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

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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 ensembles of charged amino acid monomers and dimers with some controls being carried out on tetramers. Our objective is to generate the ProCharTS spectral profile of the entire protein which arises from a spatiotemporal convolution of charged amino acid clusters of multiple orders (e.g. monomers, dimers, trimers). In this talk I will discuss our computational strategy based on classical molecular dynamics simulations and DFT-based electronic structure calculations to generate the ProCharTS profile of proteins. We hypothesize that the absorption of ProCharTS should be responsive to events that neutralize or modify the charged state of protein residues. Such events comprise biologically significant processes such as a) post-translational modifications, b) interactions between protein subunits c) protein-protein interactions, d) interactions between protein and DNA interactions, and e) protein folding. To validate this hypothesis we aim to examine the ProCharTs profiles of Human serum albumin, Bovine serum albumin, alpha3C and histone proteins. I will discuss our progress in studying some of these systems and my future plans.