

SFB  
1078



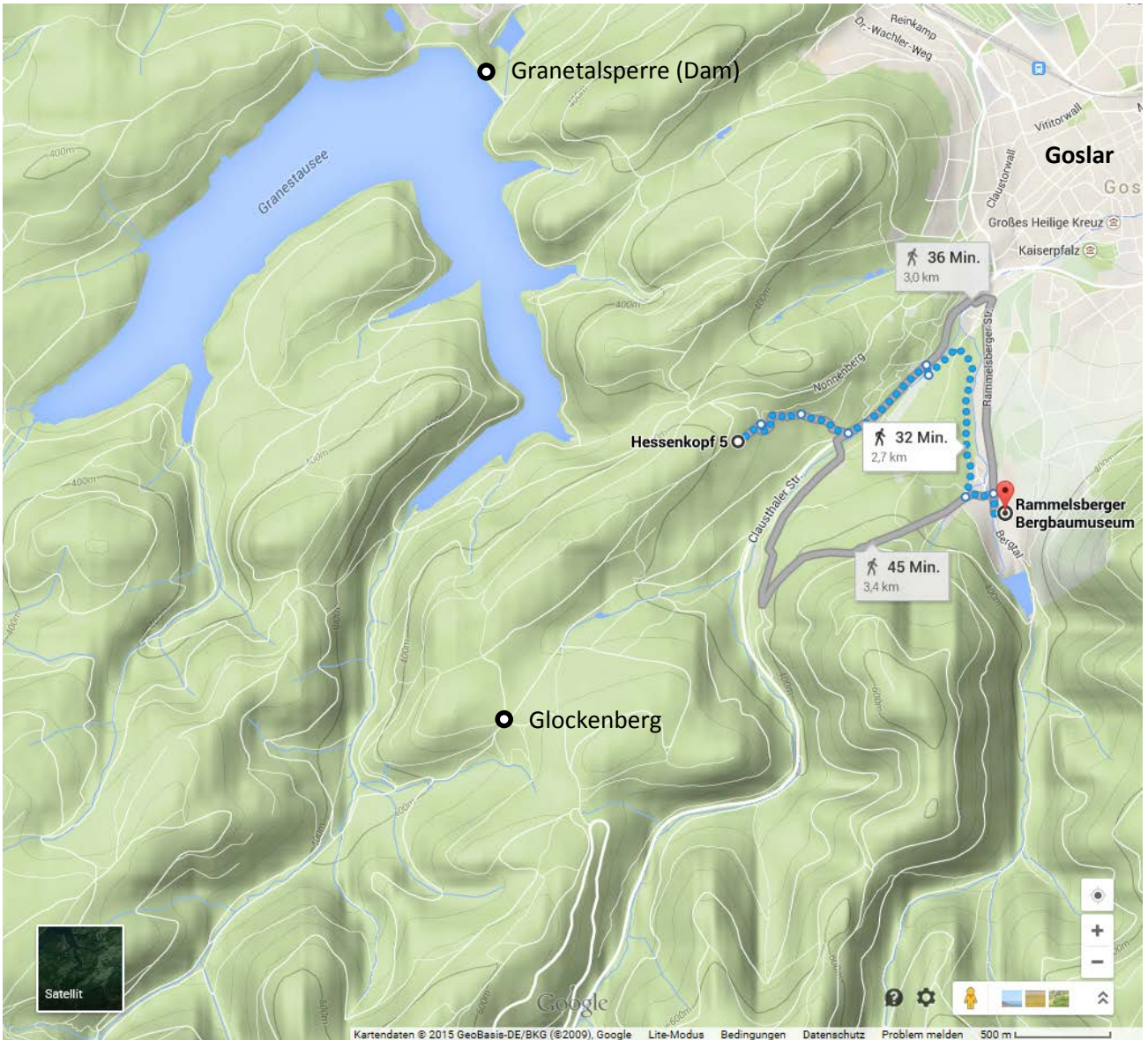
Protonation Dynamics  
in Protein Function

