

SFB
1078



Protonation Dynamics
in Protein Function

Annual Retreat 2023

Collaborative Research Center – SFB 1078

Protonation Dynamics in Protein Function

March 28-30th, 2023

Evangelische Bildungsstätte auf Schwanenwerder

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Version 3/21/2023 2:39 PM (printed version)

How to get there

1. Evangelische Bildungsstätte auf Schwanenwerder

Inselstr. 27-28

14129 Berlin

030- 847 140

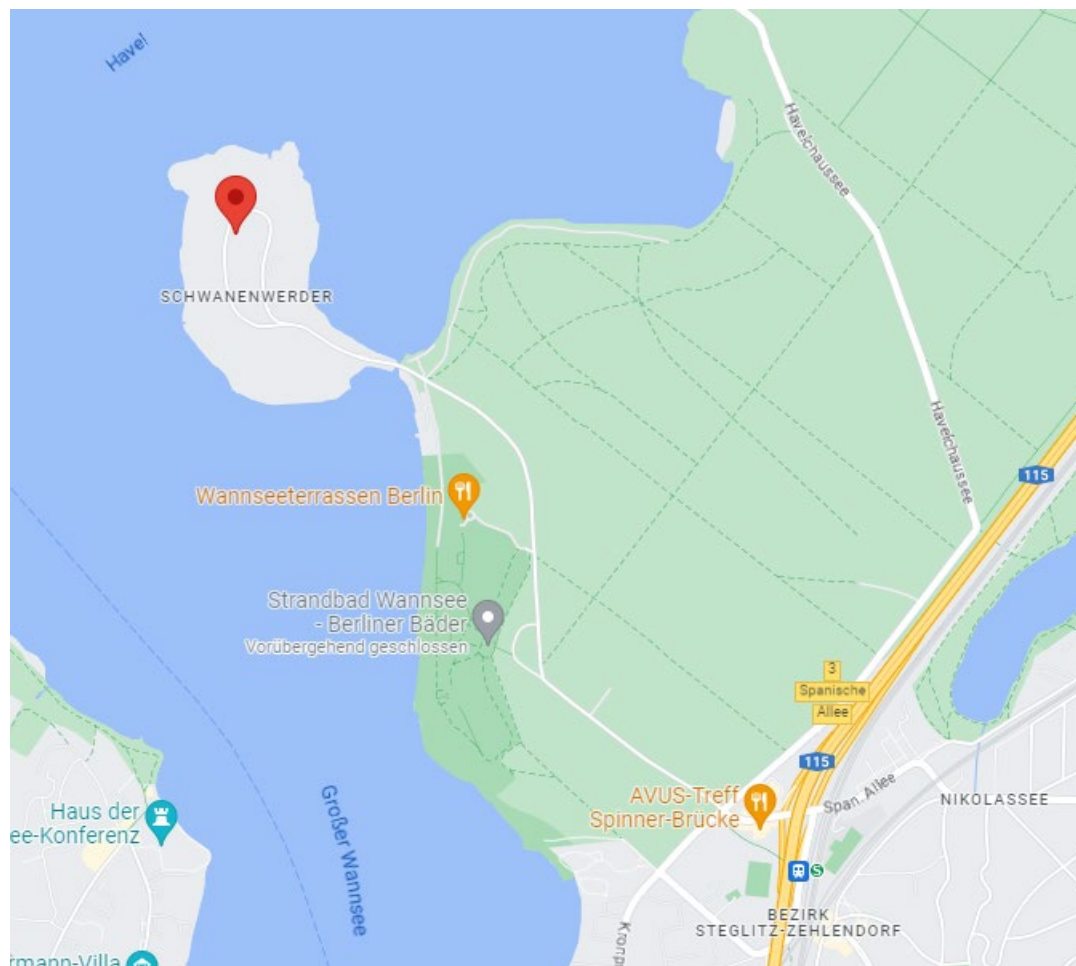
Berlin-schwanenwerder.de

2. By train

- S7 (direction Potsdam Hbf.) or S1 (direction Wannsee) to train station Nikolassee
- A shuttle service from the train station will bring you to the hotel:
Departure at 9:00 am and 9:30 am

3. By car

Freeway 115 (AVUS), exit Spanische Allee, Wannseebadweg, Inselstraße



Program

Talks are 10 min + 5 min discussion

Tuesday, March 28, 2023

09:30 Welcome at the foyer

09:30 Welcome coffee

Welcome address

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|-------|---|----------|
| 10:30 | Sabine Oldemeyer
<i>Technical advices</i> | (5 min) |
| 10:35 | Joachim Heberle , chairman
Welcome address, introduction | (15 min) |
| 10:50 | Ulrike Alexiev / Jens Balke , IGK
<i>Recent activities of the IGK</i> | (15 min) |

