SFB 1078

Protonation Dynamics in Protein Function

Collaborative Research Center – SFB 1078

International Symposium 2015

Protonation Dynamics in Redox Proteins

September 16 - 18, 2015

Freie Universität Berlin, Physics Department

Program

Wednesday, Sept. 16, 2015

9:00 Welcome at the Registration Desk

9:30 – 11:20 Chair: Joachim Heberle

9:30 **Holger Dau**, Freie Universität Berlin (20 min)
Protonation dynamics in photosynthetic water oxidation

10:00 **Robert B. Gennis**, University of Illinois, Urbana, IL, USA (30 min)
Diversity of the Heme-Copper Oxidoreductase Superfamily

10:40 **Per Siegbahn**, Stockholm University, Sweden (30 min)
Proton transfer steps in photosystem II and cytochrome c oxidase

11:20 Coffee break in the former library

11:50 – 13:10 Chair: Ana-Nicoleta Bondar

11:50 **Felix Ho**, Uppsala University, Sweden (30 min)
Water: a multitasker in Photosystem II

12:30 **Johannes Messinger**, Umea University, Sweden (30 min)
Substrate binding and exchange in biological water-oxidation

13:10 Lunch break in the Ethnological Museum

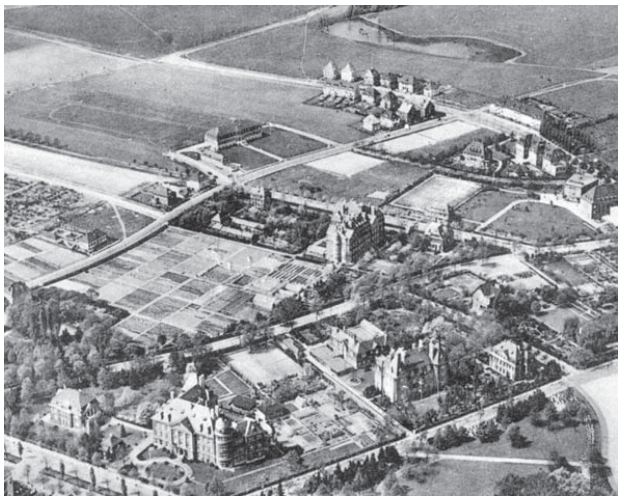
14:30 – 16:00 Guided Tour

100 Years of Research in the Science Quarter Berlin-Dahlem

Nuclear fission, the first uranium reactor, the electron microscope – a surprising number of scientific discoveries and inventions have emerged from Dahlem. From 1912 on, the elegant residential district evolved into a mecca for creative brains from around the world. Unparalleled in Germany, the first modern research campus emerged here on the greenfield site. Albert Einstein, Otto Hahn and Lise Meitner were just some of the researchers who worked or lived in Dahlem. The stimulus was provided by the Kaiser Wilhelm Society, the predecessor of the Max Planck Society, which now continues the tradition together with the Freie Universität. The tour follows the footsteps of Nobel Prize winners, leads to milestones in the history of science, and provides surprising insights into the architecture: most of the Wilhelminian-style buildings were in fact high-tech laboratories. They were the birthplace of modern molecular biology and nuclear physics.

The meeting point for the tour is in front of the Ethnological Museum.

16:30 – 17:00 Coffee / tea time in the former library




Berlin-Dahlem, around 1930. Otto Heinrich Warburg in his laboratory in the Max Planck Institute for Cell Physiology, 1950s. (www.harnackhaus-berlin.mpg.de/4210290/Guided-City-Tours-2015.pdf)

17:00 – 18:30		Chair: Inez Weidinger
17:00	**Ernst-Walter Knapp**, Freie Universität Berlin *Proton transfer in cytochrome c oxidase*	(20 min)
17:30	**Ulrike Alexiev**, Freie Universität Berlin *Protonation and conformational dynamics at the surface of proteins*	(20 min)
18:00	**Petra Imhof**, Freie Universität Berlin *Pathways in Cytochrome c Oxidase: Proton Transfer and Communication*	(20 min)
19:00	Dinner buffet in the former library	

20:00 – 21:30 Poster Session

For the list of posters, please see next page.

