

SFB
1078



Protonation Dynamics
in Protein Function

Annual Retreat 2022

Collaborative Research Center – SFB 1078

Protonation Dynamics in Protein Function

April 5 - 7, 2022

Hotel Haus Chorin and online

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How to get there

1. Hotel Haus Chorin

Neue Klosterallee 10

16230 Chorin

033366 - 500

<https://www.chorin.de/service/lage-anreise/>

2. Chorin, Bahnhof (Train)

RE3 Nord Berlin <-> Stralsund Hbf/Schwedt (Oder),

- Runs hourly between Berlin Hbf, Berlin Gesundbrunnen, Bernau, Eberswalde, Britz, Chorin
- Takes between 45 – 55 min from Berlin Hbf to Chorin
- Ticket VBB 9 € one way
- 15 min walk to the hotel or wait for the shuttle

3. By car

- You can reach us via the freeway (A11) Berlin - Prenzlau, exit Chorin:
- Please drive now **without a navigation system (you'll get lost otherwise)** via Britz and follow the signs to Chorin, past the Kloster Chorin and the Amtssee.
- After about 500m turn left towards the center of Chorin.
- The hotel's own parking lot is suitable for cars and buses and is located directly at the hotel.



In order to prepare for an efficient hybrid event, we'd like to point out the following information beforehand:

What you will need?

- Internet connection, ideally through LAN and a laptop/desktop
- Webex Software on your desktop (browser might slow the connection too much... when testing the link below, you will be prompted to download and install)
- Headphones with microphone (!), and a
- camera (if you want)

How to prepare for webex? With us together!

We offer two time slots to test your settings up front. Especially, for those who will present a talk or elevator pitch, we suggest to test out the slide sharing with us. Just pop in for 5-10 minutes through these time slots:

- Friday, 9.30 am with me: <https://fu-berlin.webex.com/fu-berlin/j.php?MTID=m9d393be56021638c624f63f4a0fc4994>

OR

- Monday, 2 pm with Fine: <https://fu-berlin.webex.com/fu-berlin/j.php?MTID=m30f25fc4485e1badace451d5fc387e76>

During the meeting!

- keep your microphone muted
- use the webex tools (chat and “raise hand”) to notify us if you want to say something
- if you experience a slow internet connection, try first to turn off your camera
- if you have technical questions, use the chat to ask the hosts directly

During the lunch and coffee breaks

- get up, stretch a leg and enjoy your break 😊
- get yourself some nice treat / food
- sitting in front of the screen all day and listening can be very tiring

Link to the retreat:

<https://fu-berlin.webex.com/fu-berlin/j.php?MTID=m33e213fc19f57b30c9ab3cd0989003a4>

Link to the council meeting:

<https://fu-berlin.webex.com/fu-berlin/j.php?MTID=mecff1a9e6028aefaa6e940ea29b26203>

For all people, who will come to Chorin, we are aware that it is going to feel very unusual to attend an in-person meeting with up to 50 participants in a hotel after such a long time.

To make this a safe experience for everyone, please take caution:

General rules and guidelines for the event (proposed by the SFB office)

- in order to attend, you must be vaccinated or recovered from COVID (within 3 months)
- bring a negative test result (lateral flow test / Antigen-Schnelltest) from within 24 hours
- wear a FFP2 mask during all time
- we'll provide lateral flow test for the second and third day

- we will air the conference room during the breaks – bring an extra sweater
- next to the conference room will be a terrace that we booked exclusively
- during lunch and evening mealtimes there will be only SFB people, however not during the breakfast
- the weather is not going to be in our favour, so taking meals outside will only be for the tough ones'

Before the event:

- be cautious about your contacts before our retreat
- test yourself regularly (lateral flow test / Antigen-Schnelltest)
- **if you have any signs of infection (headache, sore throat, runny nose), stay at home and participate online**

Program

Talks are 10 min + 5 min discussion

Webex Link

<https://fu-berlin.webex.com/fu-berlin/j.php?MTID=m33e213fc19f57b30c9ab3cd0989003a4>

Tuesday, April 05, 2022

09:30 Welcome at the reception desk

09:30 Welcome coffee

Foyer

Welcome address

11:15 **Jeannine Marquardt** (15 min)
Technical advices

11:30 **Joachim Heberle**, chairman (15 min)
Recent developments in the CRC 1078

11:45 **Ulrike Alexiev**, IGK (15 min)
Recent activities of the IGK

12:00 Lunch

Restaurant

SESSION 1:

Chair: Stephan Block

13:30 – 15:10

13:30 **Karsten Heyne** (B7) *online* (15 min)
Ultrafast dynamics of hydrogen-bonded networks in photoreceptors

