



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
SHORT ABSTRACT OF THESIS

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Thesis Title: **Investigations on Protein Charge Transfer Spectra among charged amino acids and monomeric proteins**

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**SHORT ABSTRACT**

The present thesis revolves around the central theme of photoinduced electron transfer involving side chains of charged residues and peptide backbone in proteins, its consequent absorption spectra (termed as Protein Charge Transfer Spectra or ProCharTS) and luminescence from charge transfer states. The solutions of pure charged amino acids (Lysine, Glutamate and their capped derivatives) and selected proteins rich in charged residues display similar excitation and emission spectra apart from showing significant ProCharTS. However, their drastically different extinction coefficients clearly demonstrates the crucial role of proximity of interacting side chains towards charge transfer transitions. Apart from this, similarity in their Stokes shift, quantum yield and luminescence lifetime suggests towards the common origin and that could be charge recombination dependent luminescence. The lower quantum yield and luminescence lifetime hints towards the lower rates of charge recombination. Moreover, the extinction coefficient was found to be the major contributor towards the origin of luminescence from charge transfer states.

Since, the observed luminescence are excitation wavelength dependent and are significant in UV-Visible region, they are found to modulate the fluorescence of other chromophores sharing

the same spectral region. It was found that the charged residues in the vicinity of indole not only quenched the fluorescence lifetime of Trp but also changed the decay kinetics of excited state population. This could be one of the reasons behind the multi-exponential decay of Trp in proteins. Similarly, the effect of intrinsic luminescence from charge transfer states was also observed to modulate the fluorescence of an extrinsic fluorophore, Dansyl conjugated to a moderately charged protein, human serum albumin.

Further, the ProCharTS was found suitable in monitoring protein unfolding as well as protein aggregation. Both the molecular events revealed insights on the dependence of ProCharTS on the proximal distance between the interacting side chains as well as their population and density at any given condition. The decrease in the Stokes shift upon formation of fibrillar hen lysozyme aggregates hold the assumption of their (ProCharTS luminescence) sensitivity towards the solvent exposure. Finally, the increase in intrinsic luminescence from lysozyme aggregates with time was observed in spite of decrease in their luminescence lifetime and quantum yield, which signifies the major contribution from extinction coefficient in the origin of such intrinsic luminescence.