

Table of Contents

CHAPTER 1	1
1.1 Overview	1
1.2 p-type Semiconducting Oxides	3
1.3 Conductivity Limitations and Improvements in Delafossites	6
1.3.1 Chalcogenides and Oxychalcogenides	8
1.3.2 Nitride Delafossites	9
1.3.3 Oxyhydroxides	10
1.3.4 Highly Conductive Metallic Delafossites	10
1.3.5 Applications of Delafossites	11
1.4 Goal of the Thesis and Objectives	14
1.5 Organization of Dissertation	14
References	18
CHAPTER 2	22
2.1 A summary of Density Functional Theory	22
2.2 Wave Function-based Methods to Solve Many-body Problem	24
2.2.1 The Born-Oppenheimer Approximation	24
2.2.2 Hartree Approximation	25
2.2.3 Hartree-Fock (HF) Approximation	26
2.3 Density Based Method; Density Functional Theory	27
2.3.1 Hohenberg and Kohn Theorem	27
2.3.2 The Kohn-Sham Equation	28
2.3.3 Exchange and Correlation Functionals	29
2.4 Density Functional Perturbation Theory	30
2.5 Elastic Properties	32
2.6 Optical Properties	34
2.7 Experimental Techniques	36
2.7.1 Sample Preparation	36
2.7.2 Characterization Techniques	37
References	40
CHAPTER 3	42
3.1 Introduction	42
3.2 Computational Methods	43
3.3 Results and Discussion	44

3.3.1	Structural Properties.....	44
3.3.2	Electronic Band Structure	46
3.3.3	Vibrational Properties	48
3.4	Elastic Properties.....	54
3.5	Conclusions	57
	References	57
CHAPTER 4		60
4.1	Introduction	60
4.2	Computational Methods	62
4.3	Results and Discussion.....	63
4.3.1	Structural Properties.....	63
4.3.2	Electronic Band Structure	64
4.3.3	Phonon Dispersion Curves.....	67
4.3.4	Optical Properties.....	70
4.4	Conclusions	79
	References	80
CHAPTER 5		83
5.1	Introduction	83
5.2	Methodology	85
5.2.1	Sample Preparation and Characterization	85
5.2.2	Computational Details	85
5.3	Results and Discussion.....	86
5.3.1	Structural Properties.....	86
5.3.2	X-ray Photoelectron Spectroscopy (XPS) and Electronic Properties	88
5.3.3	Phonon Dispersion Curves and Raman Spectra.....	91
5.3.4	Magnetic Properties	94
5.3.5	Optical Properties.....	95
5.4	Conclusions	101
	References	102
CHAPTER 6		105
6.1	Conclusions	105
6.2	Future Scope.....	108