Time-dependent DFT investigation of the optical response in biological materials

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Photobiological reactions, which start with the light absorption as a source of energy, play a vital role in living organisms. During the last two decades, a wide variety of computational techniques have been used to study the mechanisms of photochemical reactions. Among all computational strategies for excited state calculation, TD-DFT methods are too attractive due to the possibility to achieve reliable accuracy at a much reduced computational cost and time compared to wavefunction-based methods (CIS, CC, MP2,).

The first part of this talk devoted to a brief review of TD-DFT basic concepts and their applications in biological materials. In the following, we present the TDDFT simulations of spectroscopic properties of some well-known biological chromophores such as chlorophyll a and b. Finally, we present an extract from a study conducted by our group on various spectroscopic properties of the Aβ_{30-35} monomers employing TDDFT. This study focuses on the characterization of low-lying excitations, correlation between geometrical collective variables and the optical response, and solvatochromic shifts for these flexible peptides. Our results clarify the role of charged residues in the less-considered charge transfer states.