SFB 1078

Protonation Dynamics in Protein Function

Annual Retreat of the **Collaborative Research Center – SFB 1078**

Protonation Dynamics in Protein Function

October 4 – 5, 2017
Bildungszentrum Elstal

Program

Travel Information

Venue

Bildungszentrum Elstal
Eduard-Scheve-Allee 3a | D-14641 Wustermark | http://www.servicedienste-elstal.de/index.php | View on Google Maps
If you arrive with the 9:22-train, consider going straight to the lecture hall (building green oval, see below) and check in for your rooms at the reception desk (Gästeanmeldung) later during lunch break.

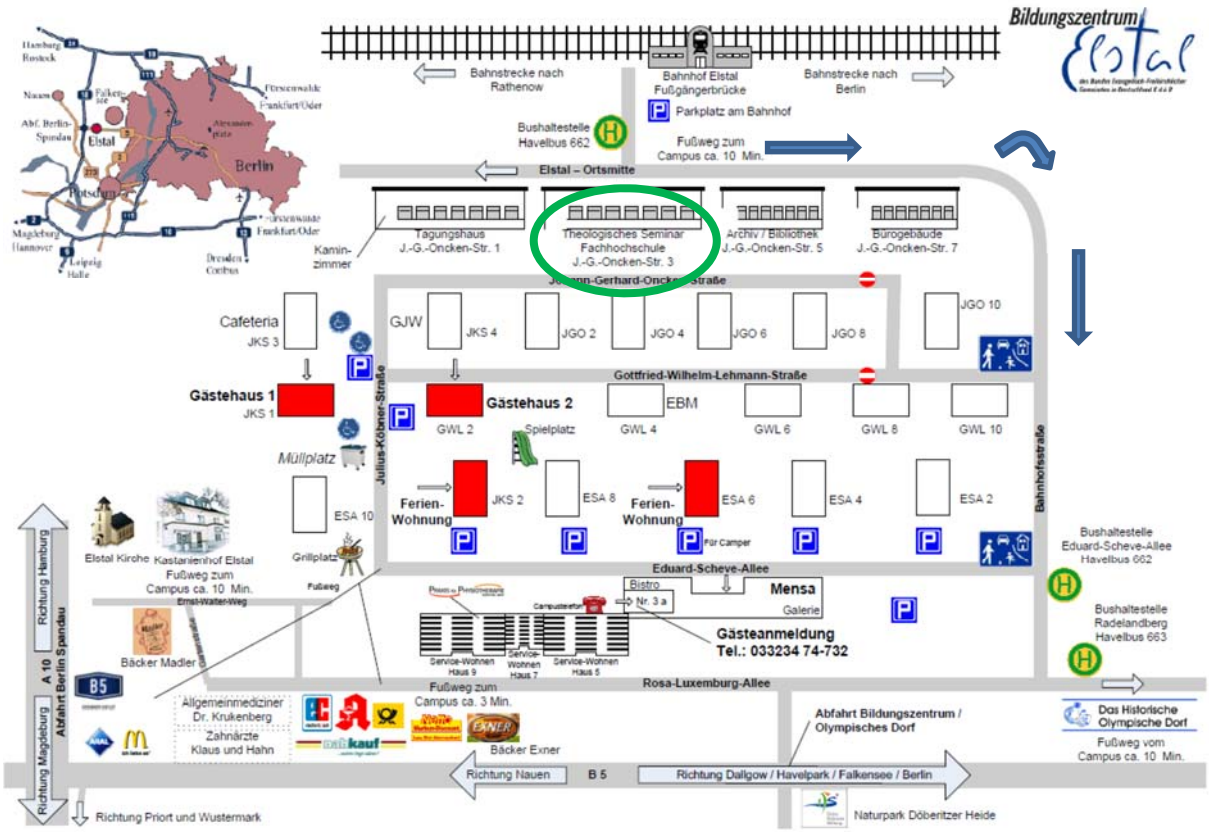
Individual Travel and Return

DB-Tickets required: **3.40 EUR** (VBB-Tarif). Please purchase your own tickets (will not be reimbursed).

