

SFB
1078



Protonation Dynamics
in Protein Function

**Annual Retreat of the
Collaborative Research Center – SFB 1078**
Protonation Dynamics in Protein Function

March 31 – April 3, 2014
Parkhotel Bad Schandau, Sächsische Schweiz

Program

Monday, 31.3.2014

Departure from Berlin by Train

- 10:26 EC 175 – Departure from Berlin-Spandau – Platform 5
10:46 EC 175 – Departure from Berlin Hbf (tief) – Platform 1 – Coach 257 (Seat 21 – 116)
10:53 EC 175 – Departure from Berlin Südkreuz – Platform 3

13:36 EC 175 – Arrival at Bahnhof Bad Schandau – Walk and Ferry Ride to the Hotel
(Luggage will be picked up)

Venue: **Parkhotel Bad Schandau**

Rudolf-Sendig-Str. 12 | D-01814 Bad Schandau | www.parkhotel-bad-schandau.de

14:30 Welcome coffee and small snacks

15:00 Welcome by Holger Dau

15:10 – 16:45 Session 1 – **Cytochrome c Oxidase** Chair: Holger Dau

- 15:10 **Murat Sezer, A1** (20 min)
Redox-dependent Structural Changes of Cytochrome c Oxidase Probed by Resonance Raman Spectroscopy
- 15:40 **Alexander Wolf, A2** (20 min)
Fluorescence correlation spectroscopy as a tool to investigate the protonation dynamics of cytochrome c oxidase
- 16:10 **Anna Lena Wölke, C2** (10 – 15 min)
Role of Lys362 for the Gating of the K-Channel in Cytochrome c Oxidase
- 16:30 **Petra Imhof, C5** (10 min)
Discrete state models for proton transfer

16:45 Coffee break

17:15 – 18:40 Session 2 – **Photosystem II & Poster Talks** Chair: Maria Andrea Mroginski

- 17:15 **Yvonne Zilliges & Zhiyong Liang, A4** (25 min)
Understanding photosynthetic water oxidation by time-resolved spectroscopy on wildtype and genetically modified photosystem II
- 17:50 **Arturo Robertazzi, C2** (10 – 15 min)
Oxygen-Evolving Complex of Photosystem II: A Quantum Chemistry and EXAFS study
- 18:10 **Poster Talks** (3 min each)
1-3, 6-10

19:00 Dinner

20:00 – 21:30 **Poster Session I**

Poster # 1- 10

[maximum talking time given in parentheses]

Poster Session I

- 1 **Fabian Kruse & Robert Götz, A1**
Setup of a Pump-Probe Experiment for Measuring Charge Transfer Dynamics of Cytochrome c Oxidase
- 2 **Hendrik Mohrmann, A1**
Rapid prototyping of microfluidics devices and their application in IR spectroscopy
- 3 **Bernd Schultz, A1**
TBA
- 4 **Alexander Wolf, A2**
Fluorescence correlation spectroscopy as a tool to investigate the protonation dynamics of cytochrome c oxidase
- 5 **Yvonne Zilliges, A4**
Identification of protonation sites and paths in photosynthetic water oxidation via site-directed mutagenesis of cyano-bacterial photosystem II
- 6 **Matthias Schönborn & Philipp Simon, A4**
Investigating protonation dynamics of photosystem II – Proceedings on time-resolved IR spectroscopy
- 7 **Emanuele Rossini, C2**
pKa's Determination for a group of di-Mn Complexes
- 8 **Jonas Wietek, B2**
Conversion of Channelrhodopsin into a light-gated chloride channel
- 9 **Nils Krause, B4**
Structural differences between the closed and open states of channelrhodopsin-2 as observed by EPR spectroscopy
- 10 **Vera Muders, B4**
Spectroscopic analysis of channelrhodopsin-1 and its chromophore

Tuesday, 1.4.2014

9:00 – 10:30 Session 3 – Channelrhodopsin Chair: Patrick Scheerer

- 9:00 **Franz Bartl, B5** (20 min)
Keyplayers of the channelrhodopsin photocycle
- 9:30 **Tom Resler, B3** (15 – 20 min)
Deuterium Kinetic Isotope Effects on Proton Transfer of Channelrhodopsin-2
- 9:55 **Victor Lorenz-Fonfria, B3** (15 min)
Conformational dynamics and channel on- and off-gating in channelrhodopsin-2
- 10:15 **Christopher Mielack, C4** (10 min)
Water and Hydrogen Bond Dynamics in Channelrhodopsin
- 10:30 Coffee break

11:00 – 12:20 Session 4 – Cytochrome c Oxidase & Poster Talks Chair: Ramona Schlesinger

