

Modeling of Phytochrome Absorption Spectra

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Phytochromes constitute a family of red/far-red absorbing photosensory proteins that function as control systems for several physiological and developmental processes in response to light conditions in plants, bacteria, cyanobacteria and fungi. Despite their important roles in Nature, comparatively few computational studies have been devoted to these proteins.

In this work [1], we assess the performance of hybrid quantum mechanics/molecular mechanics (QM/MM) methods for calculating the UV-vis absorption spectrum of the first phytochrome to be resolved by crystallography. We investigate how the choice of QM method and the size of QM system affect the computed spectrum, and demonstrate that good agreement (~ 0.15 eV) between calculated and experimental absorption maxima can be achieved for both the Q and Soret bands. Furthermore, for the Q band underlying the primary photochemistry of phytochromes, the calculations suggest that the overall long-range electrostatic effect from the protein environment tends to *red-shift* the intrinsic absorption of the bilin chromophore, whereas short-range chromophore-protein interactions overall *blue-shift* this peak.

[1] Falklöf, O., Durbeej, B. *J. Comput. Chem.*, 34:1363-1374, 2013.