Station	Time	Line – Direction
Berlin Hbf (tief)	08:58	Departure of RE 56559 – towards Rathenow
Elstal Bhf, Wustermark	09:22	Arrival Walking distance/time to Bildungszentrum 950m/ca. 10min follow sign “Bildungszentrum”

Return	
Elstal Bhf, Wustermark	from 05:33 to 22:33 – every hour
Berlin Hbf (tief)	Arrival 28 min later

Additional Information



map **not** on scale (in particular the distance “Elstal” Station – campus)

Program overview

SFB1078 Retreat - Bildungszentrum Elstal - 04/05 Oct. 2017

Time	October 04, 2017 Wednesday	
09:00 -	*Registration* *until 09:55*	
10:00 - 10:10	Welcome	J. Heberle
10:10 - 10:30	Talk A1	H. Mohrmann/ F. Kruse
10:30 - 10:50	Talk A2	U. Alexiev
10:50 - 11:10	Talk pot. A6	S. Block
11:30 - 11:50	*Coffee break*	
11:50 - 12:10	Talk C5	P. Imhof/ M. Reidelbach
12:10 - 12:30	Talk A5	M. Ibrahim
12:45 - 14:00	*Lunch*	
14:00 - 15:00	**IGK Meeting**	
15:00 - 15:20	IR sweep	M. Mangold
15:20 - 15:40	Talk A4	H. Dau
15:40 - 16:00	Talk C4	F. Guerra/ S. Adam
16:00 - 16:20	Talk B1	M. Broser/ D. Stöppler
16:40 - 17:00	*Coffee break*	
17:00 - 17:20	Talk B2	C. Grimm/ N. Budisa
17:20 - 17:40	Talk B3	M. Saita
17:40 - 18:00	Talk C1	R. Netz
18:20 - 19:20	*Dinner*	
19:30 - 21:30	**Poster Session**	

Time	October 05, 2017 Thursday	
09:00 - 09:20	Talk B4	M. Walter
09:20 - 09:40	Talk B5	J. Kaufmann
09:40 - 10:00	Mercator Fellow	I. Schapiro
10:00 - 10:20	Talk B7	Y. Yang
10:40 - 11:00	*Coffee break*	
11:00 - 11:20	Talk B8	S. Nagano
11:20 - 11:40	Talk B6	P.Hildebrandt/ L. Sauthof
11:40 - 12:00	Talk C2	M.A.Mroginski/ J. Dragelj
12:00 - 12:20	Talk C3	T. Utesch
12:45 - 14:00	*Lunch*	
14:00 -	**SFB council**	
- 15:30		
15:30	*Departure*	

Wednesday, October 4, 2017

Lecture Hall – Theologisches Seminar Fachhochschule – J.-G.-Oncken-Str. 3

10:00 **Welcome and Introduction by Joachim Heberle**

10:10 – 11:30 **Session 1** Chair: Holger Dau

10:10 **Hendrik Mohrmann** and **Fabian Kruse**, B1 (20 min)
Surface enhanced Raman investigations on the active site of cytochrome c oxidase

10:30 **Ulrike Alexiev**, B2 (20 min)
Protonation and conformational dynamics of CcO and phytochrome

10:50 **Stephan Block**, (FUB, Emmy Noether Group leader) (20 min)
Quantification of proton turnover of single cytochrome bo3 ubiquinol oxidases

11:30 Coffee break

11:50 – 12:40 **Session 2** Chair: Inez Weidinger

11:50 **Petra Imhof** and **Marco Reidelbach**, C5 (20 min)
Networks in cytochrome c oxidase: proton transfer and communication

12:10 **Mohamed Ibrahim**, A5 (20 min)
Insights into the dynamic mechanism of oxygen evolution in photosystem II based on serial femtosecond X-ray crystallography

