

SFB
1078



Protonation Dynamics
in Protein Function

**Annual Retreat of the
Collaborative Research Center – SFB 1078**
Protonation Dynamics in Protein Function

March 19 – 21, 2018
Schloss Rauschholzhausen

Program

Travel Information

Venue

Schloss Rauschholzhausen

Schlosspark 1, 35085 Ebsdorfergrund – <http://schloss.faber-management.de/>

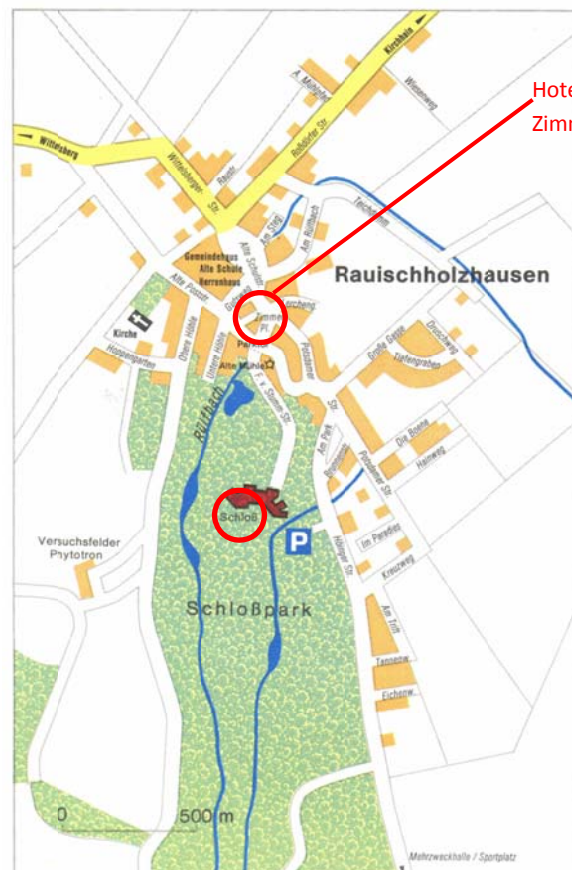
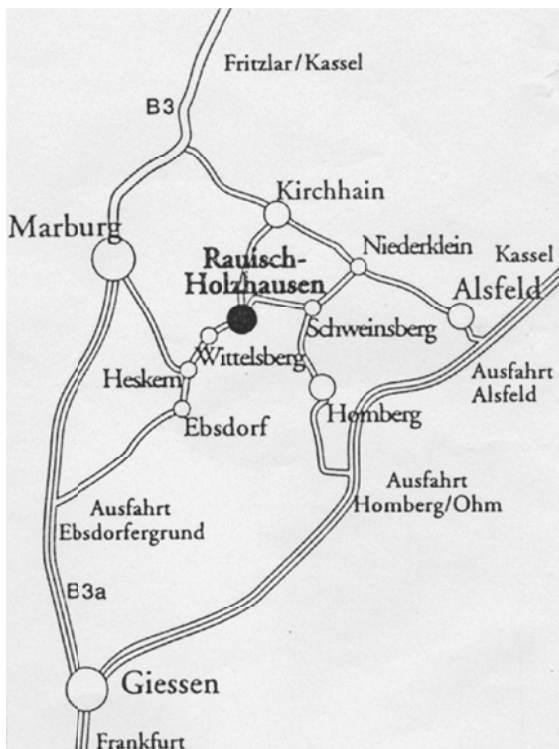
View on [Google Maps](#)

Group Travel (outward: 19/03/2018 – return: 21/03/2018)

A group ticket has been purchased. Individual tickets are only necessary if different connections are used.

Station	Time	Line – Direction
Berlin Hbf	07:59	IC 1929 – towards Hannover (coach 7)
Hannover	09:53	Arrival
Hannover	10:01	IC 2279 – towards Marburg (coach 8)
Marburg (Lahn)	12:03	Arrival
		Bus transfer to Schloss Rauschholzhausen
Return		
Marburg (Lahn)	15:50	IC 2370 – towards Hannover (coach 9)
Hannover	17:56	Arrival
Hannover	18:01	IC 1926 – towards Berlin (coach 7)
Berlin Hbf	19:54	Arrival

