



## ▪ Curriculum Vitae

### Job History

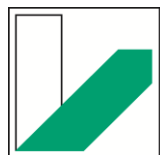
- 10/2003 - present      Professor (Structural Biology/Bioinformatics, University of Bayreuth, Faculty of Biology, Chemistry and Geo-sciences,)
- 01/2001 - 09/2003      Group Leader in the Emmy-Noether Program of the DFG at the Chair for Computational Molecular Biophysics at the IWR of the Ruprecht-Karls-Universität Heidelberg

### Education

- 01/1999 - 12/2000      Postdoc at The Scripps Research Institute in the group of Prof. David A. Case in collaboration with Prof. Louis Noodleman and Prof. Donald Bashford
- 12/1998                  Ph. D. at the Department of Chemistry of the Free University Berlin
- 1996 - 1998              Ph. D. study at the Free University Berlin in the group of Prof. E. W. Knapp (Theoretical and Computational Molecular Biophysics)
- 1994 - 1995              Diploma thesis at the Free University Berlin in the group of Prof. E. W. Knapp (Theoretical and Computational Molecular Biophysics)
- 1990 - 1995              Studies of Biochemistry at the Friedrich-Schiller University Jena and at the University Witten/Herdecke

### Awards and other responsibilities

- 1991 - 1995              Scholar of the German National Merit Foundation (Studienstiftung)
- 1996 - 1998              Ph. D. Scholar of the Boehringer Ingelheim Fonds
- 1999 - 2000              Postdoctoral Fellowship of the Deutsche Forschungsgemeinschaft (DFG)
- 2001 - 2003              Groupleader in the Emmy-Noether Program of the Deutsche Forschungsgemeinschaft (DFG)
- since 2010                Member of the international scientific board of the University of Science and Technology of Hanoi (USTH)
- seit 2013                 Mitglied des Gutachter Panel "Sciences Exactes et Naturelles-1" (SEN-1) des Fund for Scientific Research - FNRS



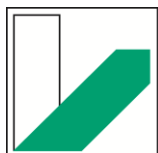
## ▪ Research Focus

In our research, we investigate the function of proteins involved in various biological energy transduction pathways. Many of these proteins are metalloproteins or cofactor-containing proteins. To study these proteins and processes, we apply a variety of theoretical methods including continuum electrostatics calculations, molecular dynamics simulations and quantum chemical calculations. Moreover, we develop methods to analyze and simulate the energetics and kinetics of charge and exciton transfer processes. Our work is at the interface of theoretical biophysics and biochemistry, bioinformatics and computational biology, bioinorganic chemistry, and structural biology

- **Docking of Electron Transfer Proteins**
- **Understanding the Protonation and Redox Behavior of Proteins**
- **Kinetics of Charge and Exciton Transfer in Proteins**
- **Density Functional Calculations of Enzyme Mechanisms**
- **Effect of Membrane Potentials on Proteins**

## ▪ Publications

1. **Mikolaj Feliks, Berta M. Martins, and G. Matthias Ullmann.** Catalytic Mechanism of the Glycyl Radical Enzyme 4-Hydroxyphenylacetate Decarboxylase from Continuum Electrostatic and QC/MM Calculations. *J. Amer. Chem. Soc.*, **135**: 14574-14585, 2013
2. **R. Thomas Ullmann and G. Matthias Ullmann.** GMCT : A Monte Carlo Simulation package for macromolecular receptors. *J. Comput. Chem.*, **33**: 887-900, 2012
3. **Silke A. Wieninger, Engin H. Serpersu and G. Matthias Ullmann.** ATP Binding Enables Broad Antibiotic Selectivity of Aminoglycoside Phosphotransferase(3)-IIIa: An Elastic Network Analysis. *J. Mol. Biol.*, **409** : 450-465, 2011
4. **Elisa Bombarda and G. Matthias Ullmann.** Continuum electrostatic investigations of charge transfer processes in biological molecules using a microstate description. *Faraday Discussions*, **148**: 173-193, 2011
5. **Elisa Bombarda and G. Matthias Ullmann.** pH-dependent  $pK_a$  Values in Proteins - A Theoretical Analysis of Protonation Energies with Practical Consequences for Enzymatic Reactions. *J. Phys. Chem. B*, **114** : 1994-2003, 2010
6. **Astrid R. Klingen, Hildur Palsdottir, Carola Hunte, and G. Matthias Ullmann.** Redox-linked Protonation State Changes in Cytochrome  $bc_1$  Identified by Poisson-Boltzmann Electrostatics Calculations. *Biochem. Biophys. Acta Bioenergetics*, **1767**, 204-221, 2007
7. **Elisa Bombarda, Torsten Becker, and G. Matthias Ullmann.** The Influence of the Membrane Potential on the Protonation of Bacteriorhodopsin: Insights from Electrostatic Calculations into the Regulation of Proton Pumping. *J. Amer. Chem. Soc.* , **128**, 12129-12139, 2006
8. **G. Matthias Ullmann.** Relations between Protonation Constants and Titration Curves in Polyprotic Acids: A Critical View. *J. Phys. Chem. B*, **107**, 1263-1271, 2003



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9. **G. Matthias Ullmann, Louis Noodleman, and David A. Case.** Density Functional Calculation of  $pK_a$  values and Redox Potentials in the Bovine Rieske Iron-Sulfur Protein. *J. Biol. Inorg. Chem.* **7**, 632-639, 2002
10. **Alexey Onufriev, David A. Case, and G. Matthias Ullmann.** A Novel View of pH Titration in Biomolecules. *Biochemistry (New Concepts)* **40**, 3413-3419, 2001



<http://www.researcherid.com/rid/H-1361-2014>

## ▪ Contact

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