Table of Contents

a. Abstract **i-vi**

b. Declaration

c. Certificate

d. Dedication

e. Acknowledgements

f. Table of Contents vii-xii

g. List of Figures xiii-xx

h. List of Abbreviations xxi-xiii

i. List of Symbols xxiv

Chapter 1: Introduction 1-28

1.1 History of Carbon Nitride 1

1.1.1 Structure of g-C_3N_4 3

1.1.2 Functional characteristics of g-C_3N_4 4

1.2 Role of Dimensionality in the era of Nanotechnology 5

1.2.1 3D Architecture of g-C_3N_4 7

1.2.2 g-C_3N_4 in its OD quantum dots dimensionality 8

1.2.3 1D tube/rod/wire arrangement of g-C_3N_4 9

1.2.4 2D nanosheets with lamellar structure 11

1.3 Intelligent Surface and interface engineering of g-C_3N_4 13

1.3.1 Engineering with Non-Metal Doping 14

1.3.2 Enhancing the functionalities with Metal Doping 16

1.3.3 Creating heterointerface for achieving brilliant performances 17

1.4 Motivation behind this work 18

1.5 Objective of This Thesis 20

References 23

Chapter 2 : Surface engineered porous magnetic graphitic sheets for rapid and efficient recovery of oil 29-48

2.1 Introduction 30

2.2 Chemicals and materials used 31

2.2.1 Preparation of $FeNi_3$ 32

2.2.2 Preparation of graphitic carbon nitride (g-C_3N_4) sheet 32

2.2.3 Preparation of composite g-C_3N_4@$FeNi_3$ 32

2.2.4 Surface modification of the prepared Nanocomposite 33

2.2.5 Crude oil 33

2.3 Results and Discussion 33

2.3.1 Microstructure and Surface morphology 33

2.3.2 Porosity and surface area analysis 36

2.3.3 Contact Angle analysis 37

2.3.4 GC-MS analysis 39

2.4 Adsorption Kinetics 39

2.5 Adsorption Isotherm 41

2.6 Oil recovery and Reusability 42

2.7 Computational Details 43

2.7.1 Atomic configuration of the system 43

2.7.2 Electronic structure of the system 44

2.8 Conclusions 45

References 46

Chapter 3: Two dimensional heterostructure for efficient quantum energy storage as in-plane micro-supercapacitor 49-74

3.1 Introduction 50

3.2 Methods 52

3.2.1 Development of 2D g-C_3N_4@$FeNi_3$ heterostructure 52
3.2.2 Materials Characterization 52
3.3 Results and discussion 52
3.3.1 Microstructural and Surface Morphology Analysis 52
3.4 Electrochemical properties 54
3.4.1 Cyclic voltammetry 54
3.4.2 Galvanostatic charge discharge (GCD) 55
3.4.3 Impedance Spectroscopy 57
3.4.4 Cyclic performances 59
3.5 Device Strategy 60
3.6 Theoretical Analysis 62
3.6.1 Density functional theory calculation 62
3.6.2 Quantum Capacitance Calculation 62
3.7 Results and Discussions 64
3.7.1 Geometrical optimization 64
3.7.2 Local densities of states (LDOS) 66
3.7.3 Projected density of states (PDOS) 67
3.7.4 Quantum capacitance 68
3.8 Conclusion 69
References 70
Chapter 4: Reinforcing 2D heterostructure to design efficient and sustainable film for food packaging 75-94
4.1 Introduction 76
4.2 Methods and Methodology 77
4.2.1 Chemicals and materials used 77
4.3 Experimental synthesis 78
4.3.1 Synthesis of 2D/2D g-C_3N_4@CuSe heterostructure 78

4.3.2 Synthesis of composite film embedding 2D/2D heterostructure within polymer matrix 78
4.4 Results and discussion 79
4.4.1 Structural and Surface Morphology 79
4.4.2 Thermal properties 80
4.4.3 Barrier properties 82
4.4.4 Mechanical properties 83
4.4.5 Contact Angle 85
4.4.6 Antimicrobial properties 86
4.4.7 Ion Migration Analysis 87
4.4.8 Degradation phenomena 89
4.4.9 Shelf Life study 90
4.5 Conclusion 91
References 92
Chapter 5: Band alignment 2D/2D heterojunction for excellent sunlight-driven photo catalytic dye degradation **95-120**
5.1 Introduction 96
5.2 Methods and Methodology 98
5.3 Experimental 98
5.3.1 Chemicals and materials used 98
5.3.2 Synthesis of 2D/2D gC_3N_4-CuSe heterostructure 98
5.4 Results and discussion 98
5.4.1 Structural and morphology studies 98
5.4.2 Spectroscopy Analysis 101
5.4.3 Photocatalytic activity 103
5.4.4 Kinetics and Surface Charge analysis 106
5.5 Theoretical Analysis 107
5.6 Computational Set-up 107
5.6.1 Electronic Structure Studies 108

5.6.2 Charge Density 109
5.6.3 Atomic Orbital Projection Analysis 110
5.6.4 Investigating the Band Alignment 112
5.6.5 Intrinsic uncertainty via proximitized hetero interface 114
5.7 Conclusion 116
References 117
Chapter 6: Fluorescence guided Superparamagnetic g-C_3N_4@$FeNi_3$-heterostructure for cancer cell imaging and detection 121-140
6.1 Introduction 122
6.2 Methodology 124
6.2.1. Experimental Details 124
6.2.1.1 Chemicals and materials used 125
6.2.1.2 Development of g-C_3N_4@$FeNi_3$ Nanocomposite 125
6.2.1.3 PEG functionalized g-C_3N_4@$FeNi_3$ Nanocomposite 125
6.2.2. Biological assays 125
6.2.2.1. Cell culture 125
6.2.2.2. Cytotoxicity assays 126
6.2.2.3 In vitro nanocomposite characterization 126
6.2.2.4 Confocal microscopy imaging of g-C_3N_4@$FeNi_3$ 126
6.3 Results and discussion 127
6.3.1 Microstructural and Morphology 127
6.3.2 Magnetic Property 128
6.3.3 UV and PL Analysis 129
6.3.4 Thermal and Surface charge Analysis 131
6.3.5 Biological properties 133
6.4 Conclusion 135

References 136
Chapter 7: Conclusion and Future outlooks 141-145
7.1 Thesis conclusions 141
7.2 Future prospects 143
Appendices **A1-A2**

List of publications **B1-B3**