

Contents

1	Introduction	1
1.1	Background	1
1.2	Thermoelectric Effect and Applications	2
1.3	Performance Parameters of Thermoelectric Materials	4
1.4	Progress in Optimization of the Thermoelectric Parameters	6
1.4.1	Individual Parameter Modulation	6
1.4.2	Two Parameters Synergistic Modulation	11
1.4.3	Three Parameters Synergistic Modulation	21
1.5	Our Main Goals	23
	References	26
2	Superionic Phase Transition Optimizing Thermoelectric Performance in Silver Chalcogenide Nanocrystals	35
2.1	Motivation	35
2.2	Results and Discussion	37
2.3	Conclusion	47
	References	47
3	Two Metal Ion Exchange Realizing Efficient Thermoelectric Properties and $p-n-p$ Conduction Type Transition	51
3.1	Motivation	51
3.2	Results and Discussion	53
3.3	Conculsion	62
	References	62
4	Toward “Phonon Glass Electron Crystal” in Solid-Solutioned Homojunction Nanoplates with Disordered Lattice	65
4.1	Motivation	65
4.2	Results and Discussion	68
4.3	Conculsion	77
	References	77

5	Magnetic Ions Dope Wide Band-Gap Semiconductor Nanocrystals Realizing Decoupled Optimization of Thermoelectric Properties	79
5.1	Motivation	79
5.2	Results and Discussion	81
5.3	Conclusion	88
	References	89
6	Magnetic Ions Fully Substituted Wide Band-Gap Semiconductor Nanocrystals for Decoupled Optimization of Thermoelectric Properties	91
6.1	Motivation	91
6.2	Results and Discussion	93
6.3	Conclusion	100
	References	101
7	Experimental Part	103
7.1	Materials	103
7.2	Samples Preparation	103
7.2.1	Synthesis of Ag_2Se and Ag_2S Nanocrystals	103
7.2.2	Synthesis of Ag_4SeS Nanocrystals	103
7.2.3	Synthesis of AgBiSe_2 Nanocrystals	104
7.2.4	Synthesis of $\text{AgBi}_{1-x}\text{Sb}_x\text{Se}_2$ Solid Solution Nanoplates	104
7.2.5	Synthesis of $\text{AgBi}_{0.5}\text{Sb}_{0.5}\text{Se}_2$ Solid-Solutioned Homojunction Nanoplates	104
7.2.6	Synthesis of Cu_2XSnS_4 Nanocrystals	105
7.2.7	Surfactants Removal Process and Bulk Samples Preparation	105
7.3	Characterizations	106
7.4	Thermoelectric Properties Measurements	106
7.5	Positron Annihilation Spectroscopy	106
7.6	Calculation Details	107
7.6.1	Calculation Details for Ag_2Se	107
7.6.2	Calculation Details for AgBiSe_2	107
7.6.3	Calculation Details for Cu_2XSnS_4	113
	References	114