

Full QM description of phytochromes

A fully quantum mechanical treatment of chromophore-protein interactions in phytochromes

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In Short

- Quantum chemical calculations
- The fragment molecular orbital (FMO) method
- Chromophore-protein interactions
- Phytochromes

This proposal aims to identify and quantify the chromophore-protein interactions underlying the photochemical process of phytochromes by means of quantum chemical calculations. To this end, we propose to use the fragment molecular orbital (FMO) method in a set of phytochromes (Figure 1).

The FMO method is a general quantum chemical method and is one of the most efficient approaches for studying biomolecules[1]. In the FMO method, a protein can be divided into small fragments, for example, each residue can be represented as a fragment. In phytochromes, the fragmentation can provide accurate information about the most significant interactions between the chromophore and the rest of the protein. Furthermore, the chromophore can be also represented as an individual fragment or can be fragmented. Thus, a deeper understanding of the activation of the photocycle in phytochromes can be achieved.

FMO has also been used for studying the effect induced by amino acid substitutions. Thus, we propose to use this quantum chemical method for

evaluating the variation types and energy changes caused by mutations surrounding the chromophore in phytochromes.

Identifying the interactions between chromophore and protein can provide accurate information on the individual contribution of each residue to the different states of the photocycle of phytochromes. To this end, a fully quantum mechanical (QM) treatment of phytochromes will be carried out by using the fragment molecular orbital (FMO) method[2].

This quantum chemical method can evaluate with high precision and detail biomolecular systems by means of a partition scheme. Additionally, pair interaction energy (PIE)[3] between a pair of fragments can be decomposed into four energy terms: electrostatics, exchange-repulsion, charge transfer, and dispersion. These energy terms provide a valuable insight into the chemical nature of non-covalent interactions between proteins and ligands or chromophores. Non-covalent interactions like salt bridges, hydrogen bonds, or polar interactions are dominated by the electrostatic and charge transfer terms while hydrophobic interactions are driven by the dispersion term[4]. For the first time a fully quantum mechanical (QM) treatment of phytochromes will be carried out by using the computational power of the HLRN.

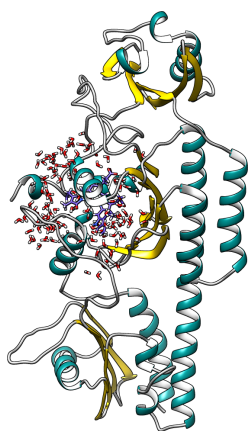


Figure 1: Phytochrome structure and water molecules within a radius of $\leq 10\text{\AA}$ around the chromophore

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<http://www.biomodeling.tu-berlin.de>

More Information

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