

SFB
1078



Protonation Dynamics
in Protein Function

Annual Retreat 2019

Collaborative Research Center – SFB 1078

Protonation Dynamics in Protein Function

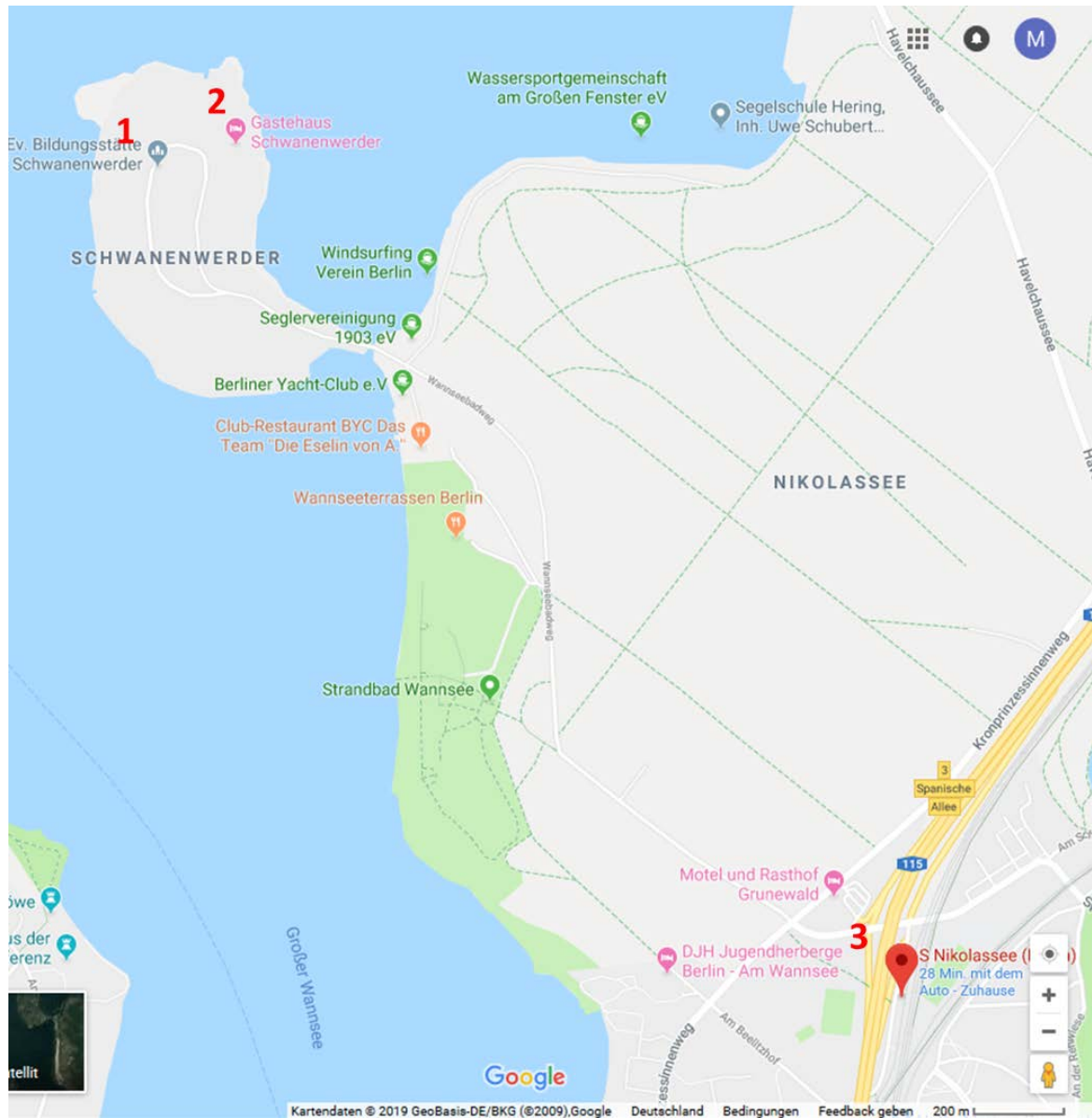
February 20 - 21, 2019

Evangelische Bildungsstätte auf Schwanenwerder

Program

Map

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



Timetable information for public transport in Berlin:

