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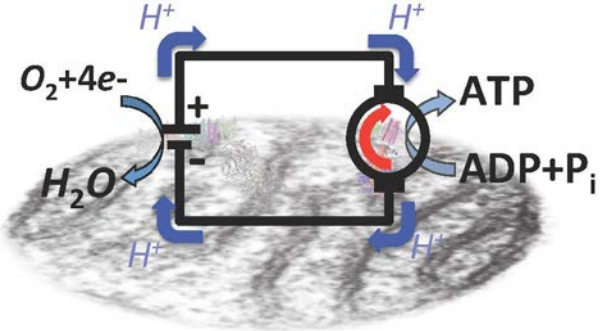
Einladung
zum
Physikalischen Kolloquium
Montag, 26.10.2015
16:15 Uhr in N24/H13

Professor Dr. Gerhard Hummer
MPI, Institut für Biophysik
Frankfurt

Molecular simulation of protein dynamics and function

We use molecular simulations to study functional protein dynamics over a broad range of time scales. Quantum-mechanics/molecular mechanics (QM/MM) descriptions allow us to follow fast, photoexcitation-driven protein motions on the picosecond scale [1]. The resulting simulation trajectories are compared directly to femtosecond time-resolved protein crystallography experiments at X-ray free electron lasers. To study the functional dynamics in molecular motors and pumps [2] on the nano- to millisecond time scales, we have used classical and QM/MM simulations [3-6]. In nonequilibrium simulations, we drive these biomolecular machines by applying mechanical bias and inducing redox transitions that mimic their operation in a biological setting. The simulations help elucidate the molecular mechanisms underlying the efficient energy transduction processes in F_oF_1-ATP synthase [3-4] and the proton pump complex I [5-6].

1. T.R.M. Barends et al., "Direct observation of ultrafast collective motions in CO myoglobin upon ligand dissociation," *Science,* in press (2015). [https://www.sciencemag.org/content/early/2015/09/09/science.aac5492.short]
2. M. Wikström, V. Sharma, V.R.I. Kaila, J. Hosler, G. Hummer, "New perspectives on proton pumping in cellular respiration," *Chemical Reviews* **115**, 2196-2221 (2015). [http://dx.doi.org/10.1021/cr500448t]
3. K.-I. Okazaki, G. Hummer, "Elasticity, friction, and pathway of γ-subunit rotation in F_oF_1-ATP synthase," *Proc. Natl. Acad. Sci. U.S.A.* **112**, 10720-10725 (2015). [http://dx.doi.org/10.1073/pnas.1500691112]
4. K.-I. Okazaki, G. Hummer, "Phosphate release coupled to rotary motion of F1-ATPase," *Proc. Natl. Acad. Sci. USA* **110**, 16468-73 (2013). [http://dx.doi.org/10.1073/pnas.1305497110]
5. V. Sharma, G. Belevich, A.P. Gamiz-Hernandez, T. Róga, I. Vattulainen, M. Verkhovskaya, M. Wikström, G. Hummer, V.R.I. Kaila, "Redox-induced activation of the proton pump in the respiratory complex I", *Proc. Natl. Acad. Sci. U.S.A.* **112**, 11571-11576 (2015). [http://dx.doi.org/10.1073/pnas.1503761112]
6. V. R. I. Kaila, M. Wikström, G. Hummer, "Electrostatics, hydration, and proton transfer dynamics in the membrane domain of respiratory complex I," *Proc. Natl. Acad. Sci. USA* **111**, 6988–6993 (2014). [http://dx.doi.org/10.1073/pnas.1319156111]



Ab 16.00 Kaffee, Tee und Kekse vor dem Hörsaal H13, Org. Prof. Dr. F. Jelezko, Tel. 23750;
Host: Prof.Michaelis Tel. 23050, off.: 23051