CYSS
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Catalytic role played by the protein environment in facilitating specific retinal photoisomerization in rhodopsins

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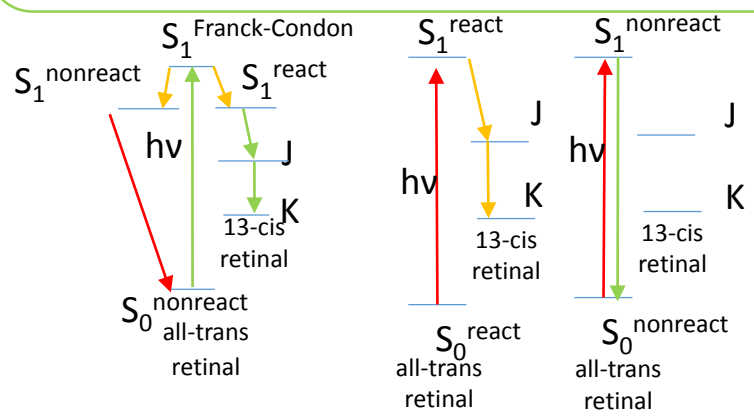
Introduction

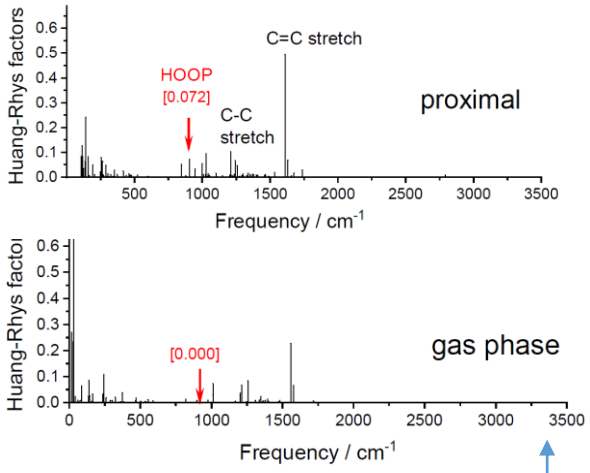
The light-driven sodium-pump Rhodopsin KR2 exhibits ultrafast photoisomerization dynamics of its all-trans protonated Schiff-base retinal (PSBR). However, the excited-state decay of KR2 also shows slow picosecond time constants, which are attributed to nonreactive states. The mechanism that produces long-lived states is unclear.

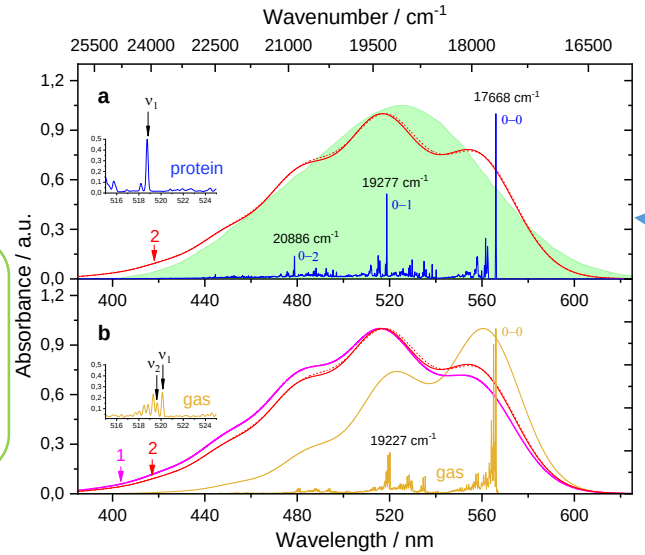


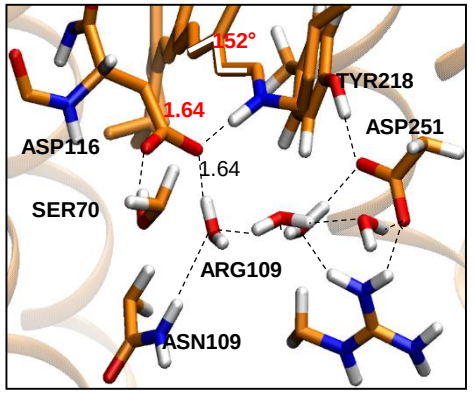
Objective

Here, by using molecular dynamics simulations and multiscale modeling based on multi-state multi-reference perturbation theory, we explore the origin of reactive and nonreactive states in KR2

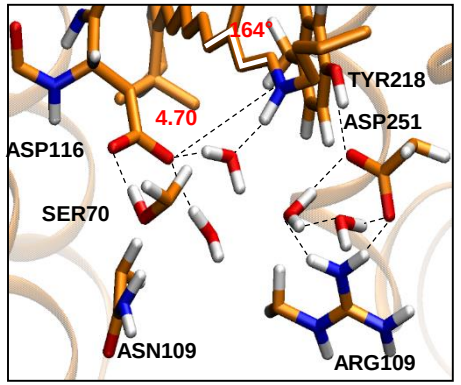
Resuts







proximal



water-bound

Methods

Molecular dynamics
Metadynamics

XMCQDPT2/CASSCF/EFP

Conclusions

- high flexibility of the retinal-binding pocket of the KR2 protein
- formation of a strong hydrogen bond results in pre-twisting of PSBR in the ground state, resulting in excitation of those vibrational modes that are particularly relevant to specific photoisomerization of PSBR in KR2

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This work is supported by the Russian Foundation for Basic Research (grant no. 19-33-90254). The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University as well as the local resources provided through the Lomonosov Moscow State University Program of Development.