Electronic Supplementary Material (ESI) for RSC Advances.

The effect of ion channel by different protonation states of E90 in Channelrhodopsin-2: Molecular Dynamics Simulation

Jie Cheng [a], Wenying Zhang [a], Shuangyan Zhou [a], Xu Ran [a], Yiwen Shang [a], Glenn V. Lo [b], Yusheng Dou [b], Shuai Yuan*[a]

a.Chongqing Key Laboratory of Big Data for Bio Intelligence, Chongqing University of Posts and Telecommunications, Chongqing 40065, China. E-mail: zhangwenying@cqupt.edu.cn, yuanshuai@cqupt.edu.cn

b.Department of Chemistry and Physical Sciences, Nicholls State University, P.O. Box 2022, Thibodaux, LA 70310, USA

Supporting Information

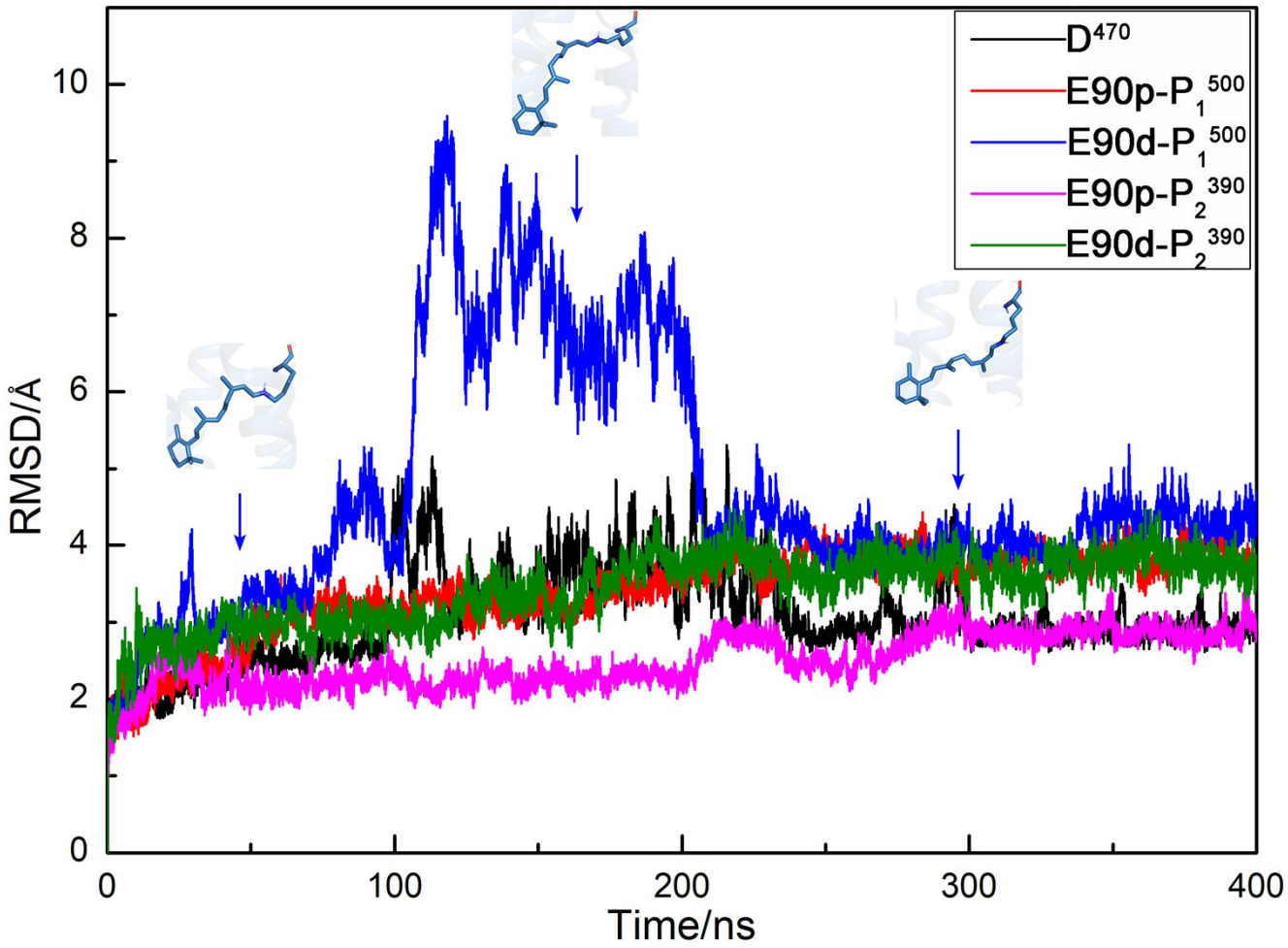

Fig. S1: Variations of root-mean-square deviation (RMSD) of skeleton atoms of channelrhodopsin-2 with time. The three diagrammatic drawings indicate the variation of retinal conformation in E90d-P_1^{500} state. The strongly fluctuations of E90d-P_1^{500} trajectory (blue curve) during 100 to 200 ns indicate the sharply conformational changes of polyene chain of retinal.

