}Bi_x Alloys	27
2.1 Historical Review	27
2.2 Method of Calculations	29
2.3 Results and discussion	30
2.3.1 Structural Properties	30
2.3.2 Electron Charge Densities, Densities of States and Band Structures	36
2.4 Conclusions	43
Part II: Bismuth-Containing Semiconductors: Linear and Nonlinear Optical Susceptibilities of GaAs_{1-x}Bi_x Alloys	47
2.1 Historical Review	47
2.2 Method of Calculation	50
2.3 Results and Discussion	51
2.3.1 Structural Properties	51
2.3.2 Linear Optical Susceptibilities	54
2.3.3 Nonlinear Optical Susceptibilities (Second Harmonic Generation)	59
2.4 Conclusions	62

CHAPTER 3

Part I: Electronic Structure, Chemical Bonding Features And Electron Charge Density of the Double-Cubane Single Crystal [Sb₇S₈Br₂](AlCl₄)₃	65
3.1 Historical Review	65
3.2 Method of Calculations	68
3.3 Results and Discussion	69
3.3.1 Band Structure and Density of States	69
3.3.2 Electronic Charge Density	72
3.4 Conclusions	75

Part II: Second Harmonic Generation and Hyperpolarizabilities of the Double-Cubane Compound $[\text{Sb}_7\text{S}_8\text{Br}_2](\text{AlCl}_4)_3$: Chalcogenide in Ionic Liquids	77
3.1 Historical Review	77
3.2 Structural Aspects	79
3.3 Theoretical Calculation	80
3.4 Results and Discussion	82
3.4.1 Linear Optical Properties	82
3.4.2 Nonlinear Optical Properties	88
3.5 Conclusions	94
CHAPTER 4	
Effect of Increasing Tellurium Content on the Electronic and Optical Properties of Cadmium Selenide Telluride Alloys $\text{CdSe}_{1-x}\text{Te}_x$: An <i>ab initio</i> Study	97
4.1 Historical Review	98
4.2 Computational Details	100
4.3 Structural Properties and Phase Transitions	102
4.4 Electronic and Optical Properties	105
4.4.1 Band Structure and Density of States	105
4.4.2 Linear Optical Susceptibilities	113
4.4.3 Second Harmonic Generation	119
4.5 Conclusions	124
CHAPTER 5	
Part I: X-Ray Photoelectron Spectrum and Electronic Properties of a Noncentrosymmetric Chalcopyrite Compound HgGa_2S_4 : LDA, GGA and EV-GGA	129
5.1 Historical Review	130
5.2 Experimental Procedure	131
5.3 Theoretical Calculation	132

5.4 Results and Discussion	133
5.4.1 Band Structure and Density of States	133
5.5 Conclusions	139
Part II: Birefringence, Linear And Nonlinear Second Order Optical Susceptibilities of a Noncentrosymmetric Chalcopyrite Compound $H_gGa_2S_4$	
5.1 Historical Review	144
5.2 Theoretical Calculation	145
5.3 Results and Discussion	146
5.3.1 Linear Optical Susceptibilities	146
5.3.2 Refraction Index and Birefringence Dispersions	149
5.3.3 Second Order Susceptibilities	150
5.4 Conclusions	155
CHAPTER 6	
Investigation of the Linear and Nonlinear Optical Susceptibilities of $KTiOPO_4$ Single Crystals: Theory and Experiment	
6.1 Historical Review	160
6.2 Experimental Details	162
6.3 Computational Details	164
6.4 Results and Discussion	166
6.4.1 Band Structure	166
6.4.2 Linear Optical Dispersion	167
6.4.3 Non-Linear Optical Dispersion	174
6.5 Conclusions	180
CHAPTER 7	
Part I: Electronic Properties of Orthorhombic $LiGaS_2$ and $LiGaSe_2$	
7.1 Historical Review	186
7.2 Computational Method	187

7.3 Results and Discussion	190
7.3.1 Band Structure and Densities of States	190
7.4 Conclusions	193
Part II: Specific Features of Nonlinear Optical Susceptibilities of LiGaX₂ (X=S, Se) Ternary Compounds	197
7.1 Historical Review	197
7.2 Computational Method	198
7.3 Results and Discussion	200
7.3.1 First Order Optical Susceptibilities	200
7.3.2 Refraction Index and Birefringence	202
7.3.3 Second Order Optical Susceptibilities	203
7.4 Conclusions	208
CHAPTER 8	
Part I: Theoretical Investigation for Li₂CuSb as Multifunctional Materials: Electrode for High Capacity Rechargeable Batteries and Novel Materials For Second Harmonic Generation	211
8.1 Historical Review	212
8.2 Method of Calculation	215
8.3 Results and Discussion	217
8.3.1 Band Structure and Density of States	217
8.3.2 The Electrochemical Properties	223
8.3.3 The Role of Structure in Electrochemical Reactions	224
8.3.4 Linear Optical Properties	225
8.3.5 Nonlinear Response	231
8.4 Conclusion	235
Part II: A Density Functional Calculation for Li₂CuSn Compound as Electrode Material for Rechargeable Batteries	239
8.1 Historical Review	239
8.2 Theoretical Calculation	241

8.3 Results and Discussion	243
8.3.1 Band Structure and Density of States	243
8.3.2 Linear Optical Properties	248
8.3.3 Nonlinear Response	254
8.4 Conclusion	256

CHAPTER 9

Part I: Electronic Band Structure And Optical Properties Of Titanium Oxyphosphates $\text{Li}_{0.50}\text{Co}_{0.25}\text{TiO}(\text{PO}_4)$ Single Crystals: An <i>ab-initio</i> Calculations	259
9.1 Historical Review	259
9.2 Structural Features and Computational Details	262
9.3 Results and Discussion	265
9.3.1 Band Structure and Density of States	265
9.3.2 Fermi Surface	273
9.3.3 First Order (Linear) Optical Susceptibility Dispersion	274
9.4 Conclusion	278
Part II: Electronic Structure and Magneto-Optic Kerr Effect in Ferromagnetic Titanium Oxyphosphates $\text{Li}_{0.50}\text{Co}_{0.25}\text{TiO}(\text{PO}_4)$: An <i>ab-initio</i> Study	281
9.1 Historical Review	282
9.2 Structural Features and Computational Details	283
9.3 Results and Discussion	286
9.3.1 Density of States and Electron Charge Density Distribution	286
9.3.2 Magneto-Optical Properties	292
9.4 Conclusion	294
INDEX	297