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

March 23 - 26, 2015

Hotel & Tagungszentrum Hessenkopf, Goslar, Harz Mountains

***Program***



## Travel Information

### Departure from Berlin by Train

- 09:23 ICE 597 – Departure from Berlin Ostbahnhof – Platform 7  
**09:34 ICE 597 – Departure from Berlin Hbf – Platform 13 – Coach 1 (Seats 22 – 57, 71 – 116)**  
09:48 ICE 597 – Departure from Berlin-Spandau – Platform 4
- 10:56 ICE 597 – Arrival at Braunschweig Hbf – Platform 6  
**11:24 erx 83741 – Departure from Braunschweig Hbf – Platform 2**
- 12:12 erx 83741 – Arrival at Goslar Bahnhof – Transfer to the Hotel Hessenkopf by Bus

### Venue

#### Hotel & Tagungszentrum Hessenkopf

Hessenkopf 5 | D-38644 Goslar | [www.hessenkopf-goslar.de](http://www.hessenkopf-goslar.de)

### Taxi

Phone +49 5321 22288 | +49 5321 1300 | +49 5321 1313

### Excursions

#### Underground Mining at Rammelsberg, a World Cultural Heritage

Bergtal 19 | D-38640 Goslar | [www.rammelsberg.de/index.php?s=51&m=82&l=en](http://www.rammelsberg.de/index.php?s=51&m=82&l=en)

- Tuesday, 24.3. 15:00 – 16:15 The Roeder Gallery – Guided tour on foot – In ENGLISH  
Tuesday, 24.3. 14:45 – 15:45 The mine train – Guided tour by train – In GERMAN  
Wednesday, 25.3. 15:00 – 16:15 The Roeder Gallery – Guided tour on foot – In ENGLISH

Price per Tour | Adults 10.50 EUR | Students 8.50 EUR | *Please sign up on Monday !!!*

### Hiking Destinations

- Historical City Center of Goslar (ca. 3 km away)  
Granetalsperre und Stausee (Grane Dam and Lake, ca. 4 km away)  
Glockenberg (ca. 2 km) – Bocksberg (ca. 6 km) – Hahnenklee-Bockswiese (ca. 7 km away)

### Individual Travel / Return

For those of you planning to stay for another day or for the weekend: There is a 'scenic route' (slow; German: Express) train travelling to Goslar on weekends and back to Berlin on Fridays/weekends. It costs at most 15 EUR per journey (payable on the train; any two people can be a family):

<http://www.hex-online.de/uploads/hee/documents/86/fahrplan-harz-berlin-express-ab-dem-14-12-2014.pdf>

## Monday, 23.3.2015

13:00 Lunch

14:00 **Welcome by Holger Dau**

14:15 – 15:45 **SFB Science Slam I** Chair: Holger Dau

14:15 **Hendrik Mohrmann, A1** (10 min)  
*Tracking protonation dynamics in non-repetitive reactions of Cytochrome C oxidase by use of flow-flash IR spectroscopy*

14:30 **Fabian Kruse, A1** (10 min)  
*Setup of a pump-probe resonance Raman experiment to probe the charge transfer and oxygen reaction of cytochrome c oxidase*

14:45 **Mahdi Bagherpoor Helabad, C5** (10 min)  
*Communication between D-and K channel in Cytochrome C oxidase*

15:00 **Celin Richter, A3** (10 min)  
*SNARF - photophysical behaviour of a new probe for pump proteins*

15:15 **Alexander Wolf & Constantin Schneider, A2** (10 min)  
*Cytochrome c oxidase and phytochrome*

15:30 **Emanuele Rossini & Jovan Dragelj, C2** (10 min)  
*Energetics of proton transport in CcO and of PSII Mn-cluster model systems*

15:45 Coffee break

16:15 – 18:15 **SFB Science Slam II & Poster Talks I** Chair: Peter Hegemann

16:15 **Philipp Simon & Matthias Schönborn, A4** (10 min)  
*Tracking reactions in Photosystem II*

