

SFB
1078



Protonation Dynamics
in Protein Function

Annual Retreat 2020

Collaborative Research Center – SFB 1078

Protonation Dynamics in Protein Function

February 26 - 28, 2020

Evangelische Bildungsstätte auf Schwanenwerder

Program

Travel Information

Venue

Evangelische Bildungsstätte auf Schwanenwerder

Inselstr. 27-28 | D-14129 Berlin | <https://www.berlin-schwanenwerder.de/>

Rooms: **Check-out before 10:00**

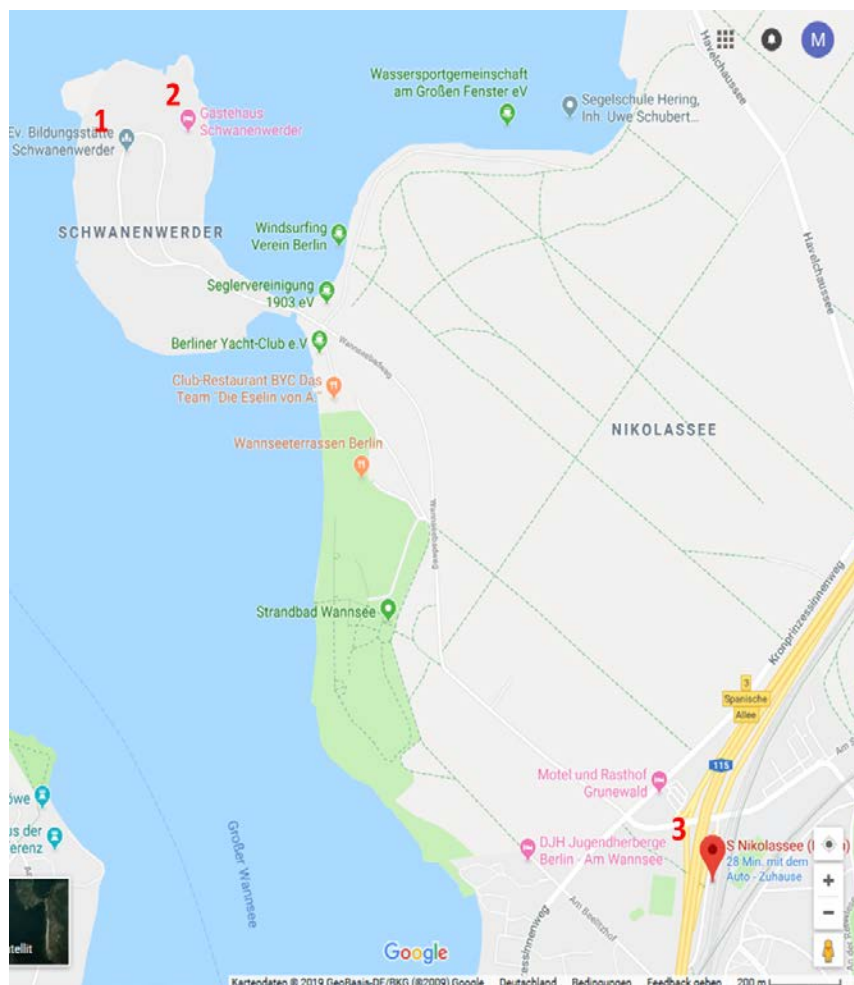
Individual Travel and Return

Ticket required: **Berlin-AB for 2.90 EUR.**

Taxi +49 (0)30 – 44 33 22 / 26 10 26 / 26 30 00 / 21 01 01 / 21 02 02

Map

- 1 Evangelische Bildungsstätte auf Schwanenwerder
- 2 Gästehaus Schwanenwerder
- 3 S-Bahnhof Nikolassee



Timetable information for public transport in Berlin:

<https://www.bvg.de/fahrinfo>

Wednesday, Feb. 26 2020

9:30 Welcome at the Registration Desk, Coffee/ tea time

10:00 – 11:30 Chair: Joachim Heberle

10:00 **Joachim Heberle**, chairman (20 min)
Recent developments in the CRC 1078

10:30 **Ville Kaila**, Mercator fellow (20 min)
Deciphering molecular mechanisms of biological energy conversion

11:00 **Holger Dau, A4** (20 min)
Tracking protonation dynamics in photosynthetic water oxidation in wild-type and mutated photosystem II

11:30 Coffee / tea time

12:00 – 13:00 Chair: Ulrike Alexiev

12:00 **Mohamed Ibrahim**, Athina Zouni, Holger Dobbek, **A5** (20 min)
Untangling Structural Evolution of Photosystem II: the S2 to S3 transition in the micro- to milliseconds time domain

12:30 **Ana-Nicoleta Bondar, C4** (20 min)
Protonation-coupled dynamics of retinal proteins and photosystem

13:00 Lunch break

14:00 – 16:00 Chair: Peter Hildebrandt

14:00 **Dennis Nürnberg, A7** (20 min)
Protonation dynamics in the interplay of redox mediator cytochrome c6 and photosystem I

14:30 Joachim Heberle, **Inez Weidinger, A1** (20 min)
Electron-driven protonation dynamics in cytochrome c oxidase

15:00 **Ulrike Alexiev, A2** (20 min)
Protonation and conformational dynamics at the surface of proteins

15:30 Coffee / tea time

16:00 – 17:30 Chair: Inez Weidinger

16:00 **Stephan Block, A6** (20 min)
Influence of the membrane composition on the proton turnover of heme-copper oxidases

16:30 **Maria Andrea Mroginski, C2** (20 min)
Understanding Protonation dynamics in CcO and Phytochrome

17:00 **Patrick Scheerer, Peter Hildebrandt, B6** (20 min)
Proton-coupled conformational changes in photoreceptors

19:00 Dinner buffet

Maximum talking time given in parentheses.

