

Table of Contents

Description	Page No.
List of Figures	xiii
List of Tables.....	xix
Symbols Used	xxi
Preface	xxiii
1. CHAPTER 1: Introduction and literature survey	1
1.1 Introduction.....	1
1.2 Composite photocatalysts	3
1.2.1 p-n heterojunction photocatalyst.....	4
1.2.2 Z-scheme photocatalysis.....	5
1.3 Importance of doping and defects in heterogeneous photocatalysis.....	6
1.4 Synthesis protocol of doped photocatalysts	8
1.4.1 Coprecipitation followed by calcination method.....	8
1.4.2 Sol-gel method.....	9
1.4.3 Reverse micelle method.....	9
1.4.4 Solvothermal or hydrothermal method	10
1.5 Synthesis of composites with doped photocatalysts	10
1.6 Computational approaches to the doped photocatalysts	11
1.7 Research gap	13

1.8	Objectives of the thesis	15
2.	CHAPTER 2: Materials and methods	17
2.1	Introduction.....	17
2.2	Chemicals	17
2.3	Sample preparation	19
2.4	Materials characterization techniques.....	19
2.4.1	Powder X-Ray Diffraction (XRD)	20
2.4.2	Transmission Electron Microscopy (TEM) sample preparation and imaging	21
2.4.3	Scanning Electron Microscope (SEM) sample preparation and imaging	22
2.4.4	UV-Visible spectroscopy	23
2.4.5	UV-visible diffuse reflectance spectroscopy (UV- DRS)	24
2.4.6	X-ray photoelectron spectroscopy (XPS).....	25
2.4.7	Spectrofluorimetry.....	26
2.5	Photocatalytic performance measurements	27
2.6	Electrochemical measurements	28
2.7	Computational protocol	29
2.7.1	Plane-wave density functional theory (DFT)	29
2.7.2	Computational protocol.....	30
3.	CHAPTER 3: Zn doped Ag₂O photocatalysts.....	31
3.1	Introduction.....	31
3.2	Experimental.....	33

3.2.1	Sample Preparation	33
3.2.2	Computational Details	34
3.2.3	Photocatalytic Performance Measurements	36
3.3	Results and Discussion.....	37
3.3.1	Structural Properties	37
3.3.2	DFT calculations.....	41
3.3.3	TEM analysis	45
3.3.4	XPS analysis	47
3.3.5	Bandgap analysis	49
3.3.6	Fluorescence spectra	50
3.3.7	Photocatalytic activity.....	51
3.4	Conclusions	59
4.	CHAPTER 4: Ni doped Ag₂O photocatalysts	61
4.1	Introduction	61
4.2	Experimental Section	64
4.2.1	Sample preparation	64
4.2.2	DFT calculations.....	65
4.2.3	Photocatalytic activity measurements.....	66
4.3	Result and discussion	67
4.3.1	Structural Properties:	67
4.3.2	XPS analysis	72
4.3.3	Photoluminescence Study	79

4.3.4	DFT calculations	80
4.3.5	Photocatalytic efficiency assessment	82
4.3.6	Proposed mechanism.....	85
4.4	Conclusions.....	86
5.	CHAPTER 5: S doped Ag₂O photocatalysts	88
5.1	Introduction.....	88
5.2	Experimental.....	91
5.2.1	Sample preparation.....	91
5.2.2	Computational details.....	92
5.2.3	Photocatalysis experimental details.....	94
5.3	Results and discussion	95
5.3.1	Structural properties	95
5.3.2	TEM and SEM analysis.....	97
5.3.3	The bandgap	99
5.3.4	Photoluminescence studies.....	100
5.3.5	XPS analysis.....	101
5.3.6	DFT calculation results	105
5.3.7	Photocatalytic properties	110
5.3.8	Plausible photocatalytic mechanism	113
5.4	Conclusions.....	115
6.	CHAPTER 6: Cd doped Ag₂O/BiVO₄ photocatalysts	116
6.1	Introduction.....	116

6.2	Experimental	118
6.2.1	Sample preparation	118
6.2.2	Computational methods	120
6.2.3	Photocatalytic experiment details	121
6.3	Results and discussion	122
6.3.1	Structural properties.....	122
6.3.2	XPS analysis	125
6.3.3	The bandgap.....	129
6.3.4	Electrochemical studies	130
6.3.5	DFT results	131
6.3.6	Photocatalytic properties.....	132
6.3.7	Plausible mechanism.....	136
6.4	Conclusions	137
7.	CHAPTER 7: Summary and conclusions	139
7.1	Summary	139
7.2	Future scope of the thesis work.....	143
8.	References	144