



UNIVERSITÄT GREIFSWALD
Wissen lockt. Seit 1456



Das **Institut für Biochemie** lädt gemeinsam mit dem Ortsverband der **Gesellschaft Deutscher Chemiker** zu einem

K o l l o q u i u m d e r G D C h

Großer Hörsaal des Instituts für Biochemie
Felix-Hausdorff-Str. 4, Greifswald

Montag, 30. Juni 2025, 16 Uhr c.t.

Prof. Dr. Matthias Ullmann

Computational Biochemistry, University of Bayreuth

spricht zum Thema:

Describing Charge Transfer in Proteins: A Microstate Model for Simple Proteins and Complex Machineries

Abstract:

Charge transfer through biological macromolecules is essential for many biological processes such as for instance photosynthesis and respiration. In these processes, protons or electrons are transferred between titratable residues or redox-active cofactors, respectively. Often their transfer is tightly coupled. Computational methods based on continuum electrostatics can be used in theoretical biochemistry to analyze the function of even very complex biochemical systems. With these methods, the pH and the redox potential of the solution can be considered in the calculations. Combining continuum electrostatic calculations with a statistical thermodynamic analysis, it is possible to calculate equilibrium parameters such as protonation or oxidation probabilities. Moreover, it is also possible to simulate reaction kinetics by using such parameters. This formalism is applied to the kinetics of electron transfer in the tetraheme-subunit and the special pair of the reaction center of *Blastochloris viridis*.

Einladende

Prof. Dr. Carola Schulzke

Dr. Christian Fischer

Vorsitzender des Ortsverbandes der GDCh