<https://fahrinfo.bvg.de/Fahrinfo/bin/query.bin/en?id=47.152&protocol=https:&>

Wednesday, Feb. 20, 2019

9:00 Welcome at the Registration Desk

9:30 – 11:30

Chair: Joachim Heberle

9:30 **Joachim Heberle**, chairman (10 min)
Recent developments in the CRC 1078

9:45 **Ulrike Alexiev, Ivelina Zaharieva**, IGK (10 min)
Activities of the IGK

10:00 **Petra Imhof, Marco Reidelbach**, C5 (20 min)
Communication and protonation dynamics in cytochrome c oxidase

10:30 **Jovan Dragelj**, C2 (20 min)
Proton loading site in cytochrome c oxidase

11:00 **Federico Baserga**, A1 (20 min)
Potential-induced difference FTIR spectroscopy on cytochrome c oxidase

11:30 Coffee break

12:00 – 13:00

Chair: Ulrike Alexiev

12:00 **Markus Göbel**, A1 (20 min)
Comparison of cytochrome c oxidase immobilization via surface-enhanced resonance Raman spectroscopy

12:30 **Stephan Block**, A6 (20 min)
Proton turnover rates of cytochrome oxidases measured at the single-enzyme level

13:00 Lunch break

14:00 – 16:00

Chair: Peter Hildebrandt

14:00 **Ulrike Alexiev**, A2 (20 min)
Interplay of conformational and protonation dynamics

14:30 **Ana-Nicoleta Bondar**, C4 (20 min)
Dynamic hydrogen-bond networks for proton transfer

15:00 **Holger Dau**, A4 (20 min)
Tracking water oxidation by time-resolved spectroscopy on wildtype and genetically modified photosystem II

15:30 **Rebeca Perez, Sarah Mäusle**, A4 (20 min)
Photosynthetic water oxidation investigated by time-resolved O₂ polarography and IR-spectroscopy

16:00 – 16:30 Coffee / tea time

Maximum talking time given in parentheses.

16:30 – 18:00

Chair: Ana-Nicoleta Bondar

- 16:30 **Hartmut Oschkinat, B1** (20 min)
tbd
- 17:00 **Johannes von Saß, B2** (20 min)
Incorporation of non-canonical amino acids into light-driven sodium pump KR2
- 17:30 **Johannes Oppermann, B1** (10 min)
Novel anion-conducting channelrhodopsins with near-complete desensitization
- 17:45 **Enrico Peter, B1** (10 min)
Development of a K^+ conducting KR2 channel
- 19:00 Dinner buffet

20:00 – 21:30 **Poster Session**

Ricardo Assunção, Ivelina Zaharieva and Holger Dau

Ammonia as a substrate-water analogue in photosynthetic water oxidation: Influence on activation barrier of the O_2 -formation step

Jens Balke

Fluorescence lifetime imaging as a tool to detect oxidative stress and associated effects of drug binding to cytochrome c oxidase

Jens Balke

Protonation state and conformational changes at the K-channel entry of cytochrome c oxidase

Federico Baserga, Sven Stripp, Moritz Senger, Joachim Heberle

Gas binding at the active center of cytochrome c oxidase studies by in-situ FTIR-ATR spectroscopy

Sarah Mäusle, Philipp Simon, Holger Dau

Time-resolved single-frequency IR-spectroscopy on PSII in H_2O and D_2O : Tracking protonation dynamics

Nicholas Oliver

Investigation into the light-driven assembly of manganese complexes in Photosystem II: Strategic overview and preliminary results

Maryam Sadeghi, Jens Balke, Constantin Schneider, John Hughes, Patrick Scheerer, Ulrike Alexiev

Conformational and protonation dynamics at the surface of phytochromes

Rebeca Perez

Mutagenesis of cyanobacterial PSII: the key to elucidate the protonation dynamics in photosynthetic water oxidation

Maximum talking time given in parentheses.

