

SFB  
1078



Protonation Dynamics  
in Protein Function

## **Annual Retreat 2019**

Collaborative Research Center – SFB 1078

*Protonation Dynamics in Protein Function*

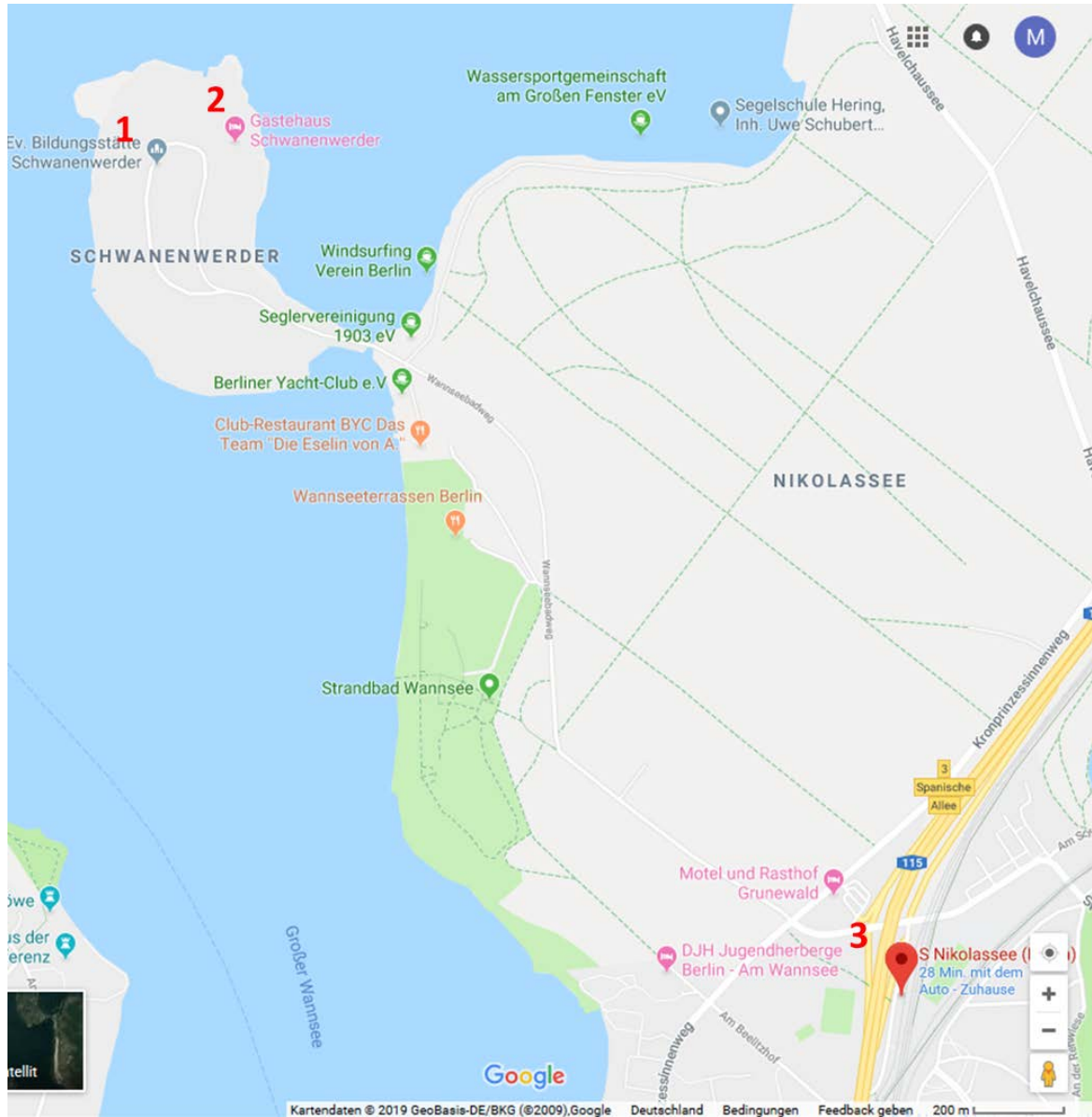
February 20 - 21, 2019

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 O<sub>2</sub> 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<sup>+</sup> 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<sub>2</sub>-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<sub>2</sub>O and D<sub>2</sub>O: 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<sup>+</sup> 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 – 15:15 Coffee / tea time

15:15 – 17:15 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.