13:50 **Swantje Mohr** (B10 Lange) (15 min)
Structural studies on viroporins using solid-state NMR

14:10 **Jacek Kozuch** (B9) (15 min)
pH-dependent structural changes of the Influenza M2 proton channel

14:30 **Florian Brünig** (C1 Netz) (15 min)
Time scales and spectroscopic signatures of excess proton dynamics

14:50 (15 min)

15:10 Coffee break

Foyer

SESSION 2:

Chair: Dennis Nürnberg

15:50 – 17:10

15:50 **Igor Schapiro** (C6) *online* (15 min)
Photoisomerization mechanism in rhodopsins and phytochromes

16:10 **Mariafrancesca La Greca** (B4 Schlesinger) (15 min)
Introduction of a Stark label via p-cyano phenylalanine into phytochrome Agp2

16:30 **Jens Balke** (A2 Alexiev) (15 min)
Recent studies of phytochrome and CcO in project A2

16:50 **Kalman Christer** (A4 Dau) (15 min)
*Investigating oxygen evolution by D1-glutamate 189 photosystem II mutants of *Synechocystis* sp. PCC 6803*

IGK elevator pitches:**Chair: Jens Balke**

17:20 – 18:20

17:20 **Elevator pitches**

(60 min)

18:20 *Dinner buffet*

Restaurant

Evening lecture:**Chair: Joachim Heberle**

19:50 – 20:50

19:50 **Anne-Frances Miller** (University of Kentucky, Einstein Visiting Fellow)

(45 min)

How proteins control electrons: Protons

Life finds ways to survive disruptive chemo-environmental catastrophes, and benefit from them. To the anaerobic organisms of the time, the rise of O₂ was a lethal wave of toxic waste, but those that acquired anti-oxidant defenses were able to exploit O₂ via respiration, and now dominate the earth. Superoxide dismutases (SODs) are central to the antioxidant defenses of life, and offer valuable insights into resilience vs. oxidative damage and tuning of the reactivity of bound transition metal ions. This presentation will review how the protein of Fe- and Mn-SODs is able to tune the reduction midpoint potential (E°) of bound Fe over almost 1 V via modulation of the strength and polarity of a few critical hydrogen bonds, as well as control over the source(s) of redox coupled protons. Indeed, the protein's exquisite control of E°s via proton energies and movements is seen in SOD's adaptation to use Mn instead of Fe, as part of evolution of tolerance to O₂.

Wednesday, April 06, 202208:00 *Breakfast***SESSION 3****Chair: Maria Andrea Mroginski**

9:00 – 10:40

09:00 **Holger Dau** (A4) *online*

(15 min)

*The electron-proton bottleneck of photosynthetic oxygen evolution*09:20 **Stephan Block** (A6)

(15 min)

*Complex proton uptake dynamics of single cytochrome c oxidases*09:40 **Iryna Zaporozhets** (C7 Clementi)

(15 min)

*Conformational transition in Slr1393g3 upon photoisomerization*10:00 **Luiz Schubert** (B3 Heberle)

(15 min)

*The usual suspects? About vectoriality in microbial proton pumps*10:20 **Manal Ebrahim** (B6 Hildebrandt / Scheerer)

(15 min)

*Structural characterization of a fluorescence optimized phytochrome in the dark- and light-adapted state*10:40 *Coffee break*

Foyer

SESSION 4: **Chair: Jacek Kozuch**
11:00 – 12:20

11:00 **Rana Hussein** (B5 Zouni) *online* (15 min)
Investigations of the structural dynamics of water and proton channels in PSII

11:20 **Sabine Oldemeyer** (B3 Heberle) (15 min)
Light-induced changes in the chloride pump NmHR detected by time resolved crystallography and FTIR spectroscopy

11:40 **Dennis Nürnberg** (15 min)
Changes in supramolecular organization of cyanobacterial thylakoid membrane complexes in response to far-red light photoacclimation

12:00 **Louis Lehmann** (C1 Netz) (15 min)
Proton transfer and Stark effect

12:20 *Lunch* Restaurant

13:40 **Field trip to Kloster Chorin**

15:10 *Coffee break* Foyer

SESSION 5: **Chair: Ulrike Alexiev**
15:30 – 16:30

15:30 **Galaan Merga** (B5 Bartl) *online* (15 min)
Photocycle of bacterial phytochromes AgP2 & AgP1

15:50 **Jheng-Liang Chen** (B4 Schlesinger) (15 min)
*Behavior of an outward proton pump from *Ustilago maydis* in acidic environment*

