Correlation between square of electron tunneling matrix element and donor-acceptor distance in fluctuating protein media

http://www.firstlight.cn 2008-10-15

Correlation between fluctuations of the square of electron tunneling matrix element TDA2 and the donor-acceptor distance RDA in the electron transfer (ET) reaction from bacteriopheophytin anion to the primary quinone of the reaction center in the photosynthetic bacteria Rhodobacter sphaeroides is investigated by a combined study of molecular dynamics simulations of the protein conformation fluctuation and quantum chemical calculations. We adopted two kinds of RDA; edge-to-edge distance REE and center-to-center distance RCC. The value of TDA2 distributed over more than 5 orders of magnitude and the fluctuation of the value of RDA distributed over more than 1.8 Å for the 106 instantaneous conformations of 1 ns simulation. We made analysis of the time-averaged correlation step by step as follows. We divide the 106 simulation data into 1000/t parts of small data set to obtain the averaged data points of t and t or t. Plotting the 1000/t sets of log10 t as a function of t or t, we made a principal coordinate analysis for these distributions. The slopes <βE>t and <βC>t of the primary axis are very large at small value of t and they are decreased considerably as t becomes large. The ellipticity for the distribution of t vs t which can be a measure for the degree of correlation became very small when t is large, while it does not hold for the distribution of t vs t. These results indicate that only the correlation between t and t for large t satisfies the well-known linear relation (“Dutton law”), although the slope is larger than the original value 1.4 Å–1. Based on the present result, we examined the analysis of the dynamic disorder by means of the single-molecule spectroscopy by Xie and co-workers with use of the “Dutton law”.

存档文本