CHAPTER IX

CONCLUDING REMARKS

This thesis explores the synthesis of supramolecular assembly as well as a detailed study of the characterization, and a comparison of the structure and dynamic properties of the inclusion complexes formed between cyclodextrins and a variety of biologically active guest compounds (i.e., TgC, RB, AMB, and UMB) in aqueous phase and in the solid state with experimental as well as computational based methods and graphene based nanomaterials and their characterization by different methodologies. The main contributions of this thesis are ***(1)*** *synthesis and characterization of inclusion complexation of biologically potent molecules with different cyclodextrins derivatives;* ***(2)*** *synthesis and characterization of GO-βCD-NB nanocomposites by covalent grafting technique and its various photophysical properties;* ***(3)*** *Comparison of traditional experimental approach through computational methodologies;* ***(4)*** *Enhancement of solubility as well as oral bioavailability of Guest molecules by cyclodextrin derivatives through complexation.*

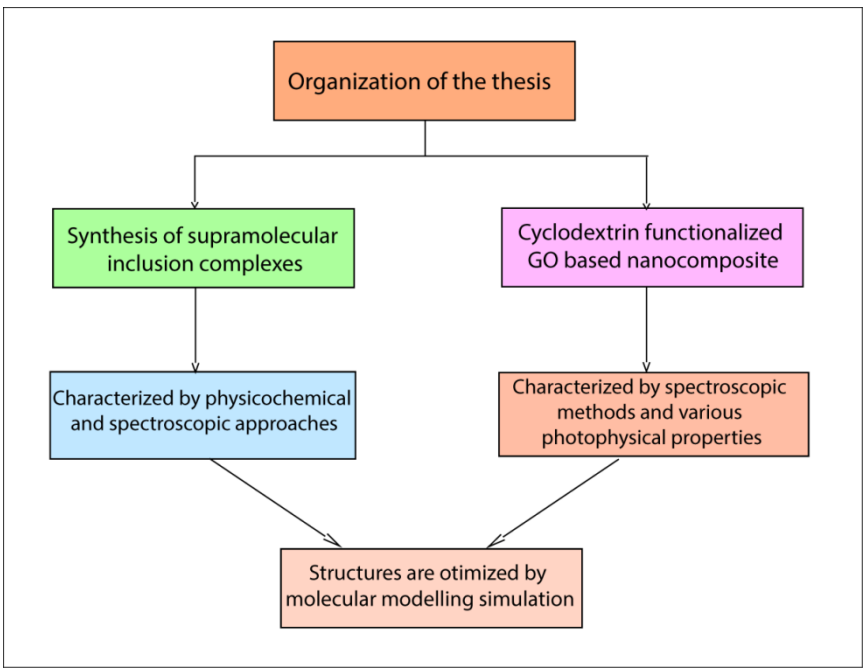
1. Significant contribution of the work:

An overall review on supramolecular chemistry, different biologically potent guest and supramolecular host, graphene and graphene based materials, carbon nanotube, etc. is given in **chapter I**. Structural properties and important applications of these subjects are also elaborated in this chapter. The materials used and experimental methods adopted for the thesis work is included in **chapter II** along with an overall idea about the principle and working of various characterization tools.

In **chapter IV**, the synthesis and characterization of ambroxol hydrochloride (AMB) with two different cyclodextrins using co-precipitation method is described. The inclusion complexes have been characterized using FTIR, UV-visible absorption spectrum, ^{1}H and 2D-NMR, ESI-MS and SEM. The mechanism for the formation of inclusion complexes proposed based on experimental evidences has been confirmed by computational simulations. Our findings are significant in such way that when

inclusion complexes are being formed, physiochemical properties as well as structure and dynamic properties of host-guest systems are getting improved.

In **chapter V**, we have designed a strategy to synthesize cyclodextrin functionalized graphene oxide based nanocomposites. The structure and photophysical properties of the whole nanocomposites were further characterized by using UV-vis, fluorescence, DLS, zeta potential and FT-IR spectroscopic, thermal analyses (TGA) methods. Study showed that fluorescence quantum yield, molar extinction coefficient, stokes shift of the nanocomposites can help to use in different biomedical applications.



Scheme 1: Research outline and organization of the PhD thesis

In **chapter VI** to **VIII**, trigonelline hydrochloride (TgC), rebamipide (RB), Umbelliferone (RB) and different host molecules (αCD, βCD, HP-β-CD) have been used to prepare supramolecular complexes. The prepared inclusion complex was characterized by ^{1}H-NMR, FTIR spectroscopy, ESI-MS, DSC, fluorescence spectroscopy and different computational methods. All the ICs are well characterized by experimental as well as optimized by molecular docking methods. Due to the increased aqueous solubility and bio-availability, they can be used for further biological as well as pharmaceutical applications.

2. Scope for future work:

Enough scope is available in both experimental and modeling of nanocomposites with this work as basis. The possibilities of future explorations with this work as a platform are discussed in this section.

The graphene based model developed in this work can be extended to biological field as this nanocomposite has all the respective properties of the materials. The synthetic strategy of nanocomposites has been carried out with an eco-friendly method. Functionalization on graphene oxide with β-cyclodextrin followed by encapsulation with nile blue can be used as sensors, imaging probes and therapeutic agents. It is known that graphene-based nanocomposites are the most widely used materials due to chemically susceptible structures. For drug delivery or therapeutics, cyclodextrin based inclusion complexes are widely used materials. Therefore, inclusion complexes that are already characterized could be extended to formulate for different clinical purposes such as targeted drug delivery, imaging, nanocarrier and therapeutics. Therefore, inclusion complexes as well as graphene based materials provide a platform for the fabrication of different supramolecular-nanomaterials with tunable chemical and photophysical properties for targeted applications in biomedical research prior to that their toxicity, availability, biocompatibility, and biodegradation need to be further investigated before proceed to future clinical uses.

3. Closures:

The comprehension of this investigation provides the insight into comparison between experimental observations with theoretical as well as computational data in a very simplified method. This thesis also depicted the scenario of cyclodextrin based supramolecular chemistry with graphene based nanocomposites and helps to correlate these two different fields. This approach can be used to create novel materials with superior properties for predicting different purposes such as sensing, drug discovery, cell imaging, which can help to broader the band of biological applications.