

CONTENTS

Chapters	Titles	Page No.
	Certificate	iii
	Declaration by the Candidate	iv
	Copyright transfer Certificate	v
	Acknowledgements	vi-vii
	Index	viii-xix
	List of Figures	xx-xxix
	List of Tables	xxx-xxxiii
	List of Abbreviations	xxxiv-xxxix
	Preface	xl-xlii
Chapter 1	Introduction	1-26
1.1	Overview	1
1.2	Introduction	2
1.3	Traditional routes for MFC production	11
1.4	Circular economy aspect of the thesis	12
1.5	Alignment of thesis chapters with different UN-sustainable development goals	14
1.6	Scope and structure of thesis	18
Chapter 2	Literature review	27-92
2.1	Introduction	27
2.2	Sources of cellulose	30
2.2.1	Wood sources	30
2.2.2	Plant sources	32
2.2.3	Bacterial sources	32
2.2.4	Tunicate sources	34
2.2.5	Algal sources	35
2.3	Types of cellulose	36
2.3.1	Microfibrilliated cellulose	36
2.3.2	Nanofibrilliated cellulose	37
2.3.3	Cellulose nanocrystal	38

2.3.4	Microcrystalline cellulose	39
2.4	Strategies of cellulose modification	39
2.4.1	Physical modification of cellulose	39
2.4.1.1	Adsorption	40
2.4.1.2	Absorption	41
2.4.1.3	<i>Ex-situ</i> and <i>in-situ</i> modification of cellulose	41
2.5	Chemical modification	45
2.5.1	Oxidation	47
2.5.2	Sulfonation	50
2.5.3	Carboxymethylation	51
2.5.4	Amidation	53
2.5.5	Silanization	54
2.5.6	Phosphorylation	56
2.6	Different routes for the production of phosphorylated cellulose	57
2.6.1	Acid derivative	57
2.6.2	Phosphate salt	60
2.6.3	Phosphorylation using deep eutectic solvent and ionic liquids	67
2.6.4	Enzymatic treatment	68
2.7	Applications of phosphorylated cellulose	72
2.7.1	Flame retardancy	73
2.7.2	Wastewater remediation	76
2.7.3	Biomedical and tissue engineering	81
2.7.4	Batteries and fuel cell	82
2.7.5	Food packaging application	84
2.8	Life cycle assessment of functionalized cellulose production	91
Chapter 3	Materials and methods	93-138
3.1	Materials	93
3.2	Methods	94
3.2.1	Delignification of biomass	94

3.2.2 Functionalization of biomass	95
3.2.2.1 <i>In-situ</i> modification of DSB/DRH using molybdate salt	95
3.2.2.2 Phosphorylation of delignified biomass	95
3.2.3 Phosphorylation of viscose	96
3.2.4 Preparation of 3D printed structures	96
3.2.5 <i>In-situ</i> growth of MoS ₂ on 3D printed structures	97
3.2.6 Fabrication of RS films	97
3.2.6.1 Fabrication of cups and other cutlery items	97
3.2.6.2 Fabrication of RS aerogels	98
3.2.7 Fabrication of SB films	98
3.2.7.1 Fabrication of SB aerogels	99
3.2.7.2 Fabrication of fruit foam	99
3.3 Analytical instrumentation and characterization	99
3.3.1 Fourier transformation infrared Spectroscopy (FTIR)	99
3.3.2 X-ray photoelectron spectroscopy (XPS) analysis	99
3.3.3 Scanning electron microscopy (SEM) and Energy dispersive -ray spectroscopy (EDS)	100
3.3.3.1 Field Emission Scanning Electron Microscopy (FESEM) and EDS	101
3.3.4 X-ray diffraction (XRD)	101
3.3.5 Thermogravimetric analysis (TGA)	101
3.3.6 Solid-state nuclear magnetic resonance (NMR) spectroscopy	102
3.3.7 Raman spectroscopy	102
3.3.8 Conductometric titration	102
3.3.9 Mechanical properties	103
3.3.9.1 Tensile property	103
3.3.9.2 Compressive property	103
3.3.10 UV-visible diffused reflection spectra (DRS)	104
3.3.11 Contact angle	104
3.3.12 Thermal conductivity	104

