Executive Summary of the UGC Minor Research Project

To understand fundamental aspects of Protein folding and to develop to predictive models to arrive at desired conformations and geometry

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As a part of studying hydrogen bonding in proteins and resulted folding the structure of DNA is intitially analysed. Optimised the DNA structure and analysed UV and IR spectrum of DNA molecule and its decomposition. The λ_{max} of the experimental spectrum is found around 260 cm^{-1}, and that of our theoretical spectrum is found around 240 cm^{-1}. These experimental and theoretical data agrees well semi-quantitatively, and this small shift in λ_{max} can be attributed to the quality of the basis set, and this can be improved by using better functional/solvation models. Since time-dependent-DFT calculation without vibronic coupling didn't reproduce the experimental UV-Visible spectrum, we calculated vibronic spectrum (ie. one-photon absorption spectrum based on Franck-Condon principle) of DNA (by adding the four Franck-Condon spectra of G, C, A, T moieties) and found a very good agreement with that of the experimental spectrum. A similar analysis was done with IR spectrum (using PM6 semi empirical theory), where the experimental IR spectrum of the DNA is compared with its constituents. The analysis suggest that, to get more correlation between the theoretical and the experimental IR intensity spectrum, more accurate level of theory is needed. The experience in the calculation will be extended to the protein structure.

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