

SFB  
1078



Protonation Dynamics  
in Protein Function

## **Annual Retreat 2021**

Collaborative Research Center – SFB 1078

*Protonation Dynamics in Protein Function*

March 17 - 18, 2021

Webex Webinar

***Program***

## Wednesday, March 17, 2021

### Welcome address

- 9:00 **Joachim Heberle**, chairman (10 min)  
*Recent developments in the CRC 1078*
- 9:10 **Ulrike Alexiev, Ivelina Zaharieva**, IGK (10 min)  
*Recent Activities of the IGK*

### SESSION 1: Viral Proton Channels

Chair: **Stephan Block**

9:20 – 10:40

- 9:20 **Adam Lange** (B10) (15 min)  
*Atomic structure and conduction mechanism of viral proton channels in liposomes studied by solid-state NMR*
- 9:40 **Han Sun** (C8) (15 min)  
*Proton permeation pathway and ion selectivity of viroporins investigated by atomistic molecular dynamics simulations*
- 10:00 **Cecilia Clementi** (C7) (15 min)  
*Structural bases of proton dynamics in viroporins by multiscale modelling and simulation*
- 10:20 **Jacek Kozuch** (B9) (15 min)  
*Dissecting the mechanism of proton and cation conductance in viroporins using vibrational spectroscopy*

10:40 *Coffee break*

### SESSION 2: Phytochromes

Chair: **Cecilia Clementi**

11:15 – 12:45

- 11:15 **Hartmut Oschkinat** (B1) (15 min)  
*Proton exchange processes in phytochromes and retinal proteins investigated by MAS NMR*
- 11:35 **Igor Schapiro** (C6) (15 min)  
*Protonation depending photochemistry in rhodopsin and phytochrome photoreceptors*
- 11:55 **Karsten Heyne / Jon Hughes** (B7) (20 min)  
*Ultrafast dynamics and structural studies of prokaryotic and plant phytochromes*

12:20 *Lunch break*

### SESSION 3: Channelrhodopsins and related systems

Chair: **Han Sun**

13:45 – 15:05

- 13:45 **Peter Hegemann** (B2) (15 min)  
*Gating and ion transport dynamics in channelrhodopsins and light-driven pumps*
- 14:05 **Joachim Heberle** (B3) (15 min)  
*Identification of proton and hydrogen bond dynamics in channelrhodopsin and related systems*

14:25	<b>Ramona Schlesinger</b> (B4) <i>Hydrogen bonding network in channel- and other rhodopsins and phytochromes analyzed by site-directed mutagenesis and labeling</i>	(15 min)
14:45	<b>Franz Bartl</b> (B5) <i>Spectroscopic investigations of proton transfer processes and hydrogen bonded networks in channelrhodopsins and phytochromes</i>	(15 min)
15:05	<b>Peter Hildebrandt / Patrick Scheerer</b> (B6) <i>Proton-coupled conformational changes in photoreceptors</i>	(20 min)
15:30	<b>Nicoleta Bondar</b> (C4) <i>Graph-based algorithms to dissect dynamic H-bond networks: from channelrhodopsins and photosystem II to spike protein S of SARS-CoV-2</i>	(15 min)
15:50	<i>Coffee break</i>	
16:30	<b>Poster Session in the IGK Gathertown room</b>	(2 h)

## Thursday, March 18, 2021

### SESSION 4: Oxidase

Chair: Jacek Kozuch

9:00 – 11:25

9:00	<b>Maria Andrea Mroginski</b> (C2) <i>Understanding proton transfer in phytochrome and cytochrome c oxidase</i>	(15 min)
9:20	<b>Joachim Heberle / Inez Weidinger</b> (A1) <i>Electron-driven protonation dynamics in cytochrome c oxidase</i>	(20 min)
9:45	<b>Ulrike Alexiev</b> (A2) <i>Surface protonation and conformational dynamics in cytochrome c oxidase and photoreceptors</i>	(15 min)
10:05	<b>Stephan Block</b> (A6) <i>Proton turnover rates of single heme copper oxidases operating against electrochemical gradients</i>	(15 min)

10:25 *Coffee break*

### SESSION 5: Photosystems

Chair: Adam Lange

11:00 – 12:25

11:00	<b>Ville Kaila</b> (Mercator) <i>Protonation dynamics in membrane-bound energy-transducing enzymes</i>	(15 min)
11:20	<b>Holger Dau</b> (A4) <i>Tracking protonation dynamics in photosynthetic water oxidation in wild-type and mutated photosystem II</i>	(15 min)
11:40	<b>Athina Zouni / Holger Dobbek (Mohamed Ibrahim)</b> (A5) <i>Structural basis of proton release from the water-oxidizing complex in cyanobacterial photosystem II</i>	(20 min)
12:05	<b>Roland Netz</b> (C1) <i>Large-scale and small-scale diffusive and dielectric aspects of proton motion</i>	(15 min)

12:25 *Lunch break*

13:30 Ratssitzung