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12:45 Lunch (Mensa – Eduard-Scheve-Allee)

14:00 – 14:55 **IGK Meeting** (Lecture Hall) Chair: Ulrike Alexiev

14:55 **Group photo** of all participants

15:00 – 16:40 **Session 3** Chair: Joachim Heberle

15:00 **Markus Mangold**, IRsweep, Zurich, Switzerland (20 min)
Single-shot sub-microsecond mid-infrared spectroscopy with quantum cascade laser frequency combs

15:20 **Holger Dau**, A4 (20 min)
Tracking protonation dynamics in photosynthetic water oxidation in wild-type and mutated photosystem II

15:40 **Federico Guerra** and **Suliman Adam**, C4 (20 min)
Molecular dynamics studies of photosystem-II and channelrhodopsin

16:00 **Matthias Broser** and **Daniel Stöppler**, B1 (20 min)
Towards structural elucidation of microbial rhodopsins

Observing structural features related to protonation dynamics by NMR spectroscopy

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16:40 Coffee break / tea time

17:00 – 18:20 **Session 4** Chair: Peter Hildebrandt

17:00 **Christiane Grimm** and **Ned Budisa**, B2 (20 min)
Electrophysiological investigation of a light-driven sodium pump

First attempts to construct an orthogonal pair for small spectroscopically valuable orthogonal amino acids

17:20 **Mattia Saita**, B3 (20 min)
Giving shape to protonated water clusters in membrane proteins with polarized FTIR

17:40 **Roland Netz**, C1 (20 min)
Spectroscopic signatures of proton transfer events

18:20 Dinner (Mensa – Eduard-Scheve-Allee)

19:30 – 21:30 Poster Session (hallways and seminar rooms, Theol. Seminar Fachhochschule – J.-G.-Oncken-Str. 3)

Posters # 1 –24

21:30 Get-together

Depending on weather condition: **Bonfire** on campus ("Grillplatz")

Thursday, October 5, 2017

Lecture Hall – Theologisches Seminar Fachhochschule – J.-G.-Oncken-Str. 3

09:00 – 10:40 Session 5 Chair: Jon Hughes

09:00 **Maria Walter**, B4 (20 min)
Mechanistic details of channelrhodopsin-1

09:20 **Joel Kaufmann**, B5 (20 min)
Proton dynamics in the photocycle of the red-activatable channelrhodopsin variant ReaChR

09:40 **Igor Schapiro**, Hebrew University Jerusalem, Mercator Fellow (20 min)
Primary photoreaction in channelrhodopsin 1

10:00 **Yang Yang**, B7 (20 min)
Ultrafast vibrational dynamics of Agp2 Pfr and related systems

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10:40 Coffee break

11:00 – 12:40 Session 6 Chair: Roland Netz

11:00 **Soshi Nagano**, B8 (20 min)
Crystal structure of sorghum phytochrome B

11:20 **Peter Hildebrandt** and **Luisa Sauthof**, B6 (20 min)
Proton-coupled conformational changes in photoreceptors

11:40 **Maria Andrea** and **Jovan Dragelj**, C2 (20 min)
Understanding proton transfer in phytochromes and cytochrome c oxidase

12:00 **Tillmann Utesch**, C3 (20 min)
Protonation-induced secondary structure changes in the tongue of phytochromes

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12:45 Lunch (Mensa – Eduard-Scheve-Allee)

14:00 – 15:30 SFB Council (Seminar Room 1 - J.-G.- Oncken-Str. 3) Chair: Joachim Heberle

Wednesday 04 Oct. 2017 - 19:30 – 21:30 **Poster Session**

1 **Fabian Kruse** et al., A1:
H/D RAMAN measurements on CN^{-1} inhibited cytochrome c oxidase