Ricardo Assuncao

Glass transition' of Photosystem II probed by X-ray absorption spectroscopy on the Mn4CaO5-core

Jens Balke

Mechanism of the redox-coupled proton-channel opening in cytochrome c oxidase

Jens Balke

Electronation dependent structural change at the proton exit side of cytochrome c oxidase as revealed by site-directed fluorescence labeling

Franz Bartl

Energy transfer from chromophore to protein is modulated by the protonation state of a glutamic acid in the active site of channelrhodopsin

Giovanni Battocchio

Secondary structural transitions in Agp2

Florian Bruenig, Roland Netz

IR line shapes from frequency-dependent friction

Krzysztof Buzar, Ana-Nicoleta Bondar

Long-distance proton transfer in photosystem II

Jheng-Liang Chen, Luiz Schubert, Joachim Heberle, Ramona Schlesinger

Mutagenesis analysis on an inward proton pump, Xenorhodopsin

David Ehrenberg

Synergy of time-resolved spectroscopy and serial X-ray crystallography in the case of KR2

Ofer Filiba, Veniamin Borin, Igor Schapiro

Involvement of the triplet state in retinal isomerization

Ronald González, Jovan Dragelj, Walter Knapp and Maria Andrea Mroginski

Quantum chemical modeling of phytochrome structures

Paul Greife

Analysis of FTIR step-scan data suggests crucial role of transient carboxylate deprotonation in the O₂-evolution transition of photosystem II

Joel Kaufmann

Energy transfer from chromophore to protein is modulated by the protonation state of a glutamic acid in the active site of channelrhodopsin

Mariafrancesca La Greca

Introduction of the unnatural aminoacid p-cyano phenylalanine into the phytochromes Agp1 and Agp2

Michalis Lazaratos, Malte Siemers, Ana-Nicoleta Bondar

Dynamic hydrogen-bond networks of channelrhodopsin variants. Developing new algorithms for efficient analyses.

Victor Manuel Loyo Cruz, Nina Mulaimovic, Jens Balke, Juliane Wonneberg, Alexander Wolf, Ulrike Alexiev

Activity dependence on the surface potential of Cytochrome c oxidase

Sarah Mäusle

Time-Resolved Single-Frequency IR-Spectroscopy on Photosystem II: Tracking Protonation Dynamics

Soshichiro Nagano, Kaoling Guan, Jon Hughes

3D structures of plant phytochrome A and B

Anh Duc Nguyen, Tui Hoang, Maria Andrea Mroginski

Electric field effects in the chromophore binding pocket of Agp2

Franziska Pranga-Sellnau, Mattia Saita, Victor Lórenz-Fonfría, Ramona Schlesinger, Joachim Heberle

Two-photon processes and proton transport reactions in channelrhodopsins

Nicholas Oliver

Investigating Manganese oxide production by Photosystem II: Experimental evidence and evolutionary implications

Maryam Sadeghi

Time-resolved Fluorescence Spectroscopy of Phytochrome

Johannes von Saß

The role of Proline residues in light-driven sodium pump KR2

Luiz Schubert

QCL-based dual comb spectroscopy in the Amide I Region on Bacteriorhodopsin

Thursday, Feb 27, 2020

9:00 – 11:00 Chair: Han Sun

9:00 **Karsten Heyne, Jon Hughes, B7** (20 min)
Ultrafast dynamics and structural studies of prokaryotic and plant phytochromes

9:30 **Franz Bartl, B5** (20 min)
Mechanistic insights into channelrhodopsin and phytochrome function

10:00 **Hartmut Oschkinat, B1** (20 min)
Structural dynamics and protonation pattern in rhodopsins and phytochromes

10:30 Peter Hegemann, **Johannes Oppermann, B2** (20 min)
Viral rhodopsins from the TARA ocean project

11:00 Coffee / tea time

11:30 – 13:00 Chair: Franz Bartl

11:30 **Ramona Schlesinger, B4** (20 min)
Hydrogen bonding network in channel- and other rhodopsins and phytochromes analysed by site-directed mutagenesis and labeling

12:00 **Igor Schapiro, C6** (20 min)
Photochemistry of phytochromes and retinal proteins

12:30 **Joachim Heberle, B3** (20 min)
Identification of proton and hydrogen-bond dynamics in channelrhodopsins and related systems

13:00 Lunch break

14:00 – 15:30 Chair: Maria Andrea Mroginski

14:00 **Jacek Kozuch, B9** (20 min)
IR-compatible membrane systems and electric fields in proteins - towards understanding viroporin function

14:30 **Adam Lange, B10** (20 min)
Structure and mechanism of viral proton channels in liposomes studied by solid-state NMR

15:00 **Han Sun, C8** (20 min)
Ion Selectivity and Proton Permeation Pathway of Viroporins Investigated by Atomistic Molecular Dynamics Simulations

15:30 – 16:00 Coffee / tea time

Maximum talking time given in parentheses.

16:30 – 18:00

Chair: Ramona Schlesinger

16:30 **Cecilia Clementi, C7** (20 min)
Structure and dynamics of viroporin proton channels by multiscale modeling and simulation

17:00 **Roland Netz, C1** (20 min)
Large-scale and small-scale diffusive and dielectric aspects of proton motion

17:30 **Ulrike Alexiev, Ivelina Zaharieva, IGK** (15 min)
Activities of the IGK

19:00 Dinner buffet

20:00 Networking, Poster session

Friday, Feb 28, 2020

9:00 – 13:00 SFB Council, IGK Meeting (parallel session) / social event

11:00 Coffee break

13:00 Farewell

13:00 optional: Lunch snack

Last update: Feb 25, 2020