

# **LAYER DEPENDENT PHYSICAL AND CHEMICAL PROPERTIES IN TWO DIMENSIONAL CARBON BASED MATERIALS AND THEIR HETEROSTRUCTURE**

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# Chapter 7

## Conclusions and Future Outlook

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### 7.1 Thesis Conclusions

The research work mainly focuses on development of 2D g-C<sub>3</sub>N<sub>4</sub> based heterostructure materials, evaluating their functionalities, and to test their efficiency in different field of applications. Various strategies were implemented such as developing hybrid nanocomposite with FeNi<sub>3</sub>, building heterojunction with CuSe to enhance functionalities towards better performances compared to its pristine form.

It was found that executing strategies such as metal doping or heterojunction, led towards formation of more active sites for photogenerated electron and holes recombination. Similarly, holes were injected to g-C<sub>3</sub>N<sub>4</sub> from the valence band of integrated species, leading towards charge transfer generation for better separation of e<sup>-</sup>/h<sup>+</sup> pairs which results in enhanced performance of the system.

Summary related to major findings and conclusions of work incorporated in this thesis are briefly discussed as follows.

✓ The study has addressed a nanocomposite system as a smart sorbent material for efficient oil recovery in presence of external magnet. This study reveals the novelty to understand the role of surface area with mesopore distribution in two dimensional sheet like composite materials and its effect towards oil adsorption capacity and response time. The oil that gets absorbed can be further separated from the developed system. Thus, combining porous 2D sheets with magnetic particles results in efficient recovery of oil within few fractions of seconds. The developed nanocomposite system demonstrates promising long-term performance for oil-in-water separation, opening a new solution to this inbuilt problem.

✓ Modern state in the arena of market concentrates on development of new equipment's with ease of construction and flexibility, added functionalities like light-weight, cost-effective and renewable features to significantly enhance the consumer's demand. In this work, we have developed a hybrid of 2D EDLC g-C<sub>3</sub>N<sub>4</sub> incorporated with pseudocapacitive FeNi<sub>3</sub>. Graphitic carbon nitride with highly mesoporous nature effectively enhanced the transmission of ions and electrons, concurrently the existence of FeNi<sub>3</sub> nanoparticles within the system helps in preventing the aggregation of graphitic layers to increase the capacitance. Looking into its high performance, promising lightweight and flexibility, the developed system can help in achieving the due requirements of higher voltages and operating currents in the pitch of flexible in-plane micro-supercapacitor.

✓ Packaging industries are using materials that are made of polymer which creates threats on the environment due to their non-degradability. In order to reduce the growing waste problem, easy degradable packaging materials could solve the problem to some extent. In content to this, correct and proper selection of materials are required which can fulfill the criteria of active packaging and also can be commercialized in future looking into the product quality. Looking into the poor barrier and mechanical properties of the natural polymers, their use in packaging applications has been limited. In this work we tried to report that small loading of 2D material increases the polymer properties in various activities such as mechanical, thermal etc. Addition to this, the antimicrobial properties of these materials helped in extending the shelf-life of the food to certain scale without spoilage. Moreover, easy biodegradability adds additional brilliance to this system which will save the earth from further soil pollution.

✓ Creating heterointerface with coupled 2D/2D heterostructure is a proficient approach to boost the systems charge separation for dye degradation activities. Thus, developing type-II band aligned 2D/2D face to face contact heterojunction facilitates rapid separation of photogenerated carriers with

complete degradation of dye. Heterojunction created between g-C<sub>3</sub>N<sub>4</sub> and CuSe were strongly attached, liable for boosting the photocatalytic ability of built systems.