Additional Information



Hotel „Zum Stern“,
Zimmerplatz 4

Program overview

SFB1078 Retreat: Schloss Rauschholzhausen – 19-21 March 2018

Time March 19, 2018
Monday

09:00 – 11:40 Session 3	
09:00 - 09:40	Talk T. Keiderling
09:40 - 10:00	Talk B3 D. Ehrenberg
10:00 - 10:20	Talk C1 R. Netz / F. Brünig
10:40 - 11:00 <i>Coffee break</i>	
11:00 - 12:40 Session 4	
11:00 - 11:20	Talk B2 J. Oppermann / J. von Saß
11:20 - 11:40	Talk B4 S. Schrottke
11:40 - 12:00	Talk C4 K. Buzar
12:00 - 12:20	Talk B1 D. Stöppler / E. Peter
12:45 - 14:00 <i>Lunch</i>	
14:00 - 15:30 SFB Council	
14:00 - 15:30 IGK Meeting	
15:30 Excursion to Marburg incl. guided city tour	
18:30 <i>Dinner in Marburg</i> <i>Restaurant "Market"</i>	
approx. 21:00 Bus transfer back to <i>Rauschholzhausen</i>	

13:30 - 14:15 <i>Lunch</i>	
14:30 - 16:20 Session 1	
14:30 - 14:50	Welcome J. Heberle / C. Frischkorn
14:50 - 15:10	Talk B8 J. Hughes
15:10 - 15:40	Talk B6 A. Kraskov / L. Sauthof
15:40 - 16:00	Talk B7 Y. Yang
16:20 - 16:40 <i>Coffee break</i>	
16:40 - 18:00 Session 2	
16:40 - 17:00	Talk MF I. Schapiro
17:00 - 17:20	Talk C2 J. Dragelj
17:20 - 17:40	Talk C3 M.A. Mroginski
18:30 - 19:30 <i>Dinner</i>	
19:30 - 21:30 Poster Session	

approx. 13:00

Expected arrival at Schloss Rauschholzhausen

Time March 20, 2018
Tuesday

Program overview: SFB1078 Retreat – 19-21 March 2018 - *continued*

Time [March 21, 2018](#)
[Wednesday](#)

09:00 - 11:50	Session 5	
09:00 - 09:20	Talk A5	M. Ibrahim
09:20 - 09:45	Talk A4	P. Simon / Z. Liang
09:45 - 10:05	Talk C5	M. Reidelbach
10:05 - 10:30	Talk A1	F. Baserga / P. Langner
10:50 - 11:10	<i>Coffee break</i>	
11:10 - 12:40	Session 6	
11:10 - 11:30	Talk B5	J. Kaufmann
11:30 - 11:50	Talk A2	U. Alexiev
11:50 - 12:10	Talk A6 (N)	S. Block
12:45 - 14:00	<i>Lunch</i>	
14:00 - 15:00	Good Scientific Practice	J. Heberle
15:00	Bus transfer to Marburg station	

Monday, March 19, 2018

Treppensaal – Schloss Rauischholzhausen

14:30 – 16:30 Session 1

Chair: Joachim Heberle

14:30 Welcome and Introduction by Joachim Heberle and Christian Frischkorn

- 14:50 **Jon Hughes**, B8 (20 min)
MAS NMR of plant phytochrome A as Pr and Pfr
- 15:10 **Anastasia Kraskov** and **Luisa Sauthof**, B6 (30 min)
Residues involved in the protonation of biliverdin in Agp2
Structural snapshot of a bacterial phytochrome in its functional intermediate state
- 15:40 **Yang Yang**, B7 (20 min)
Ultrafast vibrational dynamics of phytochromes in Pfr state
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16:20 Coffee break

16:40 – 18:00 Session 2

Chair: Petra Imhof

- 16:40 **Igor Schapiro**, Hebrew University Jerusalem, Mercator Fellow (20 min)
QM/MM simulation of spectroscopic parameters in ChRh1
- 17:00 **Jovan Dragelj**, C2 (20 min)
Modeling the proton loading site in cytochrome c oxidase
- 17:20 **Maria Andrea Mroginski**, C3 (20 min)
Computational studies on phytochrome
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18:30 Dinner

19:30 – 21:30 Poster Session (Foyer and in front of Weißer Saal)

Posters # 1 – 25

Tuesday, March 20, 2018

Treppensaal – Schloss Rauschholzhausen

09:00 – 10:40 **Session 3** Chair: Robert Bittl

09:00 **Tim Keiderling**, University of Illinois, Chicago (40 min)
Site-specific equilibria and dynamics of peptide model structures with vibrational spectra enhanced by isotope labeling

09:40 **David Ehrenberg**, B3 (20 min)
Digging into bistable opsins: light-activation in jumping spider rhodopsin-1

10:00 **Roland Netz** and **Florian Brünig**, C1 (20 min)
IR signatures of proton motion

10:40 Coffee break

11:00 – 12:40 **Session 4** Chair: Inez Weidinger

11:00 **Johannes Oppermann** and **Johannes von Saß**, B2 (20 min)
*Novel anion-conducting channelrhodopsins with near-complete desensitization
Incorporation of proline analogues into the light driven sodium pump KR2*