16:10 **Maria Andres Mroginski** (C2) (15 min)
Computational studies on phytochromes

16:30 *Coffee break* Foyer

SESSION 6: **Chair: Patrick Scheerer**
17:00 – 18:00

17:00 **Snežana Zarić** (Guest) *online* (15 min)
Pi-pi interactions

17:20 **Ville Kaila** (Mercator) (15 min)
Unified mechanisms of protonation dynamics in respiration and photosynthesis

17:40 **Hartmut Oschkinat** (B1) (15 min)
TBA

18:00 *Dinner buffet* Restaurant

Open discussion
19:30 – 21:00

Thursday, April 07, 2022

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

SESSION 7

Chair: Franz Bartl

9:00 – 10:00

- 9:00 **Inez Weidinger** (A1) (15 min)
The role of protons in the catalytic cycle of cytochrome c oxidase: old knowledge and new developments
- 9:20 **Johannes Oppermann** (B2 Hegemann) (15 min)
Metagenomically identified ACRs with optogenetic potential
- 9:40 **Jacek Kozuch** (B9) (15 min)
Nitrile infrared intensities as vibrational Stark/electric field probes

10:00 *Coffee break*

Foyer

SESSION 8:

Chair: Inez Weidinger

10:30 – 11:50

- 10:30 **Ernst-Walter Knapp** (Guest) (15 min)
Shared proton and proton-hole in water and proteins
- 10:50 **Franz Bartl** (B5) (15 min)
Protonation dynamics in photocycle and catalytic process of a rhodopsin guanylyl cyclase
- 11:10 **Frederico Baserga** (A1 Heberle) (15 min)
Some like it hot: searching for transient states of cytochrome c oxidase among heating artifacts
- 11:30 **Jon Hughes** (B7) (15 min)
Phytochrome structure and function

12:00 *Lunch*

Restaurant

Internal SFB council meeting / Internal IGK meeting

Saal 1 / Saal 2

13:30 – 15:30

IGK meeting: <https://fu-berlin.webex.com/fu-berlin-en/j.php?MTID=m27b74a2b3a2146484ae9ef65f1a755d5>

Council meeting: <https://fu-berlin.webex.com/fu-berlin/j.php?MTID=mecff1a9e6028aefaa6e940ea29b26203>

16:00 *Departure*

Participants

Principal Investigators

Weidinger, Inez	A1	TUD
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

Guests

Kaila, Ville	MF, Univ. Stockholm
Miller, Anne-Frances	Einstein Fellow, UKY
Knapp, Ernst-Walter	FUB
Zarić, Snežana*	Univ. Belgrade

Postdocs & Senior Scientists

Nürnberg, Dennis	A4	FUB
Hugentobler, Katharina*	A6	FUB
Diehl, Anne*	B1	FMP
Oppermann, Johannes	B2	HUB
Oldemeyer, Sabine	B3	FUB
Schmidt, Andrea*	B6	Charité
Kraskov, Anastasia*	B6	TUB
von Saß, Johannes*	B6	TUB
Blain-Hartung, Matthew*	B6	TUB
Nagano, Soshichiro	B7	JLU

Coordinators

Marquardt, Jeannine	Z	FUB
Frischkorn, Christian*	Z	FUB
Stuhr-Wulff, Fine	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
Oliver, Nicholas*	A4	FUB
Brandhorst, Janosch	A4	FUB
Christer, Kalman	A4	FUB
Greife, Paul	A4	FUB
Assunção, Ricardo*	A4	FUB
Mäusle, Sarah	A4	FUB
Dekmak, Yahia*	A4	FUB
Hussein, Rana*	A5	HUB
Schubert, Luiz	B3	FUB
Chen, Jheng-Liang	B4	FUB
La Greca, Mariafrancesca	B4	FUB
Große, Maximilian	B5	HUB
Merga, Galaan*	B5	HUB
Herder, Luisa*	B6	Charité
Ebrahim, Manal	B6	Charité
Guan, Kaoling	B7	JLU
Chen, Peng-Yuan	B7	JLU
Paschke, Ronja	B9	FUB
Mohr, Swantje	B10	FMP
Colinet, Hélène ^(*)	C1	FUB
Brünig, Florian	C1	FUB
Lehmann, Louis	C1	FUB
Nguyen, Anh Duc	C2	TUB
Jones, Jesse	C2	TUB
Hoang, Tu Oanh	C2	TUB
Rao, Aditya*	C6	HUJI
Filiba, Ofer*	C6	HUJI
Zaporozhets, Iryna	C7	FUB
Liu, Haoran	C8	FMP

* online participants