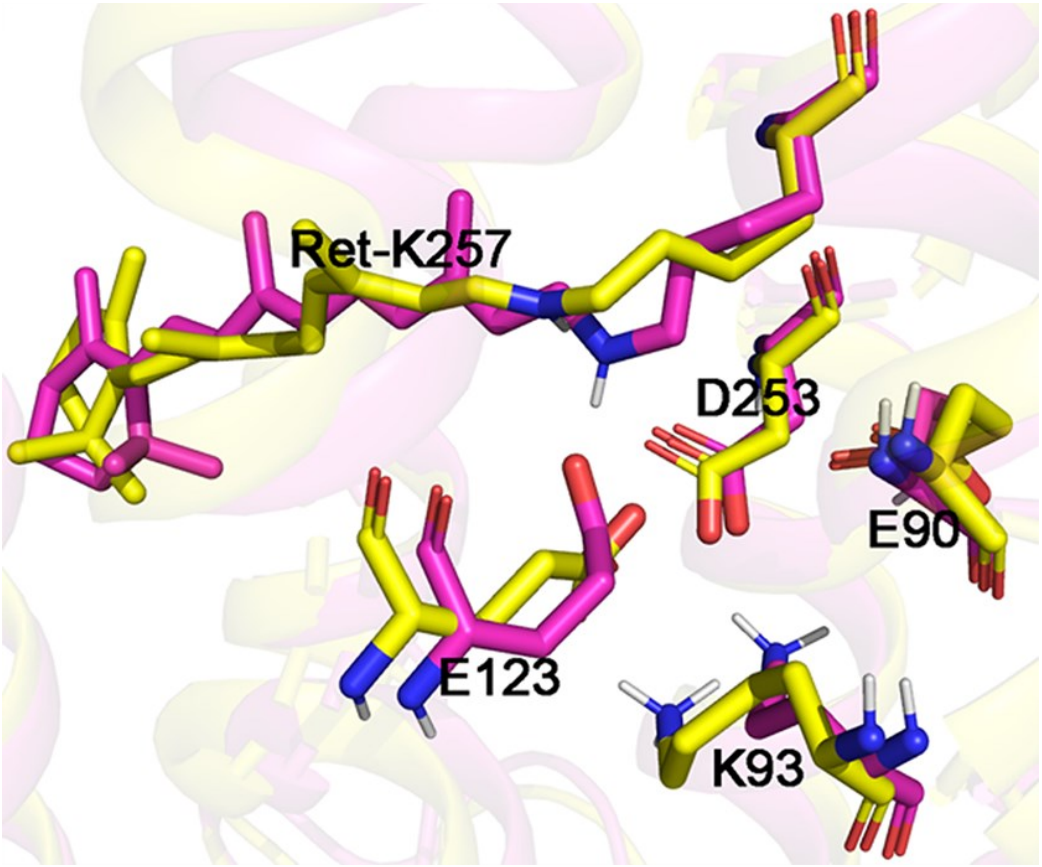

Fig. S2: The partially superimposed scheme of crystal structure of ChR2 (PDB ID: 6EID) and the structure of D^{470} state. Purple: the crystal structure of ChR2, yellow: indicates the structure of D^{470} state.

