

Table of Contents

Title	Page No.
Abstract	i
Declaration	v
Certificate	vi
Acknowledgements	vii
Table of contents	ix
List of Tables	xiv
List of Figures	xvi
List of Abbreviations	xxix
List of Symbols	xxxix
 Chapter 1. Introduction	 1-40
1.1 Background on nanomaterials	1
1.2 Two-dimensional (2D) layered materials	3
1.2.1 Graphene and graphene derivatives	3
1.2.2 Inorganic layered materials	4
1.2.3 Transitional metal dichalcogenides (TMDCs)	6
1.2.3.1 Thermal properties	8
1.2.3.2 Electrical properties	9
1.2.3.3 Mechanical properties	10
1.2.3.4 Optoelectronic and photocatalytic features	12
1.3 Irradiation-induced phenomena	15
1.4 Theoretical and computational aspects	18
1.5 Scope of this thesis	19
References	20
 Chapter 2. Experimental: processes, principles and characterization	 41-77
2.1 Introduction	41

2.2	Liquid-phase exfoliation (LPE) of tungsten disulfide (WS ₂) and tungsten diselenide (WSe ₂) systems	42
2.3	Characterization techniques	43
2.3.1	Powder X-ray diffraction	43
2.3.2	UV-visible spectroscopy	45
2.3.3	Photoluminescence spectroscopy	46
2.3.4	Raman spectroscopy	47
2.3.5	X-ray photoelectron spectroscopy (XPS)	48
2.3.6	Atomic-force microscopy (AFM)	49
2.3.7	Field-emission scanning electron microscopy (FE-SEM)	51
2.3.8	High-resolution transmission electron microscopy (HR-TEM)	52
2.3.9	Nitrogen (N ₂) adsorption-desorption technique	53
2.3.10	Universal Testing Machine (UTM)	53
2.3.11	Advanced rheometry	54
2.4	Processing of WSe ₂ and WS ₂ dispersed NaCMC polymeric nanocomposites	56
2.4.1	Processing of WSe ₂ /NaCMC nanocomposites	56
2.4.2	Processing of WS ₂ /NaCMC nanocomposites	57
2.4.3	Generating fractal patterns in NaCMC dispersed with 2D layer WS ₂ system	58
2.4.3.1	X-ray diffraction analysis	59
2.4.3.2	Raman vibrational modes	60
2.4.3.3	FT-IR spectra	62
2.4.3.4	Morphological characteristics through FE-SEM	64
2.4.3.5	Surface morphology through AFM	67
2.5	Concluding remarks	71
	References	71
	Chapter 3. γ-ray irradiation induced mechanical study of WS₂ nanosystems dispersed in NaCMC polymeric solution	78-96
3.1	Introduction	78
3.2	Physical properties of γ -irradiated WS ₂ /NaCMC films	80

3.2.1	Structural and vibrational features of γ -irradiated WS ₂ nanosystems	80
3.2.2	Elemental compositional analysis	83
3.3	Mechanical properties of γ -irradiated exfoliated WS ₂ dispersed in NaCMC	84
3.3.1	Load bearing capacity, elasticity, and breaking points	84
3.3.2	Reinforcement mechanisms of the fractured surfaces	88
3.4	Concluding remarks	92
	References	93
Chapter 4. Power dependent Raman spectra, nitrogen adsorption-desorption isotherms, and photocatalytic activity of WS₂ nanosystems exposed to UV- and β-radiation		97-113
4.1	Introduction	97
4.2	Irradiation of WS ₂ system with UV- and β -rays	98
4.3	Execution of photocatalytic experiment	98
4.4	Morphological and elemental analysis	99
4.5	Laser power-dependent Raman analysis	100
4.6	Nitrogen adsorption/desorption process and pore-size analysis	104
4.7	Congo red dye degradation activity	106
4.8	Concluding remarks	109
	References	110
Chapter 5. keV and GeV irradiation induced modification of WS₂: Excitonic features and computational perspectives		114-179
5.1	Introduction	114
5.2	Irradiation effect of WS ₂ system with 15 keV He ²⁺ , 15 keV C ²⁺ and 0.85 GeV U ²⁸⁺ ions	116
5.3	Effect of 15 keV He ²⁺ ion irradiation in few layer WS ₂	117
5.3.1	SRIM-TRIM simulations	117
5.3.2	Structural and surface compositional features	118
5.3.2.1	X-ray diffraction analysis	118
5.3.2.2	Raman spectra analysis	120

5.3.2.3	Core-level spectra analysis	122
5.3.3	Morphological and surface topographical analysis	123
5.3.3.1	Exfoliation and slipping of layers through bubble formation	123
5.3.3.2	2D surface scans, 3D topography and its height profiles	127
5.4	Effect of 15 keV C ²⁺ ion irradiation in nanoscale WS ₂ : Experimental and theoretical perspectives	129
5.4.1	SRIM/TRIM calculations	129
5.4.2	Phase structure and vibrational analysis	131
5.4.2.1	X-ray diffraction study	131
5.4.2.2	Raman spectra analysis	134
5.4.3	Elemental composition and morphological study	136
5.4.3.1	Energy dispersive X-Ray spectra and elemental mapping analysis	136
5.4.3.2	Morphological analysis	138
5.4.4	Computational study of C-incorporated WS ₂ systems	141
5.4.4.1	Computational details	141
5.4.4.2	Migration barrier energy	142
5.4.4.3	Structural and electronic properties	144
5.5	Impact of 0.85 GeV U ²⁸⁺ ions on bulk and exfoliated WS ₂ systems	149
5.5.1	SRIM analysis	149
5.5.2	Structural and vibrational analysis	150
5.5.3	Core level spectra and elemental compositional analysis	153
5.5.4	Morphological analysis	155
5.5.5	Low-temperature photoluminescence (PL) study	157
5.5.6	Photoluminescence decay measurements	165
5.6	Concluding remarks	169
	References	170
Chapter 6. Structural, morphological and rheological properties of WSe₂ with emphasis on radiation induced phenomena		180-212
6.1	Introduction	180

6.2	WSe ₂ nanosystems under γ -ray exposure and irradiation with 15 keV He ²⁺ , 15 keV C ²⁺ and 60 MeV N ⁵⁺ ions	181
6.3	Structural, vibrational and rheological study of γ -irradiated WSe ₂ systems	182
6.3.1	Structural and vibrational analysis	182
6.3.2	Rheological response of the WSe ₂ /NaCMC polymeric solution	184
6.4	Effect of 15 keV He ²⁺ ion irradiation on layered WSe ₂	188
6.4.1	SRIM analysis	188
6.4.2	Crystallographic and vibrational analysis	189
6.4.3	Inorganic fullerene (IF) like structure with He ²⁺ irradiation	191
6.5	Effect of 15 keV C ²⁺ ion irradiation on layered WSe ₂ nanosystems	193
6.5.1	SRIM analysis	193
6.5.2	Phase structure and vibrational analysis	194
6.5.3	Morphological modification and sheet fragmentation with C ²⁺ irradiation	196
6.6	Effect of 60 MeV N ⁵⁺ ion irradiation on exfoliated WSe ₂ systems	197
6.6.1	SRIM calculations	197
6.6.2	Structural analysis	198
6.6.3	Vibrational analysis	200
6.6.4	Morphological analysis	201
6.6.5	Computational details	203
6.6.6	Electronic properties of defect clusters	204
6.7	Concluding remarks	206
	References	207
Chapter 7. Conclusion and future directions		213-218
7.1	Conclusions	213
7.2	Future outlook and directions	217
Appendix		219-226
List of Publications		227
List of Conferences/Workshops attended		228