3.3.13 Rheology	105
3.3.14 Water absorption of films and aerogels	105
3.3.15 Swelling capacity	106
3.3.16 Density and porosity	106
3.4 Biodegradation of phosphorylate SB films	106
3.5 Evaluation of flame-retardant properties	107
3.5.1 Flammability test for films	107
3.5.2 Flammability test for aerogels	107
3.6 Migration study	108
3.7 High-performance application of developed composites in different sectors	108
3.7.1 Pollutant dye adsorption	108
3.7.1.1 Adsorption of MB using DSB and DSB-MoS ₂	108
3.7.1.2 Adsorption of MB using DRH and DRH-MoS ₂	109
3.7.1.3 Adsorption of MB using PC	109
3.7.1.4 Adsorption of MB using PCMo@0.5%	109
3.7.1.5 Adsorption isotherms and kinetics	110
3.7.2 Adsorption thermodynamic	112
3.7.3 Photodegradation of dyes	113
3.7.3.1 Photodegradation of MB using DSB-MoS ₂	113
3.7.3.2 Photodegradation of MB using DRH-MoS ₂	113
3.7.3.3 Photodegradation of MB using PCMo@0.5%	113
3.7.3.4 Continuous photodegradation of MB using DSB-MoS ₂	114
3.7.3.5 Continuous photodegradation of MG DRH-MoS ₂	114
3.7.3.6 Continuous photodegradation of MB using PCMo@0.5%	115
3.7.4 Adsorption and desorption cyclic study	115
3.7.5 Antibacterial properties	115

3.7.6	Simultaneous photodegradation and anti-bacterial properties of MB using PCMo@0.5%	116
3.7.7	Antioxidant activity of DRH-MoS ₂	116
3.8	Application of RS film in packaging of perishable food items	117
3.8.1	Heat sealing of RS films	117
3.8.2	Application of RS-based film in food packaging	117
3.9	Application of phosphorylated SB films for packaging of paneer	118
3.9.1	Evaluation of shelf-life of paneer	118
3.1	Surface modification of produced RS cups	118
3.10.1	Thermoregulatory performance of RS APTES modified cups	118
3.11	Evaluation of pH of butter and paneer	119
3.12	Evaluation of peroxide values of butter and paneer	119
3.13	Evaluation of microbial growth on butter and paneer	120
3.14	Application of phosphorylated RS aerogel	120
3.14.1	Evaluation of shelf-life of butter packed in RS aerogel box	120
3.14.2	Melting behavior and IR thermal imaging of the butter	121
3.15	Application of phosphorylated SB foam	121
3.15.1	Thermal insulation properties of PSCB foam	121
3.15.2	Antibacterial and antioxidant properties of the PSCB-G foam	121
3.16	Life cycle assessment studies	122
3.16.1	Comparisons of environmental impacts generated from phosphorylation and TEMPO-oxidation of VC for gel production	122
3.16.2	LCA of production of phosphorylated RS films and its comparison with TEMPO-oxidized film from kraft wood pulp	125
3.16.3	Comparisons of environmental impacts generated from the production of RS aerogel box and polyurethane (PU) foam	129

3.16.4	LCA of storage of butter in plastic packaging with refrigeration system and RS aerogel box	132
3.16.5	Comparisons of environmental impacts generated from the transportation of butter in plastic packaging with cold storage system and RS aerogel box	134
3.16.6	LCA for the production of film from phosphorylated SB	137
Chapter 4	Delignification of biomass for <i>in-situ</i> synthesis of MoS₂ for dye remediation	138-196
	Motivation	139
	Graphical abstract	140
4.1	Introduction	141
4.2	Results and discussion	146
4.2.1	Physiochemical and functional properties of DSB and DSB-MoS ₂	148
4.2.2	Structural investigation of DSB and DSB-MoS ₂	152
4.2.3	Raman spectroscopy of DSB-MoS ₂	153
4.2.4	Morphological properties of DSB and DSB-MoS ₂	155
4.2.5	Adsorption of MB with DSB	159
4.2.5.1	Effect of pH and temperature	159
4.2.5.2	Adsorption kinetics and isotherm	160
4.2.5.3	Adsorption thermodynamics	161
4.2.6	Photodegradation of MB using DSB-MoS ₂	165
4.2.6.1	Effect of pH on photodegradation of MB	166
4.2.6.2	Effect of temperature on photodegradation of MB	167
4.2.6.3	Photodegradation kinetics	167
4.2.6.4	Continuous photodegradation behaviour and recyclability studies of DSB-MoS ₂	168
4.2.7	Antibacterial properties of DSB-MoS ₂	169
4.2.8	Mechanism of the photodegradation of MB	170
4.3	<i>In-situ</i> modification of DRH using MoS ₂	173
4.3.1	Physicochemical and functional properties of DRH and DRH-MoS ₂	175