SESSION 1: Electron-driven protonation dynamics – redox proteins

11:10 – 12:30

Chair: Jon Hughes

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|-------|--|----------|
| 11:10 | Frederico Baserga (A1)
<i>Proton-coupled electron transfer in cytochrome c oxidase: Observing protonation reactions in real time</i> | (15 min) |
| 11:25 | Markus Göbel (A1)
<i>Side-chain protonation in the bi-nuclear center of Cytochrome c Oxidase and in a biomimetic catalyst</i> | (15 min) |
| 11:40 | Ulrike Alexiev / Jens Balke (A2) (Joined Talk)
<i>CcO and phytochrome: Proton-collecting antennae and water channels</i> | (15 min) |
| 11:55 | Ulrike Alexiev / Jens Balke (A2)
<i>CcO and phytochrome: Proton-collecting antennae and water channels</i> | (15 min) |

12:30 Lunch

Restaurant

SESSION 2: Chromophore-driven protonation dynamics – photoreceptors

13:30 – 14:50

Chair: Franz Bartl

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|-------|--|----------|
| 13:30 | Peter Hegemann (B2)
<i>Enzyme Rhodopsins, a new challenge</i> | (15 min) |
| 13:45 | Johannes Oppermann (B2)
<i>Metagenomically identified ACRs with optogenetic potential</i> | (15 min) |
| 14:00 | Luiz Schubert (B3)
<i>Protein conformational and protonation dynamics monitored by single-shot IR spectroscopy</i> | (15 min) |
| 14:15 | Mariafrancesca La Greca (B4)
<i>Protonation dynamics in the light-driven bacterial chloride pump NmHR</i> | (15 min) |

14:50 Poster session with coffee & Room check-in from 15:00

Room
"Dahlem"

SESSION 3: The bridge towards fundamental processes - theory

16:40 – 18:00

Chair: Karsten Heyne

16:40 **Maria Andrea Mroginski (C2)** (15 min)

Computational studies on phytochrome

16:55 **Louis Lehmann (C1)** (15 min)

Proton transfer at interfaces

17:10 **David Rosenberger (C7)** (15 min)

A multiscale simulation approach to study pore formation in M proteins

17:25 **Liu Haoran (C8)** (15 min)

Investigation of nonselective cation permeation through CNGA1 channels by molecular dynamic simulations.

18:00 *Dinner buffet*

Restaurant

Evening lecture:

19:30 – 20:30

Chair: Holger Dau

19:30 **Richard Cogdell (University of Glasgow, invited speaker)** (45 min)

Recent progress on the structure and function of purple bacterial light harvesting complexes

Wednesday, March 29, 2023

08:00 *Breakfast*

SESSION 4: Electron-driven protonation dynamics – redox proteins

9:00 – 10:20

Chair: Ulrike Alexiev

- 09:00 **Nicholas Oliver** (A4) (15 min)
Exogenous electron donation to Mn-depleted photosystem II: Kinetics and hypotheses
- 09:15 **Rana Hussein** (A5) (15 min)
The last milliseconds of Kok's photosynthetic water oxidation
- 09:30 **Stephan Block** (A6) (15 min)
Proton uptake dynamics of single cytochrome c oxidases
- 09:45 **Paul Greife** (A4) (15 min)
Tracking water oxidation through time-resolved FTIR Spectroscopy

10:20 *Coffee break*

Foyer

SESSION 5: Chromophore-driven protonation dynamics - photoreceptors

11:00 – 12:30

Chair: Igor Schapiro

- 11:00 **Franz Bartl** (B5) (15 min)
The functionality of the DC pair in a Rhodopsin Guanylyl
- 11:15 **Jheng-Lian Chen** (B4) (15 min)
The electrostatic effects from retinal surrounding in inward proton pump, NsXeR
- 11:30 **Luisa Herder / Manal Ebrahim** (B6) (Joined Talk) (15 min)
Structural Characterization of bacterial and fungal phytochromes in dark and illuminated state
- 11:45 **Luisa Herder / Manal Ebrahim** (B6) (15 min)
Structural Characterization of bacterial and fungal phytochromes in dark and illuminated state

12:30 *Lunch*

Restaurant

Guest talks

13:30 – 14:30

Chair: Han Sun

- 13:30 **Benesh Joseph** (Freie Universität Berlin, invited speaker) (30 min)
Structural and mechanistic insights on membrane transporters from pulsed dipolar electron spin resonance spectroscopy
- 14:00 **David Bührke** (Humboldt Universität Berlin, invited speaker) (30 min)
2D-IR spectroscopy reveals vibrational couplings in Bacteriophytochrome Agp1

14:30 *Coffee break*

Foyer

SESSION 6: Chromophore-driven protonation dynamics - photoreceptors

15:30 – 16:30

Chair: Peter Hegemann

- 15:30 **Jon Hughes (B7)** (15 min)
Structure/function of Cph1 and plant phytochromes
- 15:45 **Karsten Heyne (B7)** (15 min)
Impact of electric field changes on protein dynamics in photoreceptors
- 16:00 **Jacek Kozuch (B9)** (15 min)
Mapping electrostatics and H-bonding in proteins via nitrile labels – comparing IR spectroscopy and molecular dynamics