Paul Greife, Philipp Simon, Yvonne Zilliges, Robert Burnap, Holger Dau
Single-frequency IR spectroscopy with microsecond time resolution for tracking electron and proton transfer in the D1-V185N variant of photosystem II

David Ehrenberg
The two-photon reaction of JSR1, a bistable rhodopsin of the jumping spider eye

Lisa Gerland
Protonation dynamics in photosystem II subunit PsbO

Anastasia Kraskov
Protonation dynamics in the chromophore-binding pocket of a bathy phytochrome

Johannes Oppermann, Arita Salipetre, Paul Fischer, Anke Keidel, Johannes Vierock, José Flores-Uribe, Itai Sharon, Oded Béjà, Joel Kaufmann, Matthias Broser, Maike Luck, Franz Bartl, Peter Hildebrandt, Jonas Wietek, and Peter Hegemann
Novel anion-conducting channelrhodopsins with near-complete desensitization

David Buhrke, G. Battocchio, S. Wilkening, T. Friedrich, M. Mroginski and P. Hildebrandt
Vibrational characterisation of the red/green cyanobacteriochrome Slr-GAF3

Suliman Adam, Christian Wiebeler, Ana-Nicoleta Bondar and Igor Schapiro
Structural factors determining the absorption spectrum of the channelrhodopsin chimaera C1C2

Christian Wiebeler, Aditya G. Rao und Igor Schapiro
Investigations of the photoproduct tuning in cyanobacteriochromes and canonical phytochromes via quantum chemical calculations

Luiz Schubert
Spectroscopic investigations on the light-driven inward H⁺ pump xenorhodopsin

Johannes von Saß
Incorporation of non-canonical amino acids into light-driven sodium pump KR2

Kaoling Guan, Soshi Nagano, Jon Hughes
Preliminary crystal structure of plant phytochrome B

Florian Brünig, Roland Netz
IR spectral contribution of proton barrier crossing events and transition paths

Michail Lazaratos, Malte Siemers, Ana-Nicoleta Bondar
Dynamic hydrogen-bond networks of channelrhodopsin variants. Developing new algorithms for efficient analyses.

Rene Gorriz, Senta Volkenandt, Vincent Stegmaier, Marco Reidelbach, Petra Imhof
Interplay of hydrogen bonds, water dynamics, and proton transfer in cytochrome c oxidase

Anne Hartmann, Alexander Perrera i Lluna, Petra Imhof
Analysis of communication networks in cytochrome c oxidase

Thursday, Feb 21, 2019

9:00 – 11:00 Chair: Robert Bittl

9:00 **Florian Brünig, Roland Netz, C1** (20 min)
IR spectral contribution of proton barrier crossing events and transition paths

9:30 **Mattia Saita, B3** (20 min)
Infrared spectroscopy reveals continuum bands in proteins: between protonatable H-bonded networks and strongly H-bonded vibrations

10:00 **Joel Kaufmann, B5** (20 min)
Catalysis and stereoselectivity of photoreactions in channelrhodopsin

10:30 **Maria Walter, B4** (20 min)
Proton translocations in channelrhodopsin-1

11:00 Coffee break

11:30 – 13:00 Chair: Petra Imhof

11:30 **Maria Andrea Mroginski, C3** (20 min)
Phytochromes: protonation and dynamics

12:00 **Igor Schapiro, M** (20 min)
Red/Green spectral tuning in the cyanobacteriochrome Slr1393g3

12:30 **Till Stensitzki, B7** (20 min)
Ultrafast dynamics in Agp2 and impact of high intensities on protein function

13:00 Lunch break

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

14:00 **Soshi Nagano, B8** (20 min)
Updates on plant phytochrome crystal structures and development of fluorescent phytochromes

14:30 **Anastasia Kraskov, B6** (20 min)
Protonation dynamics in the chromophore-binding pocket of a bathy phytochrome

15:00 – 15:30 Coffee / tea time

15:30 – 17:00 SFB Council, IGK Meeting (parallel session)

17:00 Farewell

(Additional guests interested in joining the dinner please contact the organizing office, Mirjam Langhans.)

Last update: Feb. 18, 2019

Maximum talking time given in parentheses.