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

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Thesis Title: Anion Coordination and Gelation Study of Small Molecule based Self-assembled Systems: Recognition, Sensing and Water Remediation

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SHORT ABSTRACT

This thesis reports the design of small organic molecule-based self-assembled systems for the study of anion coordination and gelation behaviour. Artificial receptor systems were rationally designed for the recognition of anions in both solid and solution states. The solid-state anion recognition behaviour of the receptor molecules was extensively analysed by single-crystal X-ray diffraction, whereas the solution-state anion recognition study was performed by NMR. The anion recognition potential of the receptor systems could easily be modulated by synthetically tuning the structures of the receptor molecules. Subsequently, the concept of anion recognition was further applied to highly selective and sensitive sensing of toxic anions, such as cyanide, in drinking water, and its real-world applicability was demonstrated using a simple, cost-effective paper strip method. Such highly sensitive sensing of toxic anions was achieved by modulating the self-assembly of the fluorogenic nanoprobes through incorporation into micelle systems.

Furthermore, the self-assembled systems were rationally engineered to yield low-molecular-weight gelators (LMWGs) capable of forming supramolecular gels. The resulting gel was used as a stimulus-responsive material, and the concept of anion recognition and gelation was integrated to develop an anion-responsive supramolecular gel. Moreover, by combining LMWG with a polymeric gel, a hybrid gel was constructed that could sequester precious metal ions from water, followed by spontaneous in-situ reduction of the metal ions within the gel matrix, thereby forming a conductive hybrid gel nanocomposite. Afterwards, a phase-selective organogelator (PSOG) was developed for the highly selective gelation of some specific oil samples. The idea of selective gelation was utilised for the cost-effective visual detection of fuel adulteration. Lastly, this thesis demonstrates how the phase transformation of a kinetically trapped supramolecular gel can be well regulated to yield single crystals with specific crystal habits and unveils the underlying complexity of the associated pathways.

Overall, this thesis demonstrates how the high structural tunability of small-molecule-based self-assembled systems can be exploited to construct molecular systems utilised for the development of functional materials with diverse applications, including recognition, sensing, and water remediation.