16:30 *Coffee break*

Foyer

SESSION 7: The bridge toward fundamental processes - theory

17:00 – 18:00

Chair: Maria Andrea Mroginski

- 17:00 **Igor Schapiro (C6)** (20 min)
Protonation affects the excited state properties
- 17:20 **Han Sun (C8)** (20 min)
Ion permeation in channelrhodopsins studied by atomistic molecular dynamics simulations

18:00 *Dinner buffet*

Restaurant

Evening lecture

19:30 – 20:30

Chair: Joachim Heberle

- 19:30 **Karin Hauser (Universität Konstanz, invited speaker)** (45 min)
Does protein function trigger membrane dynamics? An IR-spectroscopic study of microbial rhodopsins

Thursday, March 30, 2023

08:00 *Breakfast & Room check-out by 10:00*

SESSION 8: Electron-driven protonation dynamics – redox proteins & Guest speaker

Chair: Jacek Kozuch

9:30 – 10:15

- 9:30 **Sarah Mäusle (A4)** (15 min)
Time-resolved single-frequency infrared spectroscopy for the study of electron transfer in photosystem I
- 9:45 **Ville Kaila (Universität Stockholm, Mercator Fellow)** (15 min)
Mechanistic studies of protonation dynamics in biological energy transduction
- 10:00 **Ernst Walter Knapp (Freie Universität Berlin, invited speaker)** (30 min)
pKa computations, cytochrome c oxidase: a challenging case

10:30 *Coffee break*

Foyer

SESSION 9: Chromophore-driven protonation dynamics – photoreceptors & Proton channels

Chair: Stephan Block

11:00 – 12:30

- 10:45 **Galaan Merga (B5)** (15 min)
New insights on the photocycle of phytochrome Agp1
- 11:00 **Ronja Paschke (B7)** (15 min)
A SEIRA-spectroscopic Approach to Elucidate the pH-induced Channel Opening of Influenza A M2
- 11:15 **Henry Sawczyk (B10)** (15 min)
Development of a fluoregenic activity assay of proton channel M2 for high-throughput drug screening
- 11:30 **Swantje Mohr (B10)** (15 min)
Investigation of the Influenza A M2 proton channel using solid-state NMR

12:30 *Lunch*

Restaurant

Internal SFB council meeting / Internal IGK meeting

Saal 1 / Saal 2

13:45 – 15:45

16:00 *Departure*

Participants

Principal Investigators

Heberle, Joachim	A1, B3	FUB
Alexiev, Ulrike	A2, IGK	FUB
Dau, Holger	A4	FUB
Block, Stephan	A6	FUB
Oschkinat, Hartmut	B1	FMP
Hegemann, Peter	B2	HUB
Schlesinger, Ramona	B4	FUB
Bartl, Franz	B5	HUB
Scheerer, Patrick	B6	Charité
Heyne, Karsten	B7	FUB
Hughes, Jon	B7	JLU
Kozuch, Jacek	B9	FUB
Lange, Adam	B10	FMP
Mroginski, Maria Andrea	C2	TUB
Schapiro, Igor	C6	HUJI
Clementi, Cecilia	C7	FUB
Sun, Han	C8	FMP
Kaila, Ville	MF	Univ. Stockholm

Guests

Nürnberg, Dennis	FUB
Buhrke, David	HUB
Cogdell, Roger	Univ. Glasgow
Hauser, Karin	Univ. Konstanz
Joseph, Benesh	FUB
Knapp, Ernst-Walter	FUB

Postdocs & Senior Scientists

Ali, Rana	A5	HUB
Oppermann, Johannes	B2	HUB
Schmidt, Andrea	B6	Charité
Szczepek, Michal	B6	Charité
Herder, Luisa	B6	Charité
Nagano, Soshichiro	B7	JLU
Perez Lustres, Jose Luis	B7	FUB
Sawczyk, Henry	B10	FMP
Mackintosh, Megan	C6	HUJI
Rosenberger, David	C7	FUB

Coordinators

Oldemeyer, Sabine	Z	FUB
Hoernschemeyer, Jessi	Z	FUB
Balke, Jens	IGK	FUB

PhD Students & Candidates

Baserga, Frederico	A1	FUB
Göbel, Markus	A1	TUD
Celebi, Metehan	A2	FUB
Loyo Cruz, Victor	A2	FUB
Dekmak, Mohamad Yahia	A4	FUB
Oliver, Nicholas	A4	FUB
Greife, Paul	A4	FUB
Mäusle, Sarah	A4	FUB
Hart, Olli	A5	HUB
Gerland, Lisa	B1	FMP
Schubert, Luiz	B3	FUB
La Greca, Mariafrancesca	B4	FUB
Chen, Jheng-Liang	B4	FUB
Große, Maximilian	B5	HUB
Merga, Galaan	B5	HUB
Ebrahim, Manal	B6	Charité
Paschke, Ronja	B9	FUB
Mohr, Swantje	B10	FMP
Lehmann, Louis	C1	FUB
Jones, Jesse	C2	TUB
Hoang, Tu Oanh	C2	TUB
Filiba, Ofer	C6	HUJI
Liu, Haoran	C8	FMP