4.3.2	Structural investigation of DRH and DRH-MoS ₂	180
4.3.3	Morphological properties of DRH and DRH-MoS ₂	181
4.3.4	Adsorption of MG on DRH	182
4.3.4.1	Effect of pH and temperature	184
4.3.4.2	MG adsorption kinetics on DRH	184
4.3.4.3	Adsorption isotherm	185
4.3.4.4	Adsorption thermodynamic	185
4.3.5	Photodegradation of MG under light and adsorption under dark condition by DRH-MoS ₂	187
4.3.5.1	Effect of pH and temperature on MG degradation	188
4.3.5.2	Kinetic study of MG adsorption	189
4.3.5.3	Continuous photodegradation of MG with DRH-MoS ₂ and its reusability	190
4.3.6	Free radical scavenging ability of DRH-MoS ₂	191
4.3.7	Antibacterial properties of DRH-MoS ₂	192
4.4	Summary	196
Chapter 5	Production and processing of cellulose phosphate from viscose for 3D printing application	197-254
	Motivation	197
	Graphical Abstract	198
5.1	Introduction	199
5.2	Results and discussion	205
5.2.1	PC gel production and evaluation of physicochemical properties	205
5.2.2	LCA of PC gel and its comparative analysis	206
5.2.3	Rheological behavior of PC gel	210
5.2.4	Evaluation of functional properties of PC	212
5.2.5	Water uptake and swelling behavior of 3D printed PC	218
5.2.6	Evaluation of structural and thermal properties of VC and PC	219
5.2.7	Mechanical properties of 3D printed PC structures	220
5.2.8	Morphological studies of 3D printed PC	221

5.2.9 Dye Adsorption and its kinetics studies	222
5.2.9.1 Effect of initial concentration and contact time on adsorption behaviour	222
5.2.9.2 Effects of temperature on MB adsorption	223
5.2.9.3 Effects of pH on MB adsorption	224
5.2.9.4 Adsorption kinetics	224
5.2.9.5 Adsorption isotherms	226
5.2.9.6 Adsorption thermodynamic	226
5.2.9.7 Dye adsorption-desorption study	227
5.3 <i>In-situ</i> modification of PC-3D printed structure	230
5.3.1 Rheological studies of gels	230
5.3.1.1 Shear thinning properties of gels	232
5.3.1.2 Dynamic behaviour of the gels	232
5.3.2 Evaluation of functional properties	235
5.3.2.1 FTIR analysis of PC and <i>in-situ</i> grown PCMo structures	235
5.3.2.2 XPS analysis PCMo@0.5%	236
5.3.3 XRD and Raman spectroscopy analysis of PC and <i>in-situ</i> grown PCMo structures	237
5.3.4 Thermogravimetric analysis of PC and <i>in-situ</i> grown PCMo structures	240
5.3.5 Morphological studies	241
5.3.6 MB dye remediation using with <i>in-situ</i> grown 3D printed PC-based MoS ₂	243
5.3.6.1 Effects of contact time and initial MB concentration on adsorption	243
5.3.6.2 Effects of temperature and pH on adsorption	243
5.3.6.3 Adsorption isotherm	244
5.3.6.4 Adsorption kinetics	245
5.3.6.5 Adsorption thermodynamics	246
5.3.7 Photodegradation of MB with PCMo@0.5%	247
5.3.7.1 Reusability of PCMo@0.5%	248
5.3.7.2 Antibacterial properties of PCMo@0.5%	248

