INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
PhD-17 SHORT ABSTRACT OF THESIS

Name of the Student	:	Rubi Moral
Roll Number	:	216122043
Programme of Study	:	Ph.D.

Thesis Title: Supramolecular Self-assembly of Low Molecular Weight Receptors: Aggregation, Chemosensing and Gelation Study

Name of Thesis Supervisor(s)	:	Prof. Gopal Das
Thesis Submitted to the Academic Division	:	Chemistry
Date of completion of Thesis Viva-Voce Exam	:	5/06/2026
Key words for description of Thesis Work	:	Self-assembly, AIE, Sensing, Supramolecular gel

SHORT ABSTRACT

This thesis reports the design and synthesis of small organic probes/receptors to investigate their self-assembly properties and the stimuli-responsive behaviour of the resulting self-assembled systems towards environmentally and biologically important analytes. The solid-state self-assembly patterns of the receptors were examined by single-crystal X-ray diffraction analysis. On the other hand, solution-state aggregate formation was investigated using UV-Vis, fluorescence, and DLS analyses. Furthermore, the aggregation-induced emission (AIE) properties of the synthesized receptors in a binary solvent system containing an organic solvent and water were initially verified by fluorescence spectroscopy; subsequently, the morphological analysis of these aggregated systems was performed by FESEM. Slight structural tuning of these receptors could modulate their aggregation behaviour. Afterwards, these self-assembled systems were utilized as a sensing platform for various toxic metal ions, biologically important anions, as well as small organic molecules. Cost-effective paper strips were also developed to show real world applicability of these sensor systems.

The thesis also reports the rational design of low-molecular-weight gelators (LMWGs) for the construction of a supramolecular gel. The LMWGs thus obtained were used to adsorb small molecules, such as methyl orange and bromophenol blue, from water. Further, three adipic dihydrazide-based pyridine-functionalized positional isomers were synthesized to explore the effect of positional isomerism on metallogelation behaviour. It was interesting to observe that only the para- and meta-isomers showed selective metallogelation behaviour with $AgNO_3$ and $CdCl_2 \cdot H_2O$, respectively. The silver metallogel subsequently facilitated the in-situ formation of AgNPs within the gel matrix, and the gel nanocomposite showed antibacterial activity against the bacterial strains *B. subtilis* and *E. coli*. Nevertheless, the idea of selective metallogelation of the meta-isomer only in the presence of $CdCl_2 \cdot H_2O$ was further exploited for the visual detection of Cd^{2+} via gelation in various real water samples. Moreover, a rare anion-induced supramolecular gel was also synthesized selectively in the presence of SO_4^{2-} and HSO_4^-, which could exhibit selective stimulus-responsive properties towards picric acid.

In summary, this thesis explores self-assembled systems that exhibit fascinating aggregation and stimuli-responsive properties and demonstrates modulation of their aggregation via small structural modifications. The thesis also shows the importance of the receptors' design rationale for the formation of supramolecular gels and for the utilization of such systems for various applications, thereby making them smart functional materials.