✓ Fluorescence imaging has aided as biological imaging technology for tumor diagnosis, real-time monitoring of drug release and cancer therapy. In this work, we have integrated 2D g-C<sub>3</sub>N<sub>4</sub> nanosheets with FeNi<sub>3</sub> nanoparticles for sensitive and specific identification of cancer cells through enhancing the contrast in fluorescence imaging property. Moreover, FeNi<sub>3</sub> nanoparticles with excellent magnetic targeted ability when cladded with g-C<sub>3</sub>N<sub>4</sub> acts as photosensitive agent helping to ablate the malignant cancer with no obvious side effects during the process of detection. Further, the resultant heterostructure showed superparamagnetic behavior, which can be easily guided to the desired location simply with an external magnetic field. The bio distribution of heterostructure, along with cellular uptake inside the cells was also evaluated. In addition to their effectiveness as alternate to pervasive organic dyes, the PEG functionalized heterostructure display good dispersion and biocompatibility leading towards a potential candidate for cell imaging assays. Due to its efficient versatility and non-toxicity, the developed heterostructure shows to be potential candidates as synthetic platforms for imaging techniques with imaging applicability.

## 7.2 Future direction

It is to be mentioned that the overall enactment of developed 2D heterostructure/composite material is highly dependent on properties and dimension of the 2D materials. Higher the surface area, more efficient performances can be seen. However, while noting the performing of oil separation using g-C<sub>3</sub>N<sub>4</sub> based materials, further studies can be conducted with respect to its morphology and pore dimensionality. As, designing g-C<sub>3</sub>N<sub>4</sub> based membrane with shorter and less tortuous transport pathways will further expand new ideas in maximizing the separation capacity of oil-water separation. Therefore, in further research, it is meaningful to improve the membrane performance by controlling the physical

properties rather than tailoring the chemical properties of the materials. Also, in-depth separation mechanism molecular transport behaviour occurring within the structure needs to be investigating properly.

Although many significant outcomes have been achieved for g-C<sub>3</sub>N<sub>4</sub> as a flexible supercapacitor, challenges are still remaining which restrict its applications in conducting technology in pilot scale. Such challenges are as follows: (1) Understanding the mechanism between the surface/interface and the electrolyte so that the performances can be enhanced. (2) Although significant progress has been achieved on designing flexible supercapacitors, but challenges still remain to engineer the same with high power density, energy density and stability. (3) Lastly, it can be used in the domain of flexible wearable devices. It is expected that after appropriate modification of g-C<sub>3</sub>N<sub>4</sub> with other materials, it will further expand its possibilities in flexible supercapacitors.

Currently, many applications related to dye degradation have been achieved using g-C<sub>3</sub>N<sub>4</sub> based composite. However, there are numerous disputes remained to be resolved mainly when queries raised related to (a) structural variety of dyes and its mechanism of photocatalyst processes, (b) in-depth analysis is required to understand the adsorption mechanism of dyes (organic) in g-C<sub>3</sub>N<sub>4</sub>, (c) lastly, the system stability and their recycling ability. Solving the above problems could provide a better future direction in understanding and designing high efficiency catalyst.

The innovation and strategy to add g-C<sub>3</sub>N<sub>4</sub> based nanomaterials in food packaging domain has brought many changes in food packaging, its storage and preservation. Thanks for the antimicrobial properties which helps in extending the shelf-life of the food to certain scale without spoilage. Apart from storage, more attention has been gained in solving the environment problem due to its cost effective, eco-friendly and easy degradability nature. Lastly, ethical

questions regarding toxicity and ion migration of g-C<sub>3</sub>N<sub>4</sub> is pertinent to study in details in order to use nanomaterial work better in this field.

g-C<sub>3</sub>N<sub>4</sub> has an energy band of 2.7 eV emitting blue fluorescence as their absorption is located in ultraviolet region. Although g-C<sub>3</sub>N<sub>4</sub>-based materials have been applied to biosensors and imaging based on their photoluminescence properties. However, lack of absorption above 460 nm and low surface area limits superiorities. Thus, combining g-C<sub>3</sub>N<sub>4</sub> with some 2D heterostructure/nanocomposite material will further help in achieving performers better as a photodynamic photosensitizer. Moreover, few other factors can be addressed such as (1) optical tunability that is still inadequate to ultraviolet region, (2) being a photosensitizer, g-C<sub>3</sub>N<sub>4</sub> efficiently generate free radicals but their conversion efficacy still requires to be further enhanced, (3) in-depth assessment required regarding the toxicity of g-CNs. (4) Being an excellent candidate with good electrical property, further investigations are required to develop integrated biosensing platform to monitor multiple biomolecule indicators.

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