1. Abstract

Project Code : TRG5780300

Project Title : The electrostatic effect on the photoisomerization of bacteriorhodopsin and halorhodopsin using QM/MM simulations

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Abstract: Bacteriorhodopsin (bR) and Halorhodopsin (hR) are both membrane proteins that transport ions across the cell membrane in halobacteria. Their ion transport function is triggered by the photo-activated isomerization of the retinal protonated Schiff base (RPSB) chromophore. Despite their similar structures, the RPSB isomerization rate/quantum yield are faster/larger in bR than in hR. Previously we simulated the photoisomerization reactions in bR and hR using ab initio multiple spawning (AIMS) with quantum machanical/molecular mechanical(QM/MM) method and successfully reproduced the experimental results in terms of the substantially differences in the isomerization rates and quantum yields between the two proteins. Here we continue an investigation of the role that electrostatic interactions play in the observed photoisomerization rate and quantum yield for bR and hR. The complex counterion of the positively charged chromophore is modified in bR/hR to be more/less negative than the native state. The dynamics simulations of the charge-modified systems reveal the evidently opposite results to those of the native proteins, i.e., the photoisomerization in hR becomes much faster while it is not observed in bR during the simulations of over 12 ps. This work confirms the crucial role of electrostatic interactions exerted by the complex counterion in the different isomerization rates between bR and hR, which have to be accompanied by a suitable charge delocalization within RPSB molecule upon photoexcitation.

Keywords: Photoisomerization, Bacteriorhodopsin, Halorhodopsin, Electrostatic effect, Excited state, Retinal protonated Schiff base, Simulation