

Physical Chemistry Colloquium

Virtual

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Understanding the early events of rhodopsin activation using time-resolved X-ray scattering and molecular simulation



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Dark-adapted vision in mammals starts with the absorption of a photon and the activation of rhodopsin, a G protein-coupled receptor. The early stages of rhodopsin activation involve the cis-to-trans isomerization of the receptor's ligand (retinal) and a relaxation process that drives the receptor through several non-equilibrium intermediates. These ultra-fast phenomena have been previously characterized spectroscopically. However, the structural information available that describes the femtosecond-to-picosecond scale changes involved is limited. Time-resolved small- and wide-angle X-ray scattering with free electron lasers is an emerging technique that has been shown to provide insights into the functional protein dynamics that take place at these timescales. Still, extracting structural information from scattering data is challenging. All-atom molecular dynamics is a powerful tool that can aid the interpretation of these experimental signals. Starting from dark-state simulations of bovine rhodopsin, we run and analyze thousands of 10 ps trajectories in two environments---bilayers and micelles---and two conditions---dark and light-excited---to model the process of energy dispersion across the receptor after light-excitation. Following this strategy, we observe an increase in the radius of gyration of the receptor after light-excitation and a propagation of the light-induced perturbation across the protein that occurs roughly at the speed of sound.



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