

Protein Electrostatics Berlin 2016 (PEB2016)

Program

Tuesday, 19. July

8:30 - 9:30 **Registration**

9:30 **Welcome**

The time schedule for the talks includes some time for discussions. As a rule it should be 5 min for long and 3 min for short talks.

9:40 - 11:00 **Energy and Charge Transfer**
chair: Antonio Baptista

9:40 - 10:20 **Alexei Stuchebrukhov**
Electron Tunneling in Respiratory Complex III

10:20 - 10:40 **Hajime Torii**
New Twist in the Theories on the Electrostatic
Vibrational Response of Peptides and Related
Systems

10:40 - 11:00 **Ana P. Gamiz-Hernandez**
Redox Tuning of Quinone in the Respiratory
Complex I

11:00 - 11:30 **coffee break and registration**

11:30 - 13:00 **Energy and Charge Transfer, continued**

11:30 - 12:10 **Thomas Renger**
Electrostatics of Excited Electronic States of
Chromophores in Proteins

12:10 - 12:30 **Maria Andrea Mroginski**
Elucidation of Protonation States of Key Residues
in Phytochromes: a combined Computational and
Spectroscopic Approach

12:30 - 13:10 **Hiroshi Ishikita**
Proton Transfer Reactions in Water Oxidizing
Enzyme Photosystem II

13:10 - 14:30 **lunch break and registration**

- 14:30 - 16:50** **pKa, Experiment & Theory**
chair: Thomas Simonson
- 14:30 - 15:10** **Bertrand Garcia-Moreno**
Determinants of pKa Values of Ionizable Residues
Buried in the Hydrophobic Interior of Proteins
- 15:10 - 15:50** **Marilyn Gunner**
Application of MCCE to Proton Pumping Proteins
- 16:00 - 16:30** **coffee break**
- pKa, Experiment & Theory, continued**
- 16:30 - 16:50** **Diogo Vila-Viçosa**
pH-dependent Insertion of pHLIP Peptide into
Lipid Bilayers: pK_a values of Key Residues
- 16:50 - 18:30** **Enzyme Catalysis & More**
chair: Thomas Renger
- 16:50 - 17:30** **Qiang Cui**
Electrostatics for Protein-Membrane and
Nanoparticle-Membrane Interactions
- 17:30 - 17:50** **Michael Shokhen**
Stepwise Versus Concerted Mechanisms in
General-Base Catalysis by Serine Proteases
- 17:50 - 18:10** **Petra Imhof**
Interplay of Protonation State, Conformation,
and Reactivity
- 18:10 - 18:30** **Igor Schapiro**
Space and Time Evolution of the Electrostatic
Potential During the Photoisomerization in
Rhodopsin
- 19:00 - 21:30** **buffet dinner and poster session**
There will be poster prizes chosen by the members
of the organizing and program committee.

Wednesday, 20. July

- 9:00 - 11:00** **Solvation: Water, Ions & More**
chair: Matthias Ullmann
- 9:00 - 9:40** **Alexey Onufriev**
Electrostatics of DNA and RNA: small Differences
and their Large Consequences
- 9:40 - 10:00** **Magdalena Gebala**
Dissecting the Ion Atmosphere: Understanding
the Electrostatics of Nucleic Acids
- 10:00 - 10:20** **Nicoletta Ceres**
A Continuum Electrostatic Approach applicable to
Biomacromolecules using All Atom or Coarse-
Grain Representations
- 10:20 - 11:00** **Walter Rocchia**
Coupling continuum electrostatics with integral
equations theory to include high field effects in
the study of redox-active proteins
- 11:00 - 11:30** **coffee break**
- 11:30 - 12:50** **Solvation: Water, Ions & More, continued**
- 11:30 - 11:50** **Ralf Blossey**
Interfacial Waters of Protein-Protein Complexes:
an Exploration by MD Simulations and Continuum
Electrostatics
- 11:50 - 12:30** **Roland Netz**
Dielectric Effects of Electrolytes, Charged Surfaces
and Proteins
- 12:30 - 12:50** **Maria Kurnikova**
Accurate and Efficient Calculations of Histidine
Residue pKa in Ensembles of Protein
Conformations using Molecular Dynamics
- 13:00 - 14:20** **lunch break**
- 14:20 - 16:00** **Methods in Electrostatics**
chair: Roland Netz

- 14:20 - 15:00** **Benzhuo Lu**
Electrostatics: Computing and Applications to
Electro-diffusion Processes
- 15:00 - 15:20** **Andreas Klamt**
COSMO Polarization Charge Densities: a Highly
Efficient and Accurate Alternative Representation
of Molecular and Protein Electrostatics
- 15:20 - 16:00** **Michael Feig**
Implicit Formalisms for Describing Membrane
Environments
- 16:00 - 16:40** **coffee break**
- 16:40 - 18:00** **poster session**
There will be poster prizes chosen by the members
of the organizing and program committee.
- 18:00 - 19:30** **round table discussion**
with wine, beer and brezel
and bring along some ideas!
discussion leaders are very welcome

Thursday, 21. July

- 9:00 - 11:00** **Binding & Association**
chair: Maria Andrea Mroginski
- 9:00 - 9:20** **Menachem Gutman**
The effect of regulating molecules on the structure
of the PPAR-RXR complex
- 9:20 - 9:40** **Yossi Tsfadia**
The Role of Electrostatic Attraction Forces in the
Reconstruction and Stabilization of the Binding
Site of a Homo-Trimer Enzyme
- 9:40 - 10:00** **Jim Warwicker**
Electrostatics Models for pH-Dependence and
Solubility
- 10:00 - 10:20** **Duřanka Janeřiĉ**
Protein Binding Sites Dynamics in Drug Discovery
- 10:20 - 11:00** **Mikael Lund**
Association of Like-Charged Bio-Molecules

- 11:00 - 11:40** **coffee break**
- 11:40 - 13:00** **Constant-pH MD**
chair: Walter Knapp
- 11:40 - 12:20** **Antonio Baptista**
Couplings involving Protonation and Conformation
in cytochrome c oxidase: Insights from constant-pH
MD and PB/MC simulations
- 12:20 - 12:40** **Ana Damjanovic**
Constant pH Simulations with the EDS-HREX
Method
- 12:40 - 13:00** **Miguel Machuqueiro**
Computational Methods to Calculate pK_a Values
at the Water/Membrane Interface
- 13:10 - 14:30** **lunch break**
- 14:30 - 15:50** **Constant-pH MD, continued**
- 14:30 - 15:10** **Jana Shen**
Mechanisms of pH Activation in Enzymes and
Membrane Transporters
- 15:10 - 15:50** **Charles L. Brooks III**
Constant pH Molecular Dynamics: Probing pH-
Mediated Processes from Viral Capsids to
Membranes
- 16:00 - 16:30** **last coffee**
16:30 **announcement of the poster prizes**
sponsored by the Ernst-Reuter Gesellschaft
official farewell
- 18:00** **starting for S-Bahn trip to the**
Club house of the Berliner Ruder Club (BRC)
Only for participants that have booked the dinner in advance.
A map and S-Bahn schedule to the BRC and back will be distributed.
- 19:00** **conference dinner in the Club house of the BRC**