INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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The thesis is formulated into 7 chapters along with summery. Chapter 1 is the introduction describing important aspects of fluorescence such as intramolecular charge transfer (ICT) and proton transfer (ESIPT), factors effecting ICT and ESIPT, nanoparticle-fluorophore interaction motivating for the present research works planned. Chapter 2 is about materials, methodologies and instrumentations such as UV, steady state and time resolved spectrophotometer, FESEM, TEM etc. Chapter 3 describes the interactions of the silver nanoparticles with 2-(4′-N,N-dimethylaminophenyl)benzimidazole and its nitrogen substituted analogues. These fluorophores are well efficient in stabilizing the nanoparticles. These interactions led to the formation of TICT state from the nitrogenous analogues in aprotic solvent for the first time. Complexation with β-cyclodextrin strengthen the TICT emission. Chapter 4 elaborates the extraction of same set of ICT fluorophores as in chapter 3 from nanoparticle composite by micelles of different ionic character. Silver nanoparticles in water were prepared by reducing silver nitrate salt using simple borohydride reduction method without any other common stabilizing agent. The hydroxyl ion present in solution acted as stabilizer at specific p^H of 10. All three fluorophores interact with silver nanoparticles prepared in water through the ring nitrogen with static quenching. The fluorescence of the fluorophores can be recovered by addition of surfactant. The micelles were found to be well efficient to extract the fluorophores from the nanoparticles surface into their hydrophobic cavities. It seems that the CTAB has stronger interaction with the nanoparticles than TX-100. Interaction of nanoparticles with the same set of fluorophores present inside the BSA pocket is explained in chapter 5. Addition of silver nanoparticles to these systems lead to some conformational changes in the tertiary structure of the protein leading to exposure of the fluorophores. The blue shift of the BSA emission in presence of silver nanoparticles confirms the conformational change of the BSA (instead of total denaturation). These fluorophores-nanoparticles interaction resulted in the quenching of the fluorophore emission with bathochromic shift. The magnitude of the quenching of the fluorescence of the fluorophores by nanoparticles in presence and absence of BSA confirmed that the fluorophores didn't detached from the BSA pocket. Chapter 6 is the suppression of ESIPT of 2-(2'-hydroxyphenyl)benzimidazole (HPBI) and its nitrogenous analogues on the surface of nanoparticles. HPBI and its nitrogen substituted analogous undergo ESIPT in different environments. The normal emission was obtained from the trans-enol form and the keto emission was observed due to ESIPT of cis-enol. In this chapter, the ESIPT processes of these molecules on surface of silver nanoparticles were elaborated. Silver nanoparticles reduced the fluorescence of both the emissions of HPBI without any significant shift in the spectrum. But the decrease in the fluorescence of HPIP-b and HPIP-c were accompanied by a huge bathochromic shift of the tautomer band. These red shifts

indicate that the interactions occurs through the pyridyl nitrogen which increases the conjugation. The intensity ratios depicted that the normal band intensity increases at the cost of tautomer emission in pyridoimidazoles. As the interaction occurs through pyridyl nitrogen, due to conjugation the charge flow from the azole nitrogen to pyridyl nitrogen. This reduces the basicity of the azole nitrogen which weakens the intramolecular hydrogen bond. Therefore, the ESIPT process was hindered on the surface of nanoparticles. Proton transfer is affected most in HPIP-c followed by HPIP-b and is less in case of HPBI. Chapter 7 briefs the facile synthesis of spindles, rods and niddles from HPBI and its nitrogen substituted analogous through aggregation induced enhanced emission from excited state intramolecular proton transfer. All the fluorophores aggregated in proper solvent mixture of methanol and water to form aggregates. The shape of aggregated structures varies depending on the fluorophores. HPBI is giving spindle shaped structures. Long needles and short rods are obtained from HPIP-b and HPIP-c respectively. The aggregates of all fluorophores are compatible with HeLa cell and gave good fluorescence inside cell. The monomer fails to give fluorescence inside cell. The van der Waals and weak hydrogen bonded interactions play vital role in aggregate formation as obtained from molecular dynamics simulation study.