16:30 **Mohamed Ibrahim, A5** (10 min)  
*An XFEL time-resolved structural investigation of the oxygen evolving complex in Photosystem II*

16:45 **Suliman Adam, C4** (10 min)  
*Coupling between protein, water, and protonation dynamics in channelrhodopsin-2 and photosystem II*

17:00 **Tom Resler, B3** (10 min)  
*Identification of proton and hydrogen bond dynamics in channelrhodopsin*

17:15 **Nils Krause, B4** (10 min)  
*First structural insights in the opening of Channelrhodopsin-2*

17:30 **Joel Kaufmann, B5** (10 min)  
*UV/visible and FTIR investigation on the photocycle of the red-shifted Channelrhodopsin variant ReaCh*

17:45 **Poster Talks** (3 min each)  
*# 1 – 10*

18:30 Dinner

[maximum talking time given in parentheses]

**19:30 – 21:00 Poster Session I**

*Poster # 1 – 10*

- 1 **Martin Bommer, A5**  
*Photosystem II rows-of-dimers superstructure: Natures tiny solar panels*
- 2 **Tom Resler, B3**  
*Deuterium Kinetic Isotope Effects of Channelrhodopsin-2*
- 3 **Matthias Schönborn, A4**  
*Salted Spinach*
- 4 **Daniel Stöppler, B1**  
*Structural investigations of ChR and bR using sensitivity enhanced solid-state MAS NMR*
- 5 **Zaneta Nogacz, B5**  
*Spectroscopic investigation of phytochromes with different types of chromophore*
- 6 **Chiara Pasquini, A4**  
*Water oxidation in a Co-based catalyst: H<sub>2</sub>O/D<sub>2</sub>O isotope effect studied by in-situ spectroscopy*
- 7 **Nils Krause, B5**  
*Helix movements upon opening of Channelrhodopsin-2 in a membrane environment*
- 8 **Christiane Grimm, B2**  
*Electrophysiological investigation of the red-shifted ReaChR and its slow-cycling mutants*
- 9 **Benjamin Krause & Joel Kaufmann, B1 & B5**  
*Spectroscopic investigation of the red-activatable channelrhodopsin ReaChR*
- 10 **Mattia Saita, B3**  
*Channelrhodopsin-2 reconstituted: towards the connection between spectroscopy and the study of the protein function*

**21:00 Bar / Kneipentreff "Knieste" is opening**



[www.goslar.de](http://www.goslar.de)

**Historical City Center of Goslar**

## Tuesday, 24.3.2015

### 9:00 – 10:30 **SFB Science Slam III** Chair: Inez Weidinger

- 9:00 **Daniel Stöppler**, B1 (10 min)  
*Structural investigations of ChR and bR using sensitivity enhanced solid-state MAS NMR*
- 9:15 **Peter Hegemann** on behalf of **Arend Vogt**, B2 (10 min)  
*Conversion of light driven proton pumps into light-gated ion channels*
- 9:30 **Jan Daldrop**, C1 (10 min)  
*Subnanometer-resolved proton mobilities*
- 9:45 **Bilal Qureshi**, B6 (10 min)  
*Structural and functional investigations on full-length phytochromes*
- 10:00 **Francisco Escobar Velazquez**, B6 (10 min)  
*A protonation-coupled feedback mechanism controls the signaling process in bathy phytochromes*
- 10:15 **Aref Takiden**, C2 (10 min)  
*MD simulations and QM/MM calculations of Phytochromes*
- 10:30 Coffee break

### 11:00 – 12:30 **SFB Perspectives I** Chair: Hartmut Oschkinat

- 11:00 **Peter Hegemann**, B1 & B2 (20 min)  
*New Perspectives for B1 and B2 – Novel Strange Rhodopsins*
- 11:30 **Roland Netz**, C1 (20 min)  
*Nanoscale Diffusion and Friction*
- 12:00 **Peter Hildebrandt & Patrick Scheerer**, B6 (20 min)  
*Perspectives: Structural, spectroscopic and functional investigations on phytochromes*
- 12:30 Lunch