20:00 – 21:30 Poster Session

J. Dragelj, A.L. Woelke, U. Alexiev, E.W. Knapp
Investigation of proton transfer in Cytochrome c oxidase at the entrance of the K-channel

Federico Guerra and Suliman Adam
Parametrization of Photosystem II cofactors

Mohamed Ibrahim, Jan Kern, Sergey Koroido, Martin Bommer, Holger Dobbek, Athina Zouni
Time Resolved Spectroscopy and Crystallography of Photosystem II Using Femtosecond X-ray laser

Zhiyong Liang, Ivelina Zaharieva, Oliver Karge, Holger Dau
The activation energy of the O-O bond formation step in photosynthetic water oxidation: Surprising entropy-enthalpy compensation

Hendrik Mohrmann, Bernd Schultz, Joachim Heberle
Tracking protonation dynamics in non-repetitive protein reactions by use of flow-flash IR spectroscopy

Chiara Pasquini, Ivelina Zaharieva, Holger Dau
Water oxidation in a Co-based catalyst: H_2O/D_2O isotope effect studied by in-situ spectroscopy

Marco Reidelbach, Raquel Maeusle, Duote Chen, Fridtjof Betz, Mahdi Bagherpoor Helabad, Petra Imhof
Modelling proton transfer pathways in Cytochrome c oxidase

Emanuele Rossini
Proton solvation in Protic and Aprotic Solvents

Matthias Schönborn, Petko Chernev, Holger Dau
Salted Spinach—Influence of the water analogue NH_3 on PSII water oxidation

Philipp Simon, Petko Chernev, Holger Dau
Time-resolved single-frequency IR absorption spectroscopy on photosystem II: electron-coupled proton transfer at the quinone side

P. Volz, C. Schneider, C. Richter, R. Mahrwald, N. Ernsting, U. Alexiev
Time-resolved fluorescence spectroscopy and microscopy of a pH sensitive SNARF dye suited for coupling to the surface of proteins

A. Wolf, P. Volz, T. Schlieter, J. Balke, U. Alexiev
A novel tracking-free assessment of single molecule diffusion

A. Wolf, C. Schneider, J. Wonneberg, U. Alexiev
Fluorescence correlation spectroscopy as a tool to investigate the protonation dynamics of cytochrome c oxidase

Yvonne Zilliges, Zhiyong Liang
Trapping kinetic and energetic parameters of cyanobacterial PSII D1-variants

Thursday, Sept. 17, 2015

9:30 – 11:20 Chair: Ulrike Alexiev

9:30 **Peter Rich**, University College London, UK (30 min)
Mitochondrial cytochrome c oxidases: functions of the hydrophilic channels

10:10 **Constantinos Varotsis**, Cyprus University of Technology, Lemesos, Cyprus (30 min)
Detection of functional hydrogen-bonded water molecules with protonated/ deprotonated key carboxyl side chains in the respiratory enzyme ba3-oxidoreductase

10:50 **Joachim Heberle**, Freie Universität Berlin (20 min)
Microfluidic IR spectroscopy on cytochrome c and its cognate oxidase

11:20 Coffee break in the former library

11:50 – 13:10 Chair: Yvonne Zilliges

11:50 **Robert Burnap**, Oklahoma State University, Stillwater, OK, USA (30 min)
Second sphere ligands steer the reactivity of the catalytic metal cluster of photosynthetic oxygen evolution

12:30 **Miwa Sugiura**, Emihe University, Japan (30 min)
Effects of Structural Modification around TyrZ and D1-His190 on Proton-coupled Electron Transfer in Photosystem II

13:10 Lunch break in the Ethnological Museum

14:45 Guided Tour – Option 1

The new CYANO laboratories at FU Berlin

This lab tour by Yvonne Zilliges includes a demonstration of the new CellDeg photocultivator optimized for fast and high biomass yields.

The meeting point for the tour is in the former library of the Physics Department.