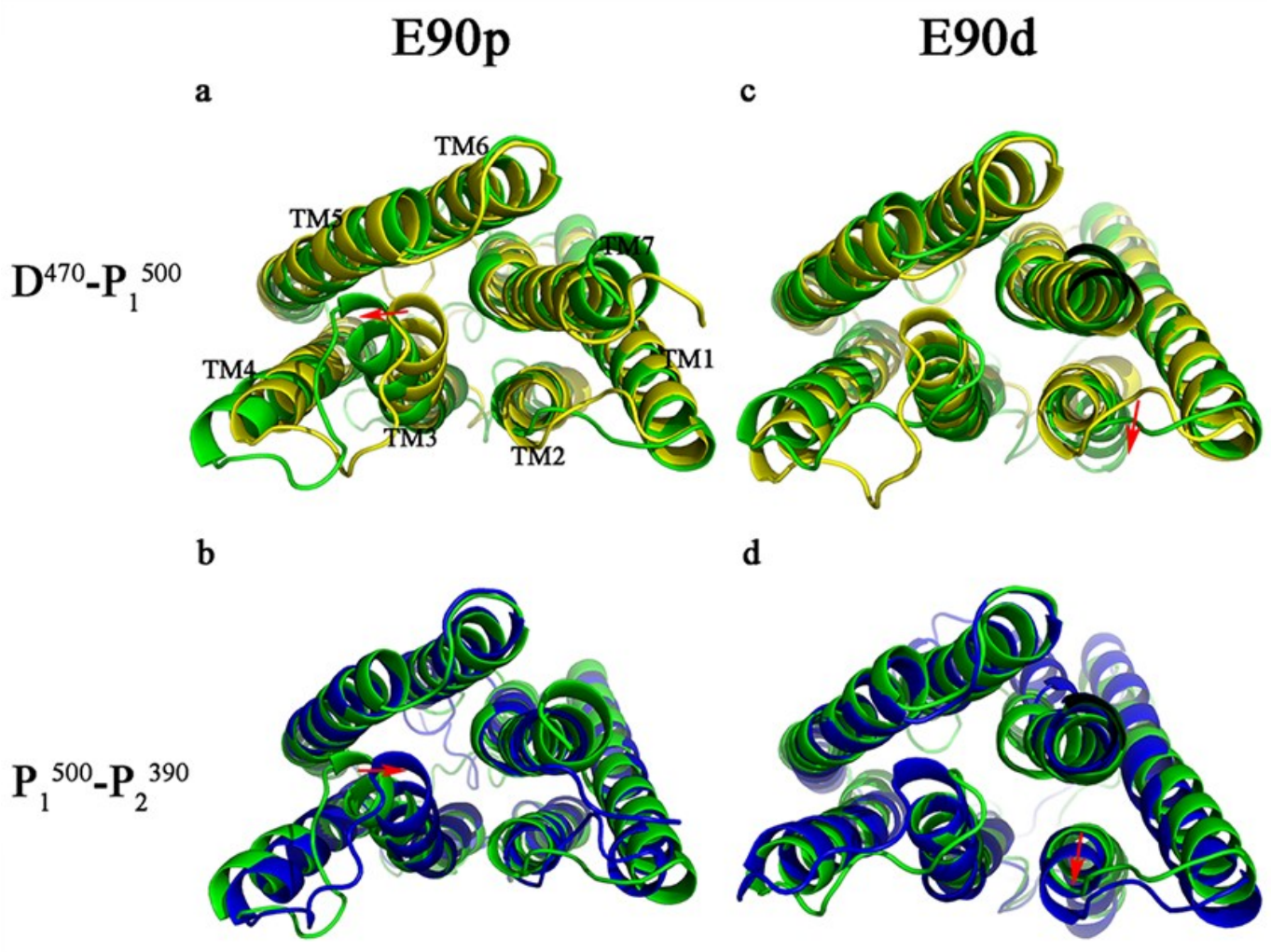

Fig. S3: The structure changes of ChR2 protein during the photocycle. (a) the superimposed conformations of D^{470} and E90p-P_1^{500}, (b) the superimposed conformations of E90p-P_1^{500} and E90p-P_2^{390}, (c) the superimposed conformations of D^{470} and E90d-P_1^{500}, (d) the superimposed conformations of E90d-P_1^{500} and E90d-P_2^{390}. The D^{470} state is displayed in yellow, the P_1^{500} state is displayed in green, and the P_2^{390} state is displayed in blue.

