

CSC-RUB PhD Project Proposal

Title: Structural characterization of ultrafast energy transfer in light harvesting proteins

Sector of research: Structural biology, Photosynthesis, Biophysics, Biochemistry

Degree awarded: PhD in Biology (Integrated Graduate School of Biology, IGB)

Keywords: Protein crystallography, cryoEM, time resolved crystallography, light harvesting, energy transfer, photosynthesis, algae, dinoflagellates, coral bleaching, primary producers, photoprotection

Supervisor of PhD project:

Prof. Dr. Eckhard Hofmann, Faculty of Biology and Biotechnology, Ruhr University Bochum

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Research focus of supervisor:

My laboratory is interested in unraveling the structural factors defining and controlling the function of proteins and enzymes. We utilize both experimental (molecular biology, protein biochemistry, protein crystallography, cryo EM, biophysics, biochemistry) and theoretical approaches to study and simulate the dynamics of these biological nanomachines. Especially the combination of these approaches allows us to gain deeper insight into the functional details. Frequently, the combination of structural information with bioinformatics on a genetic level allows us to learn about the evolutionary development of protein function.

In addition to our in house state of the art infrastructure, we rely on continuous access to synchrotron facilities to obtain time resolved data at highest resolution. Current research focuses on membrane transport proteins, plant and algal enzymes, bio-hydrogen production and light harvesting processes in photosynthetic organisms.

Publications:

H-index: 24; number of publications: 28 (last 5 years , GOOGLE- Scholar)

Winkler M, Duan J, Rutz A, Felbek C, Scholtyssek L, Lampret O, Jaenecke J, Apfel U-P, Gilardi G, Valetti F, Fourmond V, Hofmann E, Léger C, Happe T. 2021. A safety cap protects hydrogenase from oxygen attack. *Nature Comm* 12:756.

Della Corte D, van Beek HL, Syberg F, Schallmey M, Tobola F, Cormann KU, Schlicker C, Baumann PT, Krumbach K, Sokolowsky S, Morris CJ, Grünberger A, Hofmann E, Schröder GF, Marienhagen J. 2020. Engineering and application of a biosensor with focused ligand specificity. *Nature Comm* 11:4851.

Schulte T, Niedzwiedzki DM, Birge RR, Hiller RG, Polívka T, Hofmann E, Frank HA. 2009. Identification of a single peridinin sensing Chl-a excitation in reconstituted PCP by crystallography and spectroscopy. *Proc Natl Acad Sci USA* 106:20764–20769.

Hofmann E, Zerbe P, Schaller F. 2006. The crystal structure of *Arabidopsis thaliana* allene oxide cyclase: insights into the oxylipin cyclization reaction. *Plant Cell* 18:3201–3217.

Hofmann E, Wrench PM, Sharples FP, Hiller RG, Welte W, Diederichs K. 1996. Structural basis of light harvesting by carotenoids: peridinin-chlorophyll-protein from *Amphidinium carterae*. *Science* 272:1788–1791.

Second Supervisor of PhD project

Prof. Dr. Marc M. Nowaczyk, Plant Biochemistry, Faculty of Biology and Biotechnology

Summary of research plan:

Background: Photosynthetic organisms utilize accessory pigments to harvest light in spectral regions not covered by chlorophyll molecules in the core photosystems. These pigments are fixed in a protein scaffold of light harvesting (LH) proteins, thereby ensuring nearly loss-free transfer of energy towards the reaction centers. Eukaryotic dinoflagellates are ecologically important parts of the phytoplankton and as essential symbionts central in the process of coral bleaching. They have two LH-complexes: the soluble Peridinin Chl *a* Proteins (PCP), and the membrane bound Light Harvesting Complex (LHCa/c).

Study objective: In this project, two main questions will be addressed: We can routinely grow xtals of PCP diffracting to atomic resolution of 1.0Å and beyond and will use these to study the energy transfer at ultrahigh resolution by time resolved crystallography. In a second line of research, we will work towards an atomic structure of LHCa/c both using protein crystallography and using cryoEM of supercomplexes.

Expected Results: Ideally, we will obtain a picosecond molecular movie of structural changes in the PCP pigment-protein complex. This will allow us to clarify energy transfer pathways and photoprotective mechanism. LHC a/c structures, especially in supercomplexes will allow us to improve the understanding of the interaction and the coupling with the core photosystems.

Methods: Protein for structural studies will be prepared both from native algae and from heterologous sources. The full infrastructure is established in my lab. We will utilize specialized beamlines for time resolved crystallography at the ESRF (Grenoble) and DESY (Hamburg), and will also start a project at the European XFEL X-ray-laser facility (Hamburg). Femtosecond spectroscopy will be performed within established collaborations.

Candidate Requirements: MSc Biology or Biochemistry, good practical background in protein purification. Prior experience in structural biology (X-ray or CryoEM). Good English language skills and ability to integrate into a small international team are essential.

Motivation for CSC application: The PhD candidate will be embedded in the strong research environment at the Ruhr University Bochum and the Faculty for Biology and Biotechnology. Here, structured PhD programmes are offered, providing the opportunity to acquire interdisciplinary skills (e.g. IGB, RUB Research school (<https://www.research-school.rub.de/>)). Training in the Hofmann group will include photosynthesis, algal culturing, general molecular biology, advanced protein purification and all aspects of protein crystallography. Prof. Hofmann has solved numerous structures of soluble and membrane proteins, using all phasing methods available. He solved the first structure of a PCP complex and was integral in developing the spectroscopic investigation of the energy transfer processes in cooperation with leading groups for ultrafast spectroscopy.