

Contents

		Page
Abstract		vii
Acknowledgments		ix
Contents		xi
List of Figures		xiii
List of Tables		xvii
List of Symbols		xix
List of Abbreviations		xxi
Chapter 1: Introduction		1
1.1	Purpose of the study	1
1.2	Objectives and scope	3
1.3	Brief results and future perspective of the work	3
Chapter 2: Literature Review		7
2.1	Electrocatalytic Hydrogen evolution reaction	7
2.2	Degradation of Organic pollutants	9
2.3	Biodiesel and Bio-Jet fuel production	10
2.4	Impact of Gadolinium Doping into the Frustrated Antiferromagnetic Lithium Manganese Oxide Spinel.	13
Chapter 3: Role of ZnO in ZnO Nanoflake/Ti₃C₂ MXene composites in photocatalytic and electrocatalytic hydrogen evolution.		15
3.1	Experimental Section	15
	3.1.1 Synthesis of MXene	15
	3.1.2 Synthesis of ZnO-MXene	15
	3.1.3 Dye degradation test	15
	3.1.4 Electrochemical Measurements	16
	3.1.5 Scavenging test	16
	3.1.6 Preparation of working electrodes	16
3.2	Results and Discussion	16
	3.2.1 Structural and Morphological characterization	16
	3.2.2 Photocatalytic activity	23
	3.2.3 Electrocatalytic activity	28
3.3	Conclusion	30
Chapter 4: On the reduction of CO₂ footprint via selective hydrodeoxygenation by ZnO-Ti₃C₂T_x catalyst under solvent-free conditions		31
4.1	Experimental Section	31
	4.1.1 Synthesis of Ti ₃ C ₂ T _x and ZnO- Ti ₃ C ₂ T _x composite	31
	4.1.2 Hydroprocessing of methyl oleate	31
4.2	Results and Discussion	32
	4.2.1 Characterization of catalyst	32
	4.2.2 HDO reaction of Pristine Ti ₃ C ₂ T _x	37
	4.2.3 Selective HDO reaction of ZnO- Ti ₃ C ₂ T _x composites	40
	4.2.4 Selective HDO reaction with variable catalyst amount	42
	4.2.5 Recyclability test of catalyst	43
	4.2.6 Reaction pathway	44
4.3	Conclusion	46
Chapter 5: Highly selective production of bio-jet fuel grade alkanes over Fe/ SiO₂-Al₂O₃ solid acid catalyst under solvent-free conditions		47

5.1	Experimental Techniques	47
	5.1.1 Catalyst preparation	47
	5.1.2 Catalytic hydrocracking of Methyl oleate	47
	5.1.3 Catalyst Reusability	48
5.2	Results and Discussion	48
	5.2.1 Characterization of catalyst	48
	5.2.2 Catalytic Hydrocracking Reactions	53
	5.2.3 Effect of different catalysts loading	58
	5.2.4 Reusability test	59
	5.2.5 Proposed Reaction Mechanism	60
5.3	Conclusion	61
Chapter 6: Impact of Gadolinium Doping into the Frustrated Antiferromagnetic Lithium Manganese Oxide Spinel		63
6.1	Experimental Techniques	63
	6.1.1 Preparation of $\text{LiMn}_{2-x}\text{Gd}_x\text{O}_4$	63
	6.1.2 Sample preparation for magnetic measurements	64
	6.1.3 Computational details	64
6.2	Results and Discussion	64
	6.2.1 Structural and morphology analysis	64
	6.2.2 Raman analysis	67
	6.2.3 First principles calculations	68
	6.2.4 Magnetic properties	70
6.3	Conclusion	74
Chapter 7: Conclusion		75
7.1	Summary	75
7.2	Future scope	76
Publications		77
Annexure A: Materials and methods		79
A.1	Reagents	79
A.2	Instrumentation Techniques	79
A.3	Software used	80
References		81