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Orange Carotenoid Protein: Effect of Internal Dynamics on Protein Functionality

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In cyanobacteria, photosynthesis is initiated by light absorption in protein complexes referred to as phycobilisomes (PBs). In excess light, photodamage to the photosynthetic apparatus is prevented by non-photochemical quenching (NPQ). This adaptive process responsible for high light tolerance is realized by the interplay between the light-harvesting PBs, a light-sensitive effector of NPQ called Orange Carotenoid Protein (OCP), and a regulatory Fluorescence Recovery Protein (FRP). The underlying structural processes are currently a field of intensive research[1-4].
It is well known that OCP exhibits a significant structural change upon photoactivation switching from the ground state (OCPO) to the active state (OCPR). However, the knowledge about the structural changes induced by light is insufficient to describe and understand OCP's functionality. A rarely considered aspect is the importance of internal protein dynamics. Using QENS, we probe the protein dynamics of the orange carotenoid protein in the observation time range from ~0.1 picoseconds to ~26 ps. Our measurements in the dark and under (in-situ-) blue light illumination directly reveal the dynamics in the ground and the active state of OCP, respectively. It is shown that the localized internal dynamics of amino acid residues are significantly enhanced upon photoactivation. This effect is attributed to the light-induced large-scale structural changes exposing larger areas of the protein surface to the solvent. A more open structure of OCPR also causes higher flexibility of structural elements like domain linkers and N-terminal extension.
However, the latter enhancement of flexibility is significantly smaller than that observed before for the mutant OCPW288A [5]. That is an inspiring observation since the OCPW288A mutant mimics the overall structure of OCP in the active state, as shown by SANS [5]. Our observation from the QENS experiment suggests that the point mutation destabilizes a relatively rigid part of the protein structure rendering in-situ experiments indispensable to determine the proper active state dynamics. In the present study, we provide the first MD simulations that shed light on the observed difference in protein dynamic between OCP in the active state and its mutant OCPW288A.

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