### 13:30 – 17:00 **Informal Discussion Rounds**

Among project leaders on current issues and perspectives of the SFB 1078

### 13:30 – 17:00 **Time for Excursions**

Optional: Guided tour at the mine Rammelsberg (*Please sign up on Monday!*)

16:00 – 17:10 Coffee / tea time

### 17:10 – 18:30 **Invited Lecture & Poster Talks II** Chair: Peter Hildebrandt

- 17:10 **Jon Hughes**, Justus-Liebig-Universität Gießen (40 min)  
*How do phytochromes work?*
- 18:00 **Poster Talks** (3 min each)  
*# 11 – 20*
- 18:30 Dinner

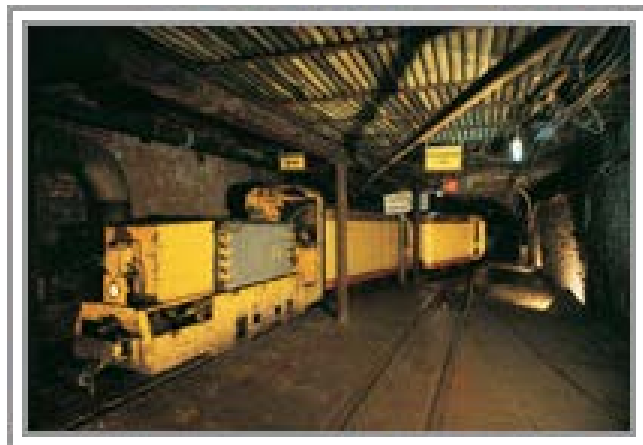
[maximum talking time given in parentheses]

**19:30 – 21:00 Poster Session II**

*Poster # 11 – 20*

- 11 **Eglof Ritter, B5**  
*Cryotrapping of Channelrhodopsin Intermediates*
- 12 **Fabian Kruse, A1**  
*Investigating charge transfer and oxygen reduction of cytochrome c oxidase via time resolved- and surface enhanced resonance Raman spectroscopy*
- 13 **Jovan Dragelj, C2**  
*Energetics of proton transport in cytochrome c oxidase*
- 14 **Mohamed Ibrahim, Rana Hussein & Miao Zhang, A5**  
*An XFEL time-resolved structural investigation of the oxygen evolving complex in Photosystem II*
- 15 **Mario Gerecke, A2**  
*Water solvation dynamics near hydrophobic groups probed by fs fluorescence Stokes shift measurements*
- 16 **Till Stensitzki, B4**  
*Observing the ultrafast photoinduced reactions in ChR1 and Phytochrome*
- 17 **Zhiyong Liang, A4**  
*Water oxidation in photosystem II from cyanobacteria and spinach investigated by time-resolved O<sub>2</sub> polarography: activation energy and influence of NH<sub>4</sub>Cl*
- 18 **Hendrik Mohrmann, A1**  
*Tracking protonation dynamics in non-repetitive reactions of Cytochrome C oxidase by use of flow-flash IR spectroscopy*
- 19 **Bernd Schultz, A1**  
*Time-resolved IR spectroscopy with tunable quantum cascade lasers*
- 20 **Katja Stehfest & Ulrike Scheib, B1 & B2**  
*The rhodopsin guanylyl cyclase of the aquatic fungus Blastocladiella emersonii enables fast optical control of cGMP signaling*

**21:00 Bar / Kneipentreff "Knieste" is opening**



[www.rammelsberg.de](http://www.rammelsberg.de)  
**Rammelsberg – The Mountain Train**

## Wednesday, 25.3.2015

### 9:00 – 10:30 SFB Perspectives II Chair: Ernst-Walter Knapp

9:00 **Maria Andrea Mroginski, C3** (20 min)  
*Perspectives in molecular modelling of Phytochromes*

