

Table of Contents

<i>Certificate</i>	<i>iii</i>
<i>Declaration by the Candidate</i>	<i>v</i>
<i>Copyright Transfer Certificate</i>	<i>vii</i>
<i>Acknowledgements</i>	<i>ix</i>
<i>Table of Contents</i>	<i>xiii</i>
<i>List of Figures</i>	<i>xviii</i>
<i>List of Tables</i>	<i>xxv</i>
<i>List of Abbreviations</i>	<i>xxvi</i>
<i>List of Symbols</i>	<i>xxviii</i>
<i>Preface</i>	<i>xxix</i>
Chapter 1 Introduction and Literature Survey	1-24
1.1 Introduction	1
1.2 Molybdenum Disulfide (MoS ₂).....	2
1.3 Structure of MoS ₂	2
1.4 Synthesis of MoS ₂	4
1.4.1 Top-Down Methods.....	4
1.4.1.1 Mechanical Exfoliation.....	4
1.4.1.2 Liquid Phase Exfoliation.....	5
1.4.1.3 Lithium Ion Intercalation.....	6
1.4.2 Bottom-Up Methods.....	7
1.4.2.1 Physical Vapor Deposition (PVD).....	7
1.4.2.2 Chemical Vapor Deposition (CVD).....	8
1.4.2.3 Solution Chemical Process.....	9
1.5 Properties of MoS ₂ Nanostructures.....	11
1.5.1 Electrical and Electronic Properties.....	11
1.5.2 Mechanical Behavior.....	13
1.5.3 Optical Behavior.....	13
1.5.4 Thermal Transport Behavior.....	15
1.6 Applications of MoS ₂ Nanostructures.....	18

1.7	Literature Survey	19
1.7.1	Literature Survey on Semiconducting Response of MoS ₂ Nanostructures..	19
1.7.2	Literature Survey on Optical Anisotropy Study of MoS ₂ Nanostructures....	20
1.7.3	Literature Survey on Thermal Transport of MoS ₂ Nanostructures.....	21
1.7.4	Literature Survey on SERS Application of MoS ₂ Nanostructures.....	22
1.8	Scope and Objective of the Present Work.....	23
Chapter 2 Synthesis and Characterization Techniques.....		25-43
2.1	Synthesis Methods.....	25
2.2	Characterization Techniques.....	30
2.2.1	Optical Microscopy	30
2.2.2	Scanning Electron Microscopy (SEM).....	32
2.2.3	Atomic Force Microscopy (AFM).....	34
2.2.4	Raman Spectroscopy.....	36
2.2.5	Photoluminescence (PL) Spectroscopy.....	40
2.2.6	UV-Visible Spectrophotometer	42
Chapter 3 Electronic Band Structure Calculation and Layer/ Morphology/ Substrate Dependence on Thermal Sensitive Excitonic Response of MoS₂.....		45-64
3.1	Introduction.....	45
3.2	Results and Discussion.....	46
3.2.1	DFT Calculation for Layer Dependent Electronic Band Structure and Total Density of States (DOS) of MoS ₂	46
3.2.2	Raman and PL Studies of Different Layered CVD Grown (1L, 3L and 5L) Triangular MoS ₂ over SiO ₂ -Si Substrate.....	50
3.2.3	Temperature-Dependent Exciton Study in Different Layered (1L, 3L and 5L) Triangular MoS ₂ over SiO ₂ -Si Substrate.....	52
3.2.4	Temperature-Dependent Exciton Study in Horizontally Grown MoS ₂ Thin Film over SiO ₂ -Si Substrate (H-MoS ₂ /SiO ₂ -Si).....	58
3.2.5	Temperature-Dependent Exciton Study in Vertically Grown MoS ₂ over SiO ₂ -Si Substrate (V-MoS ₂ /SiO ₂ -Si).....	60
3.2.6	Temperature-Dependent Exciton Study in Horizontally Grown MoS ₂ over FTO Coated Glass Substrate (H-MoS ₂ /FTO).....	62
3.3	Conclusion.....	64

Chapter 4 Phonon Calculation and Layer/ Morphology/ Substrate Dependence on Anisotropic Response of MoS₂.....65-93

