INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title: **Aggregation Aptitude in Rigid and Flexible Molecular Systems: Comparative Photophysical and Analytical Studies**

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Thesis Submitted to the Department/ Center : Chemistry

Date of completion of Thesis Viva-Voce Exam :11/10/2023

Key words for description of Thesis Work : Supramolecular Chemistry, Self-aggregation, Chemo-sensors

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SHORT ABSTRACT

This thesis elucidates the important consequences in comprehension of aggregation outlook of flexible and rigid frameworks and their response towards environmentally and biologically relevant analytes. **L_1-L_3** is designed which shows a comparative aggregation aptitude with chain length variation in amphiphiles. The entire photophysical study on aggregation process is dealt with. Then, these synthesized amphiphiles are used in creating hydrophobic surfaces due to their inherent property of hydrophobicity. Additionally, the concept of Photoinduced Electron Transfer or PET is applied in the detection of nitro antibiotics via fluorescence quenching. This chemo sensing is probed in biofluids viz; simulated gastric and body fluid. Next, a layout is provided where a comparative study between an amphiphile and a non-amphiphile is presented. The compounds designed and synthesized were substituted urea and amide (**L_4** & **L_5**). Studies on aggregation-induced emission are shown by a binary solvent system DMF-Water. Morphological change is depicted on solvent switching by electronic microscopy imaging. Both solid and solution state emissive property is described. A unique photophysical prospect is shown in this piece of work i.e., light harvesting. Förster resonance energy transfer or FRET mechanism delivers the basis for this light-harvesting phenomenon between the amphiphile and a commercial dye; Rhodamine. Again, PET is applied to detect nitro explosives in water is demonstrated. This detection proceeds via disaggregation of the aggregated state. In the allied chapter, functionalization of amphiphile was done: a comparative outline on substituted urea and thiourea (**L_4** & **L_6**). Apart from describing aggregational features through spectroscopy and microscopy, an edge on the chemo-sensing property is done. The thiourea selectively recognizes Hg (II) ions in an aqueous solution due to the soft-soft interaction between the sulfur atom and the heavy metal. Turn-On or fluorescence emission enhancement is achieved even in the presence of heavy metal during the chemosensing process. The toxic metal ion interaction causes disaggregation of the aggregated amphiphile confirmed through DLS and FESEM experiments. The chemo-sensing experiments are done in various real samples. Moreover, The Hg(II)-amphiphile ensemble detects sulfide ions in the water among all other sulfur-containing anions and amino acids.

After detailing the aspects of aggregation and chemo sensing, the thesis provides an outline on the rigid molecular framework. The quinoxaline motif was selected as the rigid template. Possible functionalization is done on the molecular framework and photophysical studies concerning the aggregation behavior is conducted. **L_7-L_{11}** proved to be AIEgen and the emission changes are shown by solvent switching of a binary solvent system (THF-Water). Both microscopy and spectroscopic studies are carried out. Not only aggregational features are shown in the solution phase but also solid-state studies i.e., crystalline packing are illustrated. Among all of them, the carboxylic acid group variant selectively interacts with a common surfactant: Cetyltrimethyl Ammonium Bromide (CTAB). This is due to the electrostatic interaction overpowering the non-covalent interaction via disaggregation of the emissive aggregated state. The detection is not limited to aqueous solution but tested with real water samples. Domestic wastewater and factory effluents are chosen as media to confirm the detection ability.

The last chapter, **L_{12}-L_{14}** shows a variation in optical and analytical prospects upon functionalization of the quinoxaline scaffold. **L_{12}** & **L_{14}** differed in aggregation aptitude. **L_{14}** showed solvatochromism and acidochromism. Now, this acid sensitivity or stimuli responsiveness is utilized in tracking urease enzyme activity and monitoring the freshness of food samples. The metalloenzyme activity is tracked via absorption, emission spectroscopy, and fluorescence microscopy.

In essence, we propose that this thesis will provide a significant contribution to the communities of supramolecular chemistry and analytical chemistry for improving in understanding and progress in the specific field of research. This thesis is intended to spark an additional investigation into exciting photophysical properties as well as sensing ability using this kind of small molecule motif with an aggregative nature.