9:30 **Ulrike Alexiev, A2** (20 min)  
*Protonation and conformational changes*

10:00 **Inez Weidinger, A1** (20 min)  
*Proton coupled electron transfer in cytochrome c oxidase*

10:30 Coffee break

### 11:00 – 13:00 SFB Perspectives III & Poster Talks III Chair: Maria Andrea Mroginski

11:00 **Joachim Heberle, A1 & B3** (20 min)  
*Identification of proton and hydrogen bond dynamics in channelrhodopsin*

11:30 **Franz Bartl, B5** (20 min)  
*Spectroscopic investigations of proton transfer processes in hydrogen-bonded networks in bacterial phytochromes and channelrhodopsins*

12:00 **Ana-Nicoleta Bondar, C4** (20 min)  
*Coupling between protein, water, and protonation dynamics in channelrhodopsin-2 and photosystem II*

12:30 **Poster Talks** (3 min each)  
# 21 – 29

13:00 Lunch

#### 14:00 – 17:30 Informal Discussion Rounds

Among project leaders on current issues and perspectives of the SFB 1078

#### 14:00 – 17:30 Time for Excursions

Optional: Guided tour at the mine Rammelsberg (*Please sign up on Monday!*)

16:30 – 17:30 Coffee / tea time

### 17:30 – 19:00 Poster Session III

*Poster # 22 – 29*

19:00 Dinner

### 20:00 Informal Discussion Round

“Integrated Graduate School – Perspectives” with Ulrike Alexiev and interested SFB members

[maximum talking time given in parentheses]



**17:30 – 19:00 Poster Session III**

*Poster # 21 – 29*

- 21 **Bilal Qureshi, B6**  
*Structural and functional investigations on full-length phytochromes*
- 22 **Yvonne Zilliges, A4**  
*Towards the very first crystallization of genetically modified PSII variants*
- 23 **Philipp Simon, A4**  
*Measuring interquinone  $e^-$ -transfer kinetics of photosystem II by single-frequency IR absorption spectroscopy*
- 24 **Christopher Mielack, C4**  
*Water and hydrogen bond dynamics in the channelrhodopsin light-gated cation channel*
- 25 **Aref Takiden, C3**  
*MD simulations and QM/MM calculations of Phytochromes*
- 26 **Anke Keidel, B6**  
*Chromophore Isomerization in Histidine Kinase Rhodopsin from *Ostreococcus tauri**
- 27 **Mahdi Bagherpoor Helabad, C5**  
*Communication Pathway Between D-channel and K-channel of Cytochrome C Oxidase*
- 28 **Suliman Adam & Federico Guerra, C4**  
*The Parametrisation of PSII Cofactors*
- 29 **Constantin Schneider, A2**  
*Reporter groups at the surface of phytochrome*

**20:00 Bar / Kneipentreff "Knieste" is opening**



[www.rammelsberg.de](http://www.rammelsberg.de)

**Rammelsberg – The Roeder Gallery**

## Thursday, 26.3.2015

9:00 – 10:30 **SFB Perspectives IV** Chair: Ulrike Alexiev

9:00 **Holger Dau, A4** (20 min)  
*Tracking protonation dynamics in photosynthetic water oxidation*

9:30 **Martin Bommer, A5** (20 min)  
*Perspectives: Crystallographic study of Photosystem II*

10:00 **Ernst-Walter Knapp, C2** (20 min)  
*Toward precise pKa computations of residues in proteins with focus on the Mn-cluster in PSII*

10:30 Coffee break

11:00 – 12:30 **SFB Perspectives V** Chair: Franz Bartl

11:00 **Christopher Engelhard, B4** (20 min)  
*Beyond distance: Investigating early intermediate states and spins inside the channel of channelrhodopsin 2*

11:30 **Hartmut Oschkinat, B2** (20 min)  
*Mission Possible: Watching Protons Hopping*

