

## Abstract

Applications implemented using nanomaterials have gained increasing prominence in modern life, considering its numerous fascinating properties such as its morphologies, surface area, electronic, mechanical, optical properties, etc [1,2]. Nanomaterials in diverse morphologies and surface engineering are technologically advanced, breaking their shortcomings and spreading in almost all the branches of science and technology. One of such material which cannot be diversion is carbon based materials, whose intriguing properties have gained increasing efforts, identifying outstanding challenges and emerging opportunities [3,4]. Carbon-based materials with its multifaceted nature are attractive for the entire scientific community due to which they are explored in dynamic field. However, major limitation of carbon-based materials that maximizes its application in mass operation is the price of the materials [5]. Moreover, present separation and regeneration practices during environmental applications are costly and still continue to be a challenging task. Hence, to overcome the aforementioned hurdles, tailoring and developing of advance carbon-based materials appears to be one of a hopeful approach. Among them, Graphitic Carbon Nitride ( $g\text{-C}_3\text{N}_4$ ), a two-dimensional (2D) material with heptazine ring structure and high condensation degree enables its applicability, wrapping the majority of scientific areas (*e.g.* physics, biology, chemistry, medicine etc.). In addition,  $g\text{-C}_3\text{N}_4$  can be easily prepared simply through polymerization of urea, thiourea, melamine etc. which are abundant and cheap feedstocks existing in nature [6]. Further, presence of carboxyl and hydroxyl functional groups stretches its potential beyond the limited range. High exposed surface area with active accessible porosity within the system enhances its efficiency making them suitable for employing in wide scope of applications. Apart from its ideal stoichiometry, presence of nitrogen content marks them superior, in comparison to other carbon nanomaterials present. Among myriads of  $g\text{-C}_3\text{N}_4$  based materials with extraordinary mechanical, thermal, electrical and optical properties, adaptable dimensionalities (one-dimensional (1D),

zero- dimensional (0D), and bulk (3D)) with its technological progress have grown into a research edge in the past decades. This dimensionality in the nanoscale regime helps in tackling the future challenges by exploiting their properties. g-C<sub>3</sub>N<sub>4</sub> is a 2D layered material with strong in-plane bonds and weak van der Waals coupling between layers [7,8]. Engineering g-C<sub>3</sub>N<sub>4</sub>-based heterostructures helps in resulting satisfactory performances, drawing the attention of scientific worldwide. Creating heterostructures/heterojunction/heterointerface confines the charge carriers in the low band gap material. This confined charge carries have remarkable applications than non-confined carriers. Heterostructure of 2D materials offers many approaches to study uncountable phenomena, and open unprecedented potentials of combining them for technological use. Charge transfer between the layers can be very broad, inducing large electric fields and offering remarkable possibilities in band interface engineering [9,10].

In this roadmap we tried to seize the utmost collection of g-C<sub>3</sub>N<sub>4</sub> used in diverse applications, and identify its owing challenges and emergent opportunities. As per the objectives, in this present thesis main focus is directed on development of different 2D g-C<sub>3</sub>N<sub>4</sub> heterostructure materials by physical and chemical techniques. After development of the systems, it will be applied in various fields of application such as environmental, medical, food packaging/ preservation etc. Few exciting, unique and unusual findings were observed which are addressed in subsequent chapters of the thesis as below;

**Chapter 1:** This chapter summarizes the use of Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) material beyond catalyst. As analogue to that of graphene, this layered material can also be optimized and engineered into various dimensions. Through this chapter, we have briefly discussed the various preparation techniques, surface modifications, and new generation applications of g-C<sub>3</sub>N<sub>4</sub> in different domains to justify the merit of this wonder material. Along with experimental aspects, theoretical strategies are also highlighted to understand its unrevealed properties.

**Chapter 2:** This chapter reveals the novelty to understand the role of surface area with mesopore distribution in two dimensional sheets like composite materials, and its effect towards oil adsorption capacity and response time. The developed magnetic hydrophobic/oleophilic g-C<sub>3</sub>N<sub>4</sub>@FeNi<sub>3</sub> nanocomposite exhibits excellent oil sorption performance and rapid removal of adsorbed oil using an external magnet. Combining porous and nanosheets structure along with magnetic FeNi<sub>3</sub>, further surface functionalized with fatty acid makes the system an efficient adsorbent for adsorbing and separating various forms of oil from water. Understanding the detailed underneath kinetics and isotherm of the adsorption process, provides a completely new prospective to this study. The nanocomposite acts as promising adsorbent material for efficient oil recovery providing feasible solution towards the upcoming oil consumption.