2 **Federico Baserga,** Pit Langner, Hendrik Mohrmann, and Joachim Heberle, A1:
Protonation dynamics in cytochrome c oxidase through IR spectroscopy: an improved setup

3 **Group member** of Ulrike Alexiev, A2:
Surface protonation dynamics and function of CcO

4 **Group member** of Ulrike Alexiev, A2:
Long-range interactions and multiple surface protonation events upon phytochrome light activation

5 **Philipp Simon** et al., A4:
Tracking photosystem-II water oxidation by time-resolved infrared spectroscopy

6 **Zhiyong Liang** et al., A4:
Suprising enthalpy-entropy compensation in photosynthetic water oxidation

7 **Ricardo Assunção** and Holger Dau, A4:
New results on photosynthetic water oxidation with bound ammonia, a substrate water analogue

8 **Constantin Schneider** et al., A4:
Future investigations on the proton antenna functionality of the heterologously expressed psbO protein of PSII

9 **Chiara Pasquini** et al., A4:
Kinetic versus energetic isotope effect in water oxidation by (remotely) biomimetic cobalt oxides

10 **Mohamed Ibrahim**, Holger Dobbek, and Athina Zouni, A5:
Insights into the dynamic mechanism of oxygen evolution in photosystem II based on serial femtosecond X-ray crystallography

11 **Matthias Broser**, Katja Stehfest, Ulrike Scheib, Roman Fudim, Yusaku, Hontani, Jonas Wietek, and Peter Hegemann, B1:

Toward structural elucidation of microbial rhodopsins

12 Jonas Wietek, **Christiane Grimm**, and Peter Hegemann, B2:
Artificial anion conducting channelrhodopsins with tuned spectra, modified kinetics and enhanced light sensitivity

13 **Arita Silapetere**, Christiane Grimm, and Peter Hegemann, B2:
Spectroscopical characterization of sodium pump KR2

14 **Maria Walter**, Stefanie Schrottke, Ramona Schlesinger, and Robert Bittl, B4:
Investigating photo-induced structural changes in CaChR1 by means of EPR, FT-IR, and UV/Vis spectroscopy

15 **Joel C.D. Kaufmann**, Benjamin S. Krause, Eglof Ritter, Peter Hegemann, and Franz J. Bartl, B5:
The protonation state of the counter-ions in channelrhodopsin mediates the energy transfer from chromophore to protein

16 **David Buhrke**, Uwe Kuhlmann, Norbert Michael and Peter Hildebrandt, B6:
Time resolved pre-resonant FT-Raman spectroscopy of Agrobacterium tumefaciens phytochromes

17 **Luisa Sauthof**, Andrea Schmidt, Michal Szczepek, Bilal Qureshi, Tammo Stevens, Maria Fernandez-Lopez, Francisco Velazquez Escobar, Norbert Michael, Nobert Krauss, Tilman Lamparter, Peter Hildebrandt, and Patrick Scheerer, B6:

Proton-coupled conformational changes in photoreceptors - 1

18 **Luisa Sauthof**, Andrea Schmidt, Michal Szczepek, Bilal Qureshi, Tammo Stevens, Maria Fernandez-Lopez, Francisco Velazquez Escobar, Norbert Michael, Jan F. Kern, Nobert Krauss, Tilman Lamparter, Vittal Yachandra, Peter Hildebrandt and Patrick Scheerer, B6:

Proton-coupled conformational changes in photoreceptors - 2

19 Florian Brünig, **Jan Daldrop**, Mattia Saita, Matthias Heyden, Joachim Heberle, and Roland Netz, C1:

IR polarization anisotropy and microscopic origin of continuum bands arising from protonated water clusters

20 **Ronald Gonzalez** and Maria Andrea Mroginski, C2:
Quantum modelling of protein-chromophore interactions in Cph1 phytochrome

21 **Giovanni Battocchio**, Tillmann Utesch, and Maria Andrea Mroginski, C3:
Role of protons in long timescale dynamics of phytochromes

