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On the mechanism of non-radiative decay of blue fluorescent protein chromophore: new insight from the excited-state molecular dynamics simulations and potential energy calculations

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Abstract

A detailed theoretical investigation based on the *ab initio* on-the-fly surface hopping dynamics simulations and potential energy surfaces calculations has been performed to unveil the mechanism of the photoinduced non-adiabatic relaxation process of the isolated blue fluorescent protein (BFP) chromophore in gas phase. The data analysis presents that the dominant reaction coordinate of the BFP chromophore is driven by a rotation motion around the CC double bridging bond, which is in remarkable difference with a previous result which supports a Hula-Twist rotation pattern. Such behavior is consistent with the double bond rotation pattern of the GFP neutral chromophore. In addition, the dynamics simulations give an estimated decay time of 1.1ps for the S_1 state, which is agrees well with the experimental values measured in proteins. The present work offers a straightforward understanding for the decay mechanism of the BFP chromophore and suggestions of the photochemical properties of analogous protein chromophores. We hope the current work would be helpful for further exploration of the BFP photochemical and photophysical properties in various environments, and can provide guidance and prediction for rational design of the fluorescent proteins catering for different demands.

Keywords: Nonadiabatic, Fluorescent proteins, Excited state, Dynamics simulation

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