11:20 **Stefanie Schrottke**, B4 (20 min)
Structural features of the rhodopsin guanylyl cyclase as measured by EPR spectroscopy

11:40 **Krzystof Buzar**, C4 (20 min)
Atomistic simulations of the photosystem II

12:00 **Daniel Stöppler** and **Enrico Peter**, B1 (20 min)
*Studying protonation dynamics by NMR
Shaping ion selectivity of the light-driven Na⁺ pump KR2 towards physiological K⁺ transfer*

12:40 **Group photo** of all participants

12:45 Lunch

14:00 – 15:30 **SFB Council** (Weißer Saal) Chair: Joachim Heberle

parallel session:

14:00 – 15:30 **IGK Meeting** (Treppensaal) self-organized by PhD students

15:30 Departure from Schloss Raischholzhausen
Excursion to Marburg (including guided city tour)

18:30 Dinner at Restaurant “Market” (Markt 11, 35037 Marburg)

21:00 Departure from Marburg back to Schloss Raischholzhausen

Wednesday, March 21, 2018

Treppensaal – Schloss Rauischholzhausen

09:00 – 10:50 **Session 5** Chair: Peter Hegemann

- 09:00 **Mohamed Ibrahim**, A5 (20 min)
Structural changes of the oxygen evolving complex during the catalytic cycle
- 09:20 **Philipp Simon** and **Zhiyong Liang**, A4 (25 min)
Electron and proton transfer of photosynthetic water oxidation in photosystem II
- 09:45 **Marco Reidelbach**, C5 (20 min)
Reaction path prediction in proton transfer systems
- 10:05 **Federico Baserga** and **Pit Langner**, A1 (25 min)
A novel setup for time-resolved IR spectroscopy on cytochrome c oxidase
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10:50 Coffee break

11:10 – 12:40 **Session 6** Chair: Jon Hughes

- 11:10 **Joel Kaufmann**, B5 (20 min)
How the protonation state of the Schiff base counter-ion 1 affects the photocycle in ReaChR
- 11:30 **Ulrike Alexiev**, A2 (20 min)
Protonation dynamics and conformational changes with site-directed probes
- 11:50 **Stephan Block**, A6 (N) (project proposal submitted Feb. 2018) (20 min)
Proton turnover rates of cytochrome bo_3 ubiquinol oxidases measured at the single-enzyme level
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12:45 Lunch

14:00 – 15:00 **Good Scientific Practice by Joachim Heberle**

15:00 **Bus departure to Marburg station**

- 1 **Fabian Kruse** and Inez Weidinger, A1:
SERRS measurements on CN^- -inhibited cytochrome c oxidase
- 2 **Markus Göbel** and Inez Weidinger, A1:
Spectro- electrochemical investigation of cytochrome c oxidase
- 3 **Federico Baserga**, Pit Langner, Hendrik Mohrmann, and Joachim Heberle, A1:
A novel setup for time-resolved IR spectroscopy on cytochrome c oxidase
- 4 **Jens Balke** et al., A2:
Protonation dynamics in phytochrome Cph1
- 5 **Alexander Wolf** et al., A2:
Protonation dynamics and conformational changes in CcO
- 6 **Ricardo Assunção** et al., A4:
Methanol decreases the activation energy of the O_2 releasing step in photosystem II
- 7 **Sarah Mäusle** et al., A4:
Time-resolved single-frequency IR spectroscopy on PS II in H_2O and D_2O : Tracking protonation dynamics
- 8 **Paul Greife** et al., A4:
Time-resolved FTIR spectroscopy of photosystem II: Heat artefact and the $S_3 \rightarrow S_0$ transition
- 9 Daniel Stöppler, Lisa Gerland, Konstantin Laun, **Constantin Schneider**, Yvonne Zilliges, Hartmut Oschkinat and Holger Dau, A4, B1:
Protonation dynamics at the protein-water-interface - the PsbO model protein of photosystem II
- 10 **Matthias Broser** et al., B1:
Crystal structure of the catalytic core of a rhodopsin-guanylyl cyclase with converted nucleotide specificity
- 11 **Enrico Peter** et al., B1:
Shaping ion selectivity of the light-driven Na^+ pump KR2 towards physiological K^+ transfer
- 12 **Johannes Oppermann** et al., B2:
Novel anion-conducting channelrhodopsins with near-complete desensitization
- 13 **Johannes von Saß** et al., B2:
Incorporation of proline analogues into the light driven sodium pump KR2
- 14 **David Ehrenberg** et al., B3:
Digging into bistable opsins: Light-activation in jumping spider rhodopsin-1
- 15 **Franziska Pranga-Sellnau**, Mattia Saita, Victor Lórenz-Fonfría, Ramona Schlesinger, and Joachim Heberle, B3:
Two-photon processes and proton transfer reactions in channelrhodopsin
- 16 **Stefanie Schrottke** et al., B4:
Structural features of the rhodopsin guanylyl cyclase as measured by EPR spectroscopy
- 17 **David Buhrke**, Anastasia Kraskov, and Peter Hildebrandt, B6:
Insights into the Agp2 photocycle reactions from vibrational Spectroscopy