	5.3.7.3 Continuous photodegradation and antibacterial properties of PCMo@0.5%	250
	5.3.8 Mechanism of photodegradation	251
5.4	Summary	252
Chapter 6	Phosphorylation of rice straw for production of heat-sealable packaging films and thermal box	255-319
	Motivation	255
	Graphical abstract	256
6.1	Introduction	257
6.2	Results and discussion	260
	6.2.1 Physiochemical properties of RS films	261
	6.2.2 LCA for production of phosphorylated RSF films and its comparison with TEMPO-oxidized films	263
	6.2.2.1 Normalization of mid-point results of production of phosphorylated RSF and TEMPO-oxidised films	264
	6.2.2.2 Sensitivity analysis for production of phosphorylated RSF and TEMPO-oxidised films	265
	6.2.3 Functional, structural and thermal properties	266
	6.2.3.1 Functional properties RSF	266
	6.2.3.2 Structural properties of RSF	267
	6.2.3.3 Thermal properties of RSF	268
	6.2.4 Mechanistic investigation: XPS studies of DRS and RSF-60	269
	6.2.5 Morphological properties of RSF-60	272
	6.2.6 Mechanical properties of RSF	273
	6.2.7 Wettability, water absorption, and swelling behavior of RSF	275
	6.2.8 Flammability test of RSF	276
	6.2.9 Migration studies of RSF	279
	6.2.10 Application of RSF for food packaging and development of beverage cups	279
6.3	Production of RS aerogel and thermal box	286

6.3.1	Density, porosity, thermal conductivity, and water absorption properties of RSA	286
6.3.2	Mechanical property of RSA	288
6.3.3	LCA of RS aerogel and its comparison with polyurethane foam production	290
6.3.3.1	Normalization of midpoint results RS aerogel polyurethane foam production	291
6.3.3.2	Sensitivity analysis RS aerogel and polyurethane foam production	294
6.3.4	Functional properties of RSA	296
6.3.5	Thermal properties of RSA	297
6.3.6	Structural properties RSA	298
6.3.7	Flammability test of RSA and RS thermal box	301
6.3.8	Morphological properties of RSA	301
6.3.9	Melting behavior and IR imaging of the butter	304
6.3.10	Packaging of butter in RS box	304
6.3.11	LCA of storage of butter in RSA and plastic boxes	308
6.3.11.1	Normalization of mid-point results from storage of butter in RSA and plastic boxes	309
6.3.11.2	Sensitivity analysis of storage of butter in RSA and plastic boxes	309
6.3.12	LCA of RS and plastic boxes production for the transportation of butter under a cold storage system	313
6.3.12.1	Normalization of mid-point results of transportation of butter in RSA and plastic boxes under cold storage conditions	313
6.3.12.2	Sensitivity analysis of the transportation of butter in RSA and plastic boxes under cold storage conditions	314
6.4	Summary	319
Chapter 7	Phosphorylation of sugarcane bagasse for the development of films and fruit foam for packaging of perishable food items	320-363

Motivation	320
Graphical abstract	321
7.1 Introduction	322
7.2 Results and discussion	324
7.2.1 Physiochemical properties of the films	325
7.2.1.1 Evaluation of charge content	325
7.2.1.2 FTIR spectra analysis of phosphorylated SB films	327
7.2.1.3 XPS analysis of DSB and SCBF	327
7.2.2 Morphological properties of phosphorylated SCB films	329
7.2.3 Structural properties of phosphorylated SCB films	330
7.2.4 Thermal properties of phosphorylated SCB films	331
7.2.5 Mechanical properties of phosphorylated SCB films	332
7.2.6 Water absorption capacity of phosphorylated SCB films	333
7.2.7 Surface wettability of the phosphorylated SCB films	334
7.2.8 Flammability	336
7.2.9 Migration studies of phosphorylated SCB films	336
7.2.10 Packaging of the paneer and evaluation of their shelf life	337
7.2.11 Biodegradation of phosphorylated SCB films	341
7.2.12 LCA of SCBF-film	342
7.2.12.1 Normalization of mid-point results	343
7.2.12.2 Sensitivity analysis	343
7.3 Production of PSCB aerogel and Fruits foam	346
7.3.1 Functional properties: FTIR and XPS studies of phosphorylated SCB aerogels	347
7.3.2 Structural Properties of phosphorylated SCB aerogels	349
7.3.3 Morphological Properties of the Foams	351
7.3.4 Thermal properties	351

7.3.5 Thermal conductivity of the foams	353
7.3.6 Mechanical properties	354
7.3.7 Water uptake capacity	355
7.3.8 Thermal insulation performance	356
7.3.9 Flame-retardant properties	357
7.3.10 Packaging of apples	358
7.3.11 Anti-oxidant properties	359
7.3.12 Antibacterial activity	361
7.4 Summary	362
Chapter 8 Conclusion and future scope	364-377
8.1 Conclusion	364
8.2 Future scope	375
References	378-447
List of Publications	448-451
Conference/Workshop Attended during PhD.	452-453