4.1 Introduction.....65

4.2 Results and Discussion.....66

4.2.1 Group Theory and Phonon Dispersion for Different Layered (1 to 6L) MoS₂.....66

4.2.2 ARPRS Study72

4.2.3 ARPRS Study of CVD Grown 1L, 3L and 5L Triangular MoS₂/SiO₂-Si...73

4.2.3.1 Characterization of CVD Grown Triangular MoS₂/SiO₂-Si.....73

4.2.3.2 Anisotropic Response.....75

4.2.4 ARPRS Study of Horizontally Grown MoS₂ over SiO₂-Si Substrate (H-MoS₂/SiO₂-Si)83

4.2.5 ARPRS Study of Vertically Grown MoS₂ over SiO₂-Si Substrate (V-MoS₂/SiO₂-Si)86

4.2.6 ARPRS Study of Horizontally Grown MoS₂ over FTO Coated Glass Substrate (H-MoS₂/FTO)89

4.3 Conclusion.....93

Chapter 5 Layer/ Morphology/ Substrate Dependence on Thermal Transport

Properties of MoS₂.....95-126

5.1 Introduction.....95

5.2 Results and Discussion.....97

5.2.1 Higher Order Phonon Scattering and Thermal Transport Properties of 1L, 3L and 5L Triangular MoS₂/SiO₂-Si Substrate.....97

5.2.1.1 Characterization of 1L, 3L and 5L Triangular MoS₂/SiO₂-Si Substrate98

5.2.1.2 Temperature-Dependent Raman Study of 1L, 3L and 5L Triangular MoS₂/SiO₂-Si Substrate98

5.2.1.3 Calculation for Thermal Conductivity of 1L, 3L and 5L Triangular MoS₂/SiO₂-Si Substrate104

5.2.2 Higher Order Phonon Scattering and Thermal Transport Properties of H-MoS₂/SiO₂-Si111

5.2.2.1 Characterization of H-MoS₂/SiO₂-Si.....112

5.2.2.2	Temperature-Dependent Raman Study of H-MoS ₂ /SiO ₂ -Si.....	112
5.2.2.3	Calculation for Thermal Conductivity of H-MoS ₂ /SiO ₂ -Si.....	114
5.2.3	Higher Order Phonon Scattering and Thermal Transport	
	Properties of V-MoS ₂ /SiO ₂ -Si.....	116
5.2.3.1	Characterization of V-MoS ₂ /SiO ₂ -Si.....	117
5.2.3.2	Temperature-Dependent Phonon Study of V-MoS ₂ /SiO ₂ -Si.....	117
5.2.3.3	Calculation for Thermal Conductivity of V-MoS ₂ /SiO ₂ -Si.....	119
5.2.4	Higher Order Phonon Scattering and Thermal Transport Properties	
	of H-MoS ₂ /FTO.....	121
5.2.4.1	Characterization of H-MoS ₂ /FTO.....	121
5.2.4.2	Temperature-Dependent Raman Study of H-MoS ₂ /FTO.....	121
5.2.4.3	Calculation for Thermal Conductivity of H-MoS ₂ /FTO.....	123
5.3	Conclusion.....	125
Chapter 6	Morphology/Substrate Dependent MoS₂ Based SERS Biosensors....	127-161
6.1	Introduction.....	127
6.2	Sample Preparation for SERS Measurement	130
6.3	Results and Discussion.....	131
6.3.1	Characterization of Dye Molecules.....	131
6.3.2	Characterization of SERS Substrates.....	133
6.3.3	SERS Application for the Detection of Bilirubin using Different	
	Prepared MoS ₂ Nanostructures.....	136
6.3.4	SERS Application for the Detection of Vitamin B ₁₂ using Different	
	Prepared MoS ₂ Nanostructures	141
6.3.5	SERS Mechanism for Biomolecules Detection using MoS ₂ Substrates	147
6.3.6	Calculation of Number of Biomolecules Probed in SERS (N _{SERS})	
	and Estimation of SERS Enhancement Factor (EF).....	151
6.3.7	Temperature-Dependent SERS Measurements.....	156
6.4	Conclusion.....	160
Chapter 7	Conclusion and Future Scope of the Work.....	163-167
7.1	Conclusion.....	163
7.2	Future Scope of the Work.....	166

References.....169
List of Patents, Publications, and Book Chapters.....194
Schools/Workshops/Conferences Attended.....196