A Computational Framework to Generate the Charge Transfer Spectral Profile of Proteins

Apoorva Badaya
Venkatramani Group, Department of Chemical Sciences,
Tata Institute of Fundamental Research, Mumbai

Recent experimental studies have shown that the spectra of monomeric proteins rich in charged amino acids span the entire UV-Visible spectral band (from 200-800 nm). Computational investigations have demonstrated that such broad absorption profiles of the proteins arise from photoexcited charge transfer (CT) transitions in spatially proximal charged amino acids such as lysine (Lys) and glutamate (Glu). This novel label-free spectral band is therefore termed Protein Charge Transfer Spectra (ProCharTS). Previous computational studies of the phenomena have been limited to generating and studying the spectra from specific ensembles of charged amino acid monomers and dimers. Our objective is to generate the ProCharTS spectral profile of the entire protein which arises from a spatiotemporal convolution of all the charged amino acid chromophores present in protein. In this talk, I will discuss the ProCharTS of protein obtained based on our computational strategy using classical molecular dynamics simulations and DFT-based electronic structure calculations. ProCharTS is dependent on charge complementarity, distance and the conformation of the charged amino acids. Thus, ProCharTS should be able to capture the biological events in the body, which modify the charged state of amino-acid residues. To validate this hypothesis, we investigated the impact of acetylation of lysine residues on the ProCharTS profiles of human serum albumin and alpha3C. We find that the ProCharTS of the protein is sensitive to the alteration of the charged state of amino-acids and I will talk about our progress in detail in studying some of these systems and my future plans.