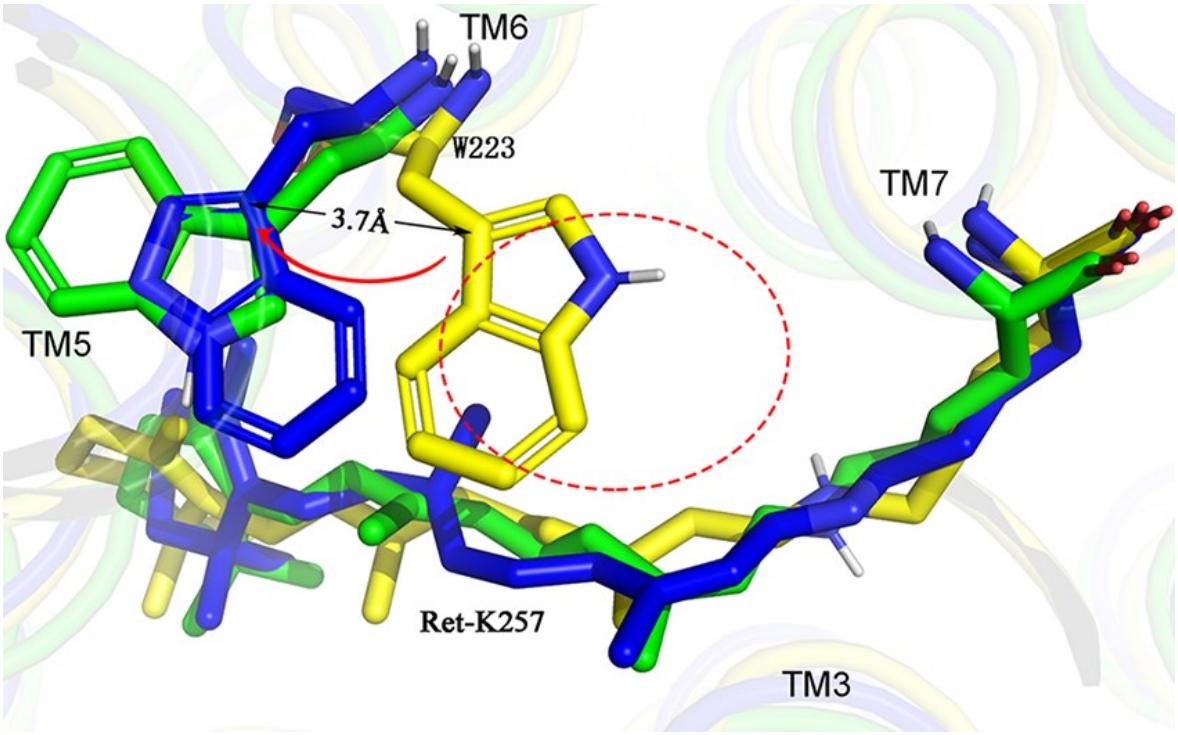

Fig. S4: The superimposed conformations of moving of the W223 residue induced by retinal isomerization. The D^{470} state is displayed in yellow, the P_1^{500} state is displayed in green, and the P_2^{390} state is displayed in blue. The position of potential ion channels on the side of retinal is indicated by a red dashed ellipse.

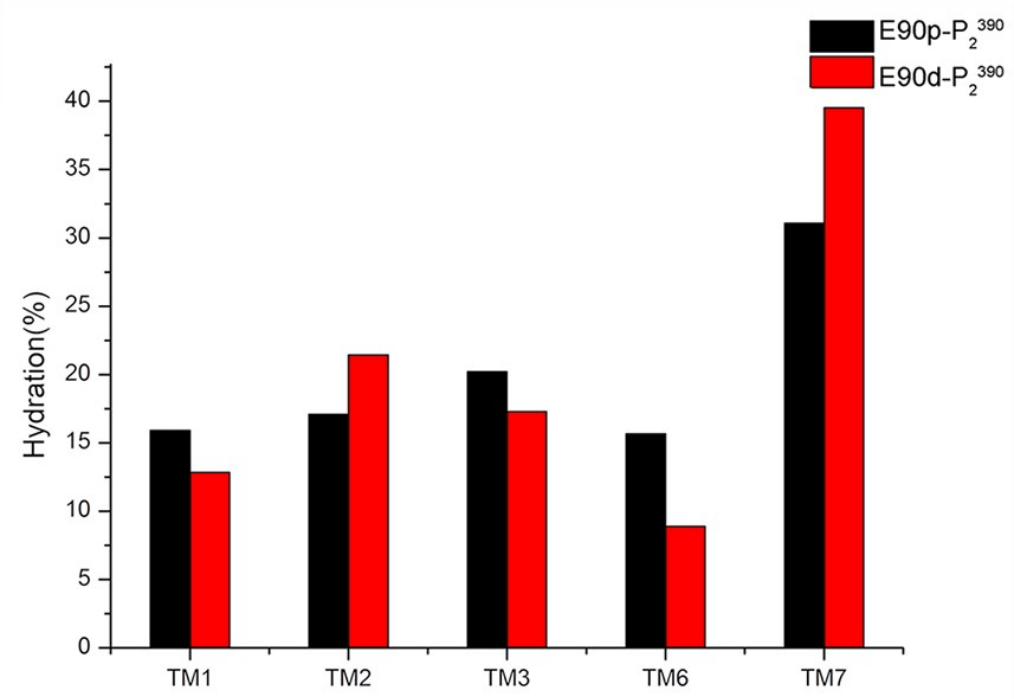

Fig. S5: Diagram of hydration degree of TM1, 2, 3, 6 and 7 in the P_2^{390} state.

Tab. S1: The pka of E90 in D^{470}, P_1^{500} and P_2^{390} states.

Intermediates	D^{470}	P_1^{500}	P_2^{390}
pKa	8.69	6.45	5.05