- 18 **Luisa Sauthof**, Andrea Schmidt, **Michal Szczeppek**, Bilal Qureshi, Tammo Stevens, Maria Fernandez-Lopez, Francisco Velazquez Escobar, Norbert Michael, Norbert Krauss, Tilman Lamparter, Peter Hildebrandt and Patrick Scheerer, B6:
Proton-coupled conformational changes in photoreceptors-1
- 19 Andrea Schmidt, **Luisa Sauthof**, **Michal Szczeppek**, Maria Fernandez-Lopez, Francisco Velazquez Escobar, Bilal Qureshi, Norbert Michael, David Buhrke, Tammo Stevens, Dennis Kwiatkowski, David von Stetten, Maria Andrea Mroginski, Norbert Krauss, Tilman Lamparter, Peter Hildebrandt and Patrick Scheerer, B6:
Proton-coupled conformational changes in photoreceptors-2
- 20 **Florian Brünig**, Jan Daldrop, and Roland Netz, C1:
IR signatures of proton motion
- 21 **Soshi Nagano** et al., B8
A high-resolution crystal structure of Sorghum phytochrome B
- 22 **Giovanni Battocchio**, Katrina Forest, and Maria Andrea Mroginski, C3:
Computational study on the role of the knot structure of deinococcus radiodurans bacteriophytochrome
- 23 **Ronald Gonzalez Medina**, C2:
Effect of the knot structure of Deinococcus radiodurans bacteriophytochrome on the chromophore-protein interactions
- 24 **Krzysztof Buzar** et al., C4:
The study of proton transfer in photosystem II
- 25 **Marco Reidelbach** et al., C5:
Reaction path prediction in proton transfer systems

List of Participants

Principal Investigators

Weidinger, Inez	A1	TU Dresden
Heberle, Joachim	A1, B3	FUB
Alexiev, Ulrike	A2	FUB
Hegemann, Peter	B1, B2	HUB
Bittl, Robert	B3	FUB
Scheerer, Patrick	B6	Charité
Hughes, Jon	B8	JLU
Netz, Roland	C1	FUB
Knapp, Ernst-Walter	C2	FUB
Mroginski, Maria Andrea	C2, C3	TUB
Utesch, Tillmann	C3	TUB
Imhof, Petra	C5	FUB
Schapiro, Igor	MF	HUJI
Block, Stephan	A6 (N)	FUB

Invited Guests

Keiderling, Tim	U Illinois, Chicago
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Postdocs, Senior Scientists

Ibrahim, Mohamed	A5	HUB
Broser, Matthias	B1	HUB
Szczeppek, Michal	B6	Charité
Yang, Yang	B7	FUB
Nagano, Soshi	B8	JLU

Coordinator

Frischkorn, Christian	Z	FUB
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PhD Students

Göbel, Markus	A1	TU Dresden
Kruse, Fabian	A1	TU Dresden
Baserga, Federico	A1	FUB
Langner, Pit	A1	FUB
Balke, Jens	A2	FUB
Sadeghi, Maryam	A2	FUB

PhD Students

continued

Wolf, Alexander	A2	FUB
Assunção, Ricardo	A4	FUB
Greife, Paul	A4	FUB
Liang, Zhiyong	A4	FUB
Mäusle, Sarah	A4	FUB
Schneider, Constantin	A4, IGK	FUB
Simon, Philipp	A4	FUB
Stöppler, Daniel	B1	FMP
Peter, Enrico	B1	HUB
Oppermann, Johannes	B1, B2	HUB
von Saß, Johannes	B2	TUB
Ehrenberg, David	B3	FUB
Pranga-Sellnau, Franziska	B3	FUB
Schubert, Luiz	B3	FUB
Schrottke, Stefanie	B4	FUB
Kaufmann, Joel	B5	Charité
Buhrke, David	B6	TUB
Kraskov, Anastasia	B6	TUB
Sauthof, Luisa	B6	Charité
Stensitzki, Till	B7	FUB
Guan, Kaoling	B8	JLU
Nayak, Anindita	B8	JLU
Brünig, Florian	C1	FUB
Dragelj, Jovan	C2	FUB
Gonzalez Medina, Ronald	C2	TUB
Battocchio, Giovanni	C3	TUB
Nguyen, Anh Duc	C3	TUB
Buzar, Krzysztof	C4	FUB
Lazaratos, Michail	C4	FUB
Reidelbach, Marco	C5	FUB