- 11:00 **Mario Gerecke, A3** (10 min)
Fluorescence non-collinear optical parametric amplification spectroscopy
- 11:15 **Celin Richter, A3** (15 min)
Ethylamino-SNARF. A new bioapplicable SNARF-derivative with a short amine-functionalized chain
- 11:40 **Poster Talks** (3 min each)
12-21
- 12:30 Lunch

13:30 – 16:30 Hiking Time

Possible Route: Kirnitzschtal – Lichtenhainer
Wasserfall – Kuhstall

16:30 Coffee break

17:00 – 18:30 Poster Session II

Poster # 11- 21

19:00 Dinner

20:00 – 21:30 General Discussion

Subjects: IGK program and related issues / Lange Nacht der Wissenschaft / ...



Kuhstall

Poster Session II

- 11 **Tom Resler, B3**
Deuterium Kinetic Isotope Effects on Proton Transfer of Channelrhodopsin-2
- 12 **Mattia Saita, B3**
Applying a membrane potential to channelrhodopsin proteoliposomes
- 13 **Till Stensitzki, B3**
Polarization resolved femtosecond IR spectroscopy of sensory Rhodopsin II in the amide I region
- 14 **Stefan Milenkovic, C4**
TBA
- 15 **Group Bartl, B5**
Spectroscopy of the red shifted channelrhodopsin variant ReaCh
- 16 **Group Bartl, B5**
Infrared studies of the channelrhodopsin photocycle intermediates
- 17 **Franziska Schneider, B2**
pHoenix - a new optogenetic tool for acidifying synaptic vesicles
- 18 **Jan Daldrop, C1**
Simulation of proton transfer along water wires
- 19 **Bilal Qureshi & Patrick Scheerer, B6**
*Towards crystal structures of bacterial phytochromes from *Agrobacterium tumefaciens**
- 20 **Nils Schuth, A4**
Influence of NH_4Cl on O_2 production of photosystem II investigated by time-resolved O_2 polarography
- 21 **Martin Bommer, Julia Hellmich & Mohamed Ibrahim, A5**
The role of detergent in crystal packing upon dehydration of photosystem II crystals

Wednesday, 2.4.2014

9:00 – 10:30 Session 5 – Photosystem II Chair: Peter Hegemann

- 9:00 **Mohamed Ibrahim, A5** (20 min)
Quality Improvement of Photosystem II Microcrystals For Femtosecond X-ray Crystallography
- 9:30 **Martin Bommer, A5** (20 min)
Photosystem II at 2.44 Å resolution in a crystal that resembles thylakoid membrane packing
- 10:00 **Suliman Adam & Federico Guerra, C4** (20 min)
The CHARMM Parametrisation of PSII Cofactors
- 10:30 Coffee break

11:00 – 12:40 Session 6 – Phytochrome Chair: Joachim Heberle

- 11:00 **Bilal Qureshi, B6** (20 – 25 min)
Towards a crystal structure of the full-length phytochrome Agp1
- 11:30 **Aref Takiden, C3** (10 – 15 min)
QM/MM Calculation on Phytochrome
- 11:50 **Francisco Velazquez Escobar, B6** (20 – 25 min)
Modulation of the signal transduction activity in bathy phytochromes via photo-induced and thermal cofactor isomerisations
- 12:20 **Patrick Piwowarski, B5** (10 – 15 min)
Elucidating the photo-induced chromophore structural changes along the Pfr-to-Pr conversion in bathy phytochrome
- 12:45 Lunch

14:00 – 18:30 Hiking Time

Possible Destination: *Schrammsteine*

19:00 Dinner

20:00 – 21:30 Scientific Discussions in Groups

Groups / Sections: *TBA*



Schrammsteine

Thursday, 3.4.2014

9:00 – 10:35 Session 7 – **Channelrhodopsin** Chair: Inez Weidinger

9:00 **Katja Stehfest**, B1 (20 min)
TBA

9:30 **Benjamin Krause**, B1 (15 min)
Unnatural amino acid mutagenesis in channelrhodopsin

9:50 **Andrew Nieuwkoop**, B1 (15 min)
Solid-State NMR Investigations of Bacteriorhodopsin

10:10 **Franziska Schneider**, B2 (15 – 20 min)
pHoenix - a new optogenetic tool for acidifying synaptic vesicles

10:35 Coffee break

11:00 – 12:00 Final Discussion

Subjects: Prize for Best Talk and Poster / Retreat 2014 Evaluation / Retreat 2015 / ...

12:15 Lunch

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17:08 EC 174 – Arrival at Berlin Südkreuz

17:15 EC 174 – Arrival at Berlin Hbf (tief)

17:32 EC 174 – Arrival at Berlin-Spandau