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Protonation Dynamics  
in Protein Function

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Freie Universität Berlin

Hörsaal B

## ➤ Colloquium

### ➤ Prof. Ville R. I. Kaila

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### Exploring the Molecular Principles of Protonation Dynamics in Biological Energy Conversion

Biological energy conversion is catalyzed by remarkable membrane-bound proteins that catalyze elementary electron-, proton-, charge-, and energy transfer reactions across large molecular dimensions. Despite many resolved experimental structures of these proteins in recent years, their molecular mechanisms still remain unclear, and of major challenge for biochemical research. In this talk, I describe our recent mechanistic explorations of long-range proton-coupled electron transfer (PCET) dynamics in the highly intricate respiratory chain enzyme Complex I, which catalyzes a 300 Å fully reversible PCET process. Our work suggests transient charge transfer reactions lead to changes in the internal hydration state of key regions, local electric fields, and the conformation of conserved ion-pairs, which in turn modulate the dynamics of functional steps along the reaction cycle. Similar functional principles are also found in other energy converting enzymes such as cytochrome c oxidase and photosystem II, suggesting that enzymes may employ conserved principles in the catalysis of biological energy transduction processes.

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