**Chapter 3:** In this chapter we have addressed an in-plane micro supercapacitor by combining pseudocapacitive FeNi<sub>3</sub> and faradaic (redox electroactive) g-C<sub>3</sub>N<sub>4</sub> materials for fabricating miniature electronic devices, also implementing experimental studies supported by density functional theory calculation. The study reveals the novelty to understand the role of synergic effect of both electro double layer and pseudocapacitive components during the development of g-C<sub>3</sub>N<sub>4</sub>@FeNi<sub>3</sub> heterostructure, providing several electron channels for ion transfers within the system. We also envision that the present strategy may be extended to fabricate other ternary oxides as well as applications for flexible and lightweight electronics to expand the requirement of sustainability.

**Chapter 4:** Food wares are hygienically packaged to protect and preserve the food items from any unseemly alteration in terms of quality and shelf life. With time and human demands, there is continuous innovative evolution in food packaging. In order to stand by the needs in packaging, technological advance is mainly chaired

by nanotechnology. Nanomaterials in association with polymer can augment the benefits associated with existing technology, addressing better safety and environmental concerns. In this present chapter, for the first time we will be discussing the development of 2D/2D g-C<sub>3</sub>N<sub>4</sub>@CuSe heterostructure with lamellar architecture, creating tortuous pathway and hindering the penetration of water and gas molecules, protecting and preserving the food for longer duration. The enhancement in antibacterial activity, mechanical, thermal, barrier, shelf-life and biodegradable functionalities of the developed film promote to perchance the use for food packaging applications. Moreover, active packaging further controls the release of nanomaterial in to the food items leading towards safe packaging.

**Chapter 5:** Rapid recombination of photogenerated charge carriers in a single-component could not meet the required photocatalytic efficiency in dye degradation, and hence construction of *type II heterojunction* can improve the photocatalytic activity where individual component promote the separation of photogenerated carriers and integration respectively. This chapter is one of the novel attempts to explain the metallic nature, developed while generating heterostructure of p type CuSe and n type g-C<sub>3</sub>N<sub>4</sub> semiconductor. Developed 2D/2D g-C<sub>3</sub>N<sub>4</sub>@CuSe heterojunction promotes easy separation of photogenerated carriers that maintains the initial strong redox ability which helps in achieving catalyst with highly desired dye degradation.

**Chapter 6:** In this chapter we have discussed the development of g-C<sub>3</sub>N<sub>4</sub>@FeNi<sub>3</sub> heterostructure as a fluorescence imaging probe to detect and monitor the growth of cancer cells in human. Unique properties of the developed system mark itself as a key target next generation applicant, used in biomedical applications. The developed heterostructure with multiple abilities such as wide absorbance range, biocompatibility and in-built fluorescent will help in early detection of cancer cells to improve survival outcomes.

**Chapter 7:** Lastly, this chapter covers the broad conclusions drawn from all the chapters explaining development and characterizations of individual systems, used in a wide range. Moreover, this chapter also projects the future possibilities of g-C<sub>3</sub>N<sub>4</sub> in fundamental and applied research.

**Bibliography:**

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## List of keywords

Chapter Number	Keywords
1	Graphitic carbon nitride, Dimensions, Heterostructure, Multifunctional, Surface and interface
2	Graphitic carbon nitride, Hydrophobicity and oleophilicity, Magnetic nanocomposite, Oil-water separation and Oil sorbent
3	in-plane micro-supercapacitor, pseudocapacitor, electrochemical double layer capacitor, heterostructure materials and density functional theory
4	Plastics, Food packaging, Polymers, Two dimensional and 2D heterostructure
5	2D/2D heterojunctions, band alignment, CuSe nanoflakes, dye degradation and g-C <sub>3</sub> N <sub>4</sub> nanosheets
6	Fluorescence imaging, 2D nanomaterials Heterostructure, Superparamagnetic and Cancer Cells