Chapter 7

7. Conclusion and Future Scope

7.1 Conclusions

In summary, it may be concluded that a facile and one-pot method is reported for the reproducible synthesis of ultra-stable BSA-capped MgNCs in an aqueous medium with multifluorescent emission and high relative quantum yield of 1.2% and 4.6% for blue and green emission. The evolution was further probed by several microscopic and spectroscopic techniques such as HR-TEM, UV-Vis spectroscopy, Fluorescence spectrophotometer, XRD, XPS, FTIR, CD spectroscopy, confocal microscopy, lifetime decay analysis, and MALDI-TOF. The as-prepared particle exhibited tunable fluorescence with board FWHM (120 nm), excellent biocompatibility, wide-range pH stability, persistent photostability, and good ionic strength tolerability. This characteristic of prepared MgNCs makes them ideal candidates for biomedical applications and ascertains their candidature for better bioimaging and labeling purposes. The prepared clusters exhibit prolonged shelf life in terms of fluorescence in both solution and powder form (only ~20% decrease in intensity after one year of storage). For the appraisal of their labeling capacity, in-vitro studies have been performed in HaCaT (Keratinocyte cell lines) cells.

Furthermore, Lysozyme-capped MgNCs have been synthesized to examine the effect of positively charged proteins on the synthesis and fluorescence properties. The prepared Lyz-MgNCs were used to label U-87 MG cells using confocal microscopy. For the estimation of the penetration depth of Lyz-MgNCs, CTCF analysis was performed for all red, green, and blue channels. Additionally, the biocompatibility results demonstrate negligible toxicity and remarkable proliferation capability in the U-87 MG cell line. In order to evaluate their applicability in real life, we also demonstrated their efficacy in terms of biocompatibility and fluorescence emission in rodents. Their histopathology reports in Charles foster rats after 28 days of administration of Lyz-MgNCs suggested negligible lesions and structural deformation in vital organs. Furthermore, the calculated hemolysis percentage in the blood of healthy rats lies in the prescribed percentage range. For the analysis of imaging capacity in real-time, we performed an in vivo imaging system in healthy rats and concluded that significant accumulation and excellent signal acquisition. The IVIS images show the highest accumulation in the brains of rats, which suggests the penetrability of Lyz-MgNCs in the blood-brain barrier. However, We found that negligible change in the fluorescence behaviour and stability of lysozyme-capped MgNCs (Lyz-MgNCs) compared to BSA-capped MgNCs (FMNCs).

Apart from bioimaging application, magnesium-based nanomaterial was utilized to combat microbial growth. For this purpose, Magnesium gel derived from peppermint essential oil has been developed for the first time using a one-pot, simpler, and sustainable method. The well-characterized Magnogel (30-40 nm) is suitable for various advanced applications in view of the adopted greener methodology supported by plant-based essential oil used in aqueous medium and devoid of harmful chemicals. Prepared gel endowed with a remarkable antibacterial, antifungal, and angiogenic. Consequently, it is safe to suggest that the incorporation of peppermint oil into nanomaterials can serve as a natural bio-adsorbent in materials science, and similar strategies can be applied to other abundant, renewable, natural, and safer extractives. Due to their significant antifungal, antibacterial, and angiogenic activity, the study paves the way for the fabrication of essential oil-mediated MgNPs to develop smart infectious disease-fighting strategies.

Besides understanding their nucleation process and phase transformation from amorphous to crystals in a high-temperature range, we utilized thermogravimetric non-isothermal models to compute nucleation rate and interfacial energy at each conversion point and temperature. For this purpose, raw TGA data of ultrasmall metallic Mg nanoclusters were obtained and utilized to compute the apparent value of activation energy using several models such as KAS, FWO, Starink, Tang, Vyazovkin and Vyazovkin AIC. Afterward, the KAS equation derived the pre-exponential factor, and computed activation energy values were employed to determine thermodynamic parameters such as ΔH, ΔG, and ΔS in all conversion points. In order to predict the degradation pathway of MgNCs, a differential function $f(\alpha) = (1 - \alpha)^3$ of random nucleation mechanism was detected using $z(\alpha)$ master plots. Mathematically, the derivation of nucleation rate and interfacial energy models suggested the exponential and linear relation, respectively, with temperature and conversion points. The nucleation rate was also computed concerning different heating rates (10, 15, and 20 °C/min) and observed an increasing trend with a rise in heating rate and this phenomenon is due to a decrease in heat and mass resistance with an increase in temperature. At the same time, the average value of interfacial energy was found to be 125.95, 127.07, and 127.86 mJ/m^2 at 10, 15, and 20 ^{0}C/min, respectively. Current research opens a door in nanoscience and technology for the determination of nucleation rates and interfacial energy of ultra-small clusters at high temperatures and respective conversions.

7.2 Future Scope

In the future, magnesium nanoclusters will hold great promise and potential across various fields due to their unique properties and applications. These nanoclusters are expected to play a significant role in the following areas:

- The obtained antibacterial property and angiogenic response of magnesium nanoclusters could be utilized for wound healing applications.
- Due to their ultrasmall size and high surface-to-volume ratio, the nano-enzymatic, such as the peroxidase-like and oxidase-like activity of nanoclusters, should be investigated.
- The fluorescence capacity of MgNCs could be avail in the biosensing application of metals and biological compounds.
- Magnesium acts as an important element for the human body; in the future, it could also be utilized as a theragnostic agent.
- Demonstration of their stability at higher temperatures makes it also liable towards optoelectronics applications.