

Contents

1	Introduction	1
1.1	Global Energy Crisis	1
1.2	The Case for Solar Power	5
1.3	Solar Cells	6
2	Organic-Inorganic Halide Perovskites	13
2.1	Organic-Inorganic Hybrid Materials	13
2.2	Perovskites for Solar Cells	14
2.2.1	Perovskite Material	14
2.2.2	Perovskite-based Solar Cells	18
2.2.3	Crystal Structure	21
2.2.4	Stability and Compositional Engineering	22
2.3	Components of Typical Perovskite Solar Cells	38
2.3.1	The Compact Layer	38
2.3.2	The Mesoporous Layer	39
2.3.3	The Perovskite Absorber	40
2.3.4	The Hole Transport Layer	41
2.3.5	Back-contact	43
2.4	Chemical and Physical Techniques	43
2.4.1	Solution Processes	44

Contents

2.4.2	Deposition Techniques	45
2.4.3	Morphology Control	48
2.5	The Physics of Solar Cells	53
2.5.1	Introduction	53
2.5.2	Air Mass	54
2.5.3	Properties of Photovoltaics	56
2.5.4	Perovskite Bandgap Origin	72
2.5.5	Hysteresis in Current-Voltage Measurements	73
3	Characterization Techniques	79
3.1	X-ray Diffraction	79
3.2	Photoluminescence	81
3.3	Atomic Force Microscope	81
3.4	Field Emission Scanning Electron Microscope	82
3.5	Optical Spectroscopy	82
4	Synthesis and Bandgap Tuning of $MAPbX_{3-x}Y_x$ ($X, Y = I, Br, Cl$) Hybrid Perovskites	85
4.1	Motivation	85
4.2	Experimental	88
4.2.1	Synthesis of Pure Perovskite Powders	88
4.2.2	Synthesis of Thin Film Perovskites	88
4.3	Results and Discussion	89
4.3.1	X-ray Diffraction	89
4.3.2	Absorbance	97
4.3.3	Photoluminescence	99
4.3.4	FESEM Analysis	105
4.4	Conclusion	107

5 Role of the Chemical Substitution in the Structural and Luminescence Properties of the Mixed Halide Perovskite $MAPbI_{3-x}Br_x$ ($0 \leq x \leq 1$) thin films	109
5.1 Motivation	109
5.2 Experimental Procedure	110
5.3 Results and Discussion	111
5.3.1 X-ray Analysis	111
5.3.2 FESEM and AFM Analyses	114
5.3.3 UV-vis Spectra and Luminescence Properties	117
5.4 Conclusion	121
6 $MAPbI_{2.9-x}Br_xCl_{0.1}$ Hybrid Halide Perovskites: Shedding Light on the Effect of Chloride and Bromide Ions on Structural and Photoluminescence Properties	123
6.1 Motivation	123
6.2 Experimental Procedure	124
6.3 Results and Discussion	125
6.3.1 X-ray Analysis	125
6.3.2 FESEM Analysis	132
6.3.3 Absorbance	133
6.3.4 Photoluminescence	136
6.4 Conclusion	138
7 Impact of Iodide Substitution on the Physical Properties and Stability of Cesium Lead Halide Perovskite Thin Films $CsPbBr_{3-x}I_x$ ($0 \leq x \leq 1$)	139
7.1 Motivation	139
7.2 Experimental section	140

Contents

7.3	Results and Discussion	141
7.3.1	X-ray Analysis	141
7.3.2	FESEM Analysis	147
7.3.3	UV-vis Spectra and Luminescence Properties	148
7.4	Conclusion	153
8	Effect of Guanidinium on the Optical Properties and Structure of the Methylammonium Lead Halide Perovskite	155
8.1	Motivation	155
8.2	Experimental procedure	157
8.3	Results and Discussion	157
8.3.1	X-Ray Diffraction	157
8.3.2	Absorbance	163
8.3.3	Photoluminescence	166
8.3.4	FESEM Analysis	170
8.4	Conclusions	172
9	Improving Structural and Optical Properties via Imidazolium Cation Integration on Methylammonium Lead Iodide Perovskite	175
9.1	Motivation	175
9.2	Experimental Procedure	177
9.2.1	Perovskite Fabrication	177
9.3	Results and Discussion	178
9.3.1	X-ray Diffraction	178
9.3.2	Absorbance	184
9.3.3	Photoluminescence	186
9.3.4	FESEM analysis	188

Contents

9.4 Conclusions	189
10 Conditions for Fabricating Efficient Devices with Methylammonium Lead Halide Perovskite	193
10.1 Motivation	193
10.2 Experimental Procedure	195
10.2.1 Materials and Precursor Solutions	195
10.2.2 Photovoltaic Devices Fabrication	195
10.3 Results and Discussion	197
10.3.1 UV-vis Spectra and Photoluminescence	197
10.3.2 FESEM analysis	198
10.3.3 Current-Voltage Measurements	199
10.4 Conclusions	202
11 Conclusions	203
Bibliography	207