**12:00 – 12:20 Closing Remarks**

*Prize for Best "SFB Science Slam" and Best Poster /  
Retreat 2015 Evaluation / Symposium 2015 / ...*

12:20 Lunch

## Travel Information

### Departure from Goslar by Train

**13:20 Departure at the Hotel** – Bus transfer to the train station Goslar

**14:03 erx 83710** – Departure from Bahnhof Goslar – Platform 4

14:14 erx 83710 – Arrival at Salzgitter-Ringelheim – Platform 2

**14:29 RB 14320** – Departure from Salzgitter-Ringelheim – Platform 7

14:51 RB 14320 – Arrival at Braunschweig Hbf – Platform 5

**14:59 ICE 690** – Departure from Braunschweig Hbf – Platform 7 – Coach 2 (Seats 11–68, 101–116)

16:07 ICE 690 – Arrival at Berlin-Spandau

16:22 ICE 690 – Arrival at Berlin Hbf

16:35 ICE 690 – Arrival at Berlin Ostbahnhof

[maximum talking time given in parentheses]

## List of Participants

### Principal Investigators

Weidinger, Inez	A1	TUB
Heberle, Joachim	A1, B3	FUB
Alexiev, Ulrike	A2	FUB
Dau, Holger	A4	FUB
Oschkinat, Hartmut	B1	FMP
Hegemann, Peter	B1, B2	HUB
Bartl, Franz	B5	Charité
Hildebrandt, Peter	B6	TUB
Scheerer, Patrick	B6	Charité
Netz, Roland	C1	FUB
Knapp, Ernst-Walter	C2	FUB
Mroginski, Maria Andrea	C3	TUB
Bondar, Ana-Nicoleta	C4	FUB

### Invited Guest

Hughes, Jon	Universität Gießen	
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### Postdocs & Senior Scientists

Zilliges, Yvonne	A4	FUB
Bommer, Martin	A5	HUB
Diehl, Anne	B1	FMP
Nieuwkoop, Andrew	B1	FMP
Stehfest, Katja	B1	HUB
Ritter, Eglof	B5	Charite
Qureshi, Bilal	B6	Charité

### Coordinator

Wagner, Kerstin	Z	FUB
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### PhD Students & Candidates

Kruse, Fabian	A1	TUB
Mohrmann, Hendrik	A1	FUB
Schultz, Bernd	A1	FUB
Schneider, Constantin	A2	FUB
Wolf, Alexander	A2	FUB
Gerecke, Mario	A3	HUB
Richter, Celin	A3	HUB
Christiana, Rebecca	A4	FUB
Liang, Zhiyong	A4	FUB
Pasquini, Chiara	A4	FUB
Schönborn, Matthias	A4	FUB
Simon, Philipp	A4	FUB
Hussein, Rana	A5	HUB
Ibrahim, Mohamed	A5	HUB
Zhang, Miao	A5	HUB
Krause, Benjamin	B1	HUB
Scheib, Ulrike	B1	HUB
Stöppler, Daniel	B1	FMP
Grimm, Christiane	B2	HUB
Vogt, Arend	B2	HUB
Resler, Tom	B3	FUB
Saita, Mattia	B3	FUB
Stensitzki, Till	B3	FUB
Engelhard, Christopher	B4	FUB
Krause, Nils	B4	FUB
Walter, Maria	B4	FUB
Kaufmann, Joel	B5	Charité
Nogacz, Zaneta	B5	Charite
Piwowarski, Patrick	B5	Charité
Fernandez Lopez, Maria	B6	TUB
Keidel, Anke	B6	TUB
Velazquez Escobar, Francisco	B6	TUB
Daldrop, Jan	C1	FUB
Dragelj, Jovan	C2	FUB
Rossini, Emanuele	C2	FUB
Takiden, Aref	C3	TUB
Adam, Suliman	C4	FUB
Guerra, Federico	C4	FUB
Mielack, Christopher	C4	FUB
Bagherpoor Helabad, Mahdi	C5	FUB