14:45 – 15:45 Guided Tour – Option 2

History and Overview of the Botanic Garden in Berlin-Dahlem

"The world in a single garden" – this was the plan of Adolf Engler, the first director of the Gardens of Dahlem in 1889. Today, the Botanic Garden of Berlin counts as one of the largest and most important botanical gardens in the world. This is not only due to its surface, but also to the variety of its plants, that count over 20,000 types. In the Botanic Garden, nature always has a season. Taking a stroll in woods and meadows, we can wander in only a few minutes from Alps to Caucasus, discover Far-Eastern plants, and feel the Tropical Rainforest. The Main Tropical Greenhouse (Great Pavilion) is an architectonical masterpiece in Art Nouveau style. Those who enter this place forget space and time – and the outside weather does not play a role anymore.

The meeting point for the tour is at the main entrance of the Botanic Garden.

16:30 – 17:00 Coffee / tea time in the former library

The Botanic Garden in Berlin-Dahlem (www.bgbm.org)

17:00 – 18:30		Chair: Ernst-Walter Knapp
17:00	**Martin Bommer**, Humboldt-Universität zu Berlin *Photosystem II in a crystalline packing that resembles its native membrane*	(20 min)
17:30	**Ivelina Zaharieva**, Freie Universität Berlin *Structural and functional parallels between the biological water oxidation site and a synthetic manganese-oxide catalyst*	(20 min)
18:00	**Ana-Nicoleta Bondar**, Freie Universität Berlin *Dynamic carboxylate/water networks on the surface of the PsbO component of Photosystem II*	(20 min)
19:00	Dinner in the former library	

20:00 – 21:30 Discussion Round

Introduction and Moderation: Holger Dau

Friday, Sept. 18, 2015

9:30 – 11:20 Chair: Joachim Heberle

9:30 **Ville Kaila**, Technische Universität München, Germany (30 min)
Functional water in respiratory and photosynthetic enzymes

10:10 **Qiang Cui**, University of Wisconsin, Madison, WI, USA (30 min)
QM/MM analysis of proton pumping in cytochrome c oxidase

10:50 **Inez Weidinger**, Technische Universität Berlin (20 min)
Voltage driven electron and proton transfer of cytochrome c oxidase on electrodes probed by surface enhanced resonance Raman spectroscopy

11:20 Coffee break in the former library

11:50 – 12:50 Chair: Petra Imhof

11:50 **Roland Netz**, Jan Daldrop, Freie Universität Berlin (20 min)
Proton transition paths are hot

12:20 **Michael Haumann**, Freie Universität Berlin (20 min)
Photosynthetic water oxidation studied by x-ray emssion spectroscopy

12:50 Lunch break in the Ethnological Museum

14:00 – 16:30 Chair: Holger Dau

14:00 **Stenbjörn Styring**, Uppsala University, Sweden (30 min)
Proton reactions around the redox active tyrosines in Photosystem II

14:40 **Peter Brzezinski**, Stockholm University, Sweden (30 min)
Cytochrome c oxidase - mechanism and regulation

15:20 **Concluding Discussion**

16:30 – 17:00 Coffee / tea time in the former library

19:00 Conference dinner for all speakers at the Restaurant Englers
(Additional guests interested in joining the dinner please contact the organizing office, Kerstin Wagner or Sylvia Luther.)

1 Physics Department (Arnimallee 14, 14195 Berlin-Dahlem)
2 Ethnological Museum
3 Seminaris Campus Hotel
4 Entrance to the Botanic Garden
5 Restaurant Englers

Wireless Network Access for Guests

Connect to the wireless network with the SSID **"conference"** and open an arbitrary web page. Instead of that page a form will appear, which asks for the following key: **2v9yb27y**

Note: For technical reasons the connection to the wireless network may be interrupted at midnight. The key is also valid for the following day and must be re-entered in order to continue using the wireless network.

Attention: Connections to the wireless network "conference" are not encrypted and can be eavesdropped. To ensure confidentiality and encryption, please use appropriate protocols (https, ssh, VPN).