22 **Federico Guerra**, Malte Siemers, and Ana-Nicoleta Bondar, C4:
Dynamic hydrogen bonding networks in photosystem II

23 **Suliman Adam** et al., C4:
Stabilising the Schiff base proton in channelrhodopsin

24 **Marco Reidelbach**, Marcus Weber, and Petra Imhof, C5:
Proton transfer in cytochrome c oxidase - calculation and prediction of transition networks

Presenters' names in bold

List of Participants

Principal Investigators

Weidinger, Inez	A1	TU Dresden
Heberle, Joachim	A1, B3	FUB
Alexiev, Ulrike	A2	FUB
Dau, Holger	A4	FUB
Zouni, Athina	A5	HUB
Oschkinat, Hartmut	B1	FMP
Budisa, Ned	B2	TUB
Schlesinger, Ramona	B3	FUB
Bartl, Franz	B5	HUB
Hildebrandt, Peter	B6	TUB
Heyne, Karsten	B7	FUB
Hughes, Jon	B8	JLU
Netz, Roland	C1	FUB
Mroginski, Maria Andrea	C2, C3	TUB
Utesch, Tillmann	C3	TUB
Bondar, Ana-Nicoleta	C4	FUB
Imhof, Petra	C5	FUB
Schapiro, Igor	MF	HUJI

Invited Guests

Block, Stephan	FUB
Mangold, Markus	IRsweep, Zürich

Postdocs & Senior Scientists

Zilliges, Yvonne	A4	FUB
Schneider, Constantin	IGK, A4	FUB
Broser, Matthias	B1	HUB
Szczepek, Michal	B6	Charité
Yang, Yang	B7	FUB
Nagano, Soshi	B8	JLU

Coordinator

Frischkorn, Christian	Z	FUB

PhD Students & Candidates

Göbel, Markus	A1	TU Dresden
Kruse, Fabian	A1	TU Dresden
Baserga, Federico	A1	FUB
Langner, Pit	A1	FUB
Mohrmann, Hendrik	A1	FUB
Balke, Jens	A2	FUB
Sadeghi, Maryam	A2	FUB
Volz, Pierre	A2	FUB
Wolf, Alexander	A2	FUB
Assunção, Ricardo	A4	FUB
Greife, Paul	A4	FUB
Laun, Konstantin	A4	FUB
Liang, Zhiyong	A4	FUB
Mäusle, Sarah	A4	FUB
Pasquini, Chiara	A4	FUB
Simon, Philipp	A4	FUB
Ibrahim, Mohamed	A5	HUB
Stöppler, Daniel	B1	FMP
Fudim, Roman	B2	HUB
Grimm, Christiane	B2	HUB
Silapetere, Arita	B2	HUB
von Saß, Johannes	B2	TUB
Ehrenberg, David	B3	FUB
Maia, Raiza	B3	FUB
Saita, Mattia	B3	FUB
Sellnau, Franziska	B3	FUB
Baumann, Axel	B4	FUB
Krause, Nils	B4	FUB
Schrottke, Stefanie	B4	FUB
Walter, Maria	B4	FUB
Kaufmann, Joel	B5	Charité
Piwowarski, Patrick	B5	Charité
Koch, Anja	B5, B6	Charité
Battocchio, Giovanni	B6	TUB
Buhrke, David	B6	TUB
Sauthof, Luisa	B6	Charité
Schmidt, Andrea	B6	Charité
Brünig, Florian	C1	FUB
Daldrop, Jan	C1	FUB
Dragelj, Jovan	C2	FUB
Peters, Enrico	C2	FUB
Gonzalez Medina, Ronald	C3	TUB
Adam, Suliman	C4	FUB
Buzar, Krzysztof	C4	FUB
Guerra, Federico	C4	FUB
Gorriz, Rene	C5	FUB
Reidelbach, Marco	C5	FUB

PhD Students & Candidates *continued*