SFB 1078 Protonation Dynamics in Protein Function

Colloquium

Mon, **Apr. 29,** 2024

15:15 – 17:30

Freie Universität Berlin
SupraFAB, Room
(Altensteinstr. 23a, 14195 Berlin)

Dr. Nataliya Archipowa – University of Gothenburg, Sweden & University of Uppsala, Sweden

Photoactivation of bacterial phytochromes studied by time-resolved crystallography and spectroscopy

Plants, fungi and bacteria use phytochrome photosensor proteins to collect information about ambient light conditions. Upon photoactivation of a biliverdin cofactor, the chromophore and protein undergo a series of structural changes on multiple time and length scales in order to alter the biochemical output activity. The structures of the resting and light-activated states of bacteriophytochromes are known, but the structural mechanism with which light cues are transferred into structural rearrangements are not well understood. In particular, the primary structural response of the chromophore and the surrounding residues remains elusive.

Here, we present crystallographic snapshots structures of two bacterial phytochromes, time-resolved at room-temperature by serial femtosecond X-ray crystallography at the Japanese X-ray free electron laser (SACLA). We present a series of snapshot from 0 to 3ps, and at 3 ns and milliseconds after photoexcitation and discuss implications for the primary photoresponse of phytochrome proteins.[1), 2)] The snapshots confirm rotation of the D-ring as the primary event of photoactivation and reveal how this leads to a concomitant liberation of the chromophore from the protein scaffold. Subsequently, we observe global changes of the entire phytochrome. Our mechanism also implicates displacement of the pyrrole water and ultrafast protonation reactions. Infrared spectroscopic results point to protein relaxation in the lumi-R state. The results provide a structural basis for understanding the primary photoresponse of phytochromes.

1) Claesson et al., eLife, 2020; 2) Carillo et al., Structure 2021

Prof. Denis Rousseau – Albert Einstein College of Medicine, New York, USA

Ultrafast terahertz spectroscopy: probing and controling fundamental motions of electrons and molecules in condensed matter

Structures of intermediates in the catalytic cycle of bovine cytochrome c oxidase (bC*c*O) will be described. The ligand structures during the reduction of oxygen were determined by resonance Raman spectroscopy several years ago. Now crystal structures of the intermediates can be determined by serial femtosecond X-ray crystallography (SFX). In SFX, diffraction, obtained with an X-ray free electron laser (XFEL), allows determination of crystal structures of reactive intermediates at near physiological conditions. In addition, as the diffraction is obtained by 30 femtosecond X-ray pulses, structures are obtained without the radiation damage that is present in structures determined with synchrotron radiation. In addition to the structure of a reactive intermediate a new structure of the oxidized state will be described. This provides new insights into the structural basis for the control of proton translocation in bCcO.

Coffee and tea will be available during the break at 16:15. www.sfb1078.de

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