

Physikalisches Kolloquium

Gerhard Hummer, MPI Frankfurt

»Molecular simulation of protein dynamics and function«

Einführung: U. Nienhaus

The combination of modern molecular simulations and quantum chemical computations makes it possible to study the molecular function of proteins in unprecedented detail. We have been using this combination to elucidate the molecular mechanisms and chemical reaction principles underlying the enzymatic catalysis of complex multistep reactions, with the processing of nucleic acids using two-metal ion catalysis [1,2] as a paradigmatic example. A combination of quantum chemical calculations and molecular simulations also helped clarify the early time evolution of the molecular structure of the light-activated signaling protein PYP, in combination with picosecond time-resolved X-ray crystallography [3,4]. On larger scales of space and time, simulations help us explore the motions and function of the molecular machines involved in biological energy transduction, including the F_1 rotary motor ATP synthase [5] and the proton pump Complex I [6]. Remarkably, common physical principles emerge in the function of these proteins, despite large variations in their structure and function, including water and hydration effects, extended protein motions, and long-range electrostatic couplings.

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2. E. Rosta, W. Yang, G. Hummer, J. Am. Chem. Soc. 136, 3137 (2014).
3. F. Schotte, H.-S. Cho, V. R. I. Kaila, H. Kamikubo, N. Dashdorj, E. Henry, T. Graber, R. Henning, M. Wulff, G. Hummer, M. Kataoka, P. A. Anfinrud, Proc. Natl. Acad. Sci. USA 109, 19256 (2012).
4. V. R. I. Kaila, F. Schotte, H.-S. Cho, G. Hummer, P. A. Anfinrud, Nature Chemistry 6, 258 (2014).
5. K.-I. Okazaki, G. Hummer, Proc. Natl. Acad. Sci. USA 110, 16468 (2013).
6. V. R. I. Kaila, M. Wikström, G. Hummer, Proc. Natl. Acad. Sci. USA, in press (2014).

Freitag, 30.05.2014, 17 Uhr c.t.,

KIT, Campus Süd,

Otto-Lehmann-Hörsaal, Physik-Flachbau (Geb. 30.22).

Anschließend Nachsitzung im Gastdozentenhaus „Heinrich Hertz“