AKB 55 Molecular Motors

Zeit: Dienstag 14:00–15:45 Raum: TU H2013

Hauptvortrag AKB 55.1 Di 14:00 TU H2013

The Role of Diffusion in the Mechanism of Motor Proteins - Thermal Ratchets and all that — •Jonathon Howard — Max Planck Institute for Molecular Cell Biology and Genetics

Motor proteins such as myosin, dynein and kinesin are enzymes that convert chemical energy, derived from the hydrolysis of ATP, into mechanical work used to power cellular motility. These proteins are unusual engines because the conversion into mechanical energy is direct rather than via an intermediate such as heat or electrical energy, as in everyday engines. A key concept for understanding the mechanism of energy transduction by motor proteins is the lever. Small, atom-sized conformational changes in the ATP-binding pocket of the protein (a few Angstroms) are amplified ten- to one hundred-fold into large conformational changes of the whole protein (several nanometers). The amplification is achieved via rigid-body rotations and translations of comparatively rigid protein domains. The transition between different chemical states is activated by thermal energy. In the case of motor proteins the transition is associated with large displacements corresponding to the protein conformational changes; for this reason, diffusion is expected to play an important role in the motor reaction. I discuss recent experimental and theoretical work on this question.

Hauptvortrag AKB 55.2 Di 14:30 TU H2013

Bacterial motion: molecular motors and switches — •Berenike Maier — CeNS, LMU München

Bacteria are the smallest free-living organisms. Having a diameter of only one micrometer, bacteria undergo random walks in aqueous solution. Bacteria have developed various molecular machines to overcome Brownian motion and to generate directed movement. In this talk we will explore kinetics, force generation and switching of the molecular machine responsible for 'twitching motility' at surfaces.

AKB 55.3 Di 15:00 TU H2013

Molecular dynamics simulations of spontaneous and forced motions of isolated subunits of F_1-ATPase — •U. Kleinekathöfer[1], B. Isralewitz[2], M. Dittrich[2], and K. Schulten[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Beckman Institute, University of Illinois, Urbana, USA.

The F_1 unit of ATP synthase converts a torque applied to its central stalk into chemical synthesis of ATP at binding sites nearly 100 Å away. F_1 has three-fold pseudo-symmetry, consisting of three non-catalytic α-subunits and three catalytic β-subunits. During synthesis, the torque-driven central stalk rotation causes the β-subunit to assume several different conformations at different points in the synthesis cycle. The reverse happens during hydrolysis: conformation changes in the β-subunits drive rotation of the central stalk. We examine the tendency towards spontaneous conformation change of isolated open, half-closed, and closed β-subunits of bovine mitochondrial F1-ATP synthase. In 10-ns molecular dynamics equilibrations, the subunit structural changes can be decomposed into two motions: one parallel to the pseudo-symmetry axis of F1 and one perpendicular to this axis. We also examine the behavior of the central stalk when a β-subunit is forced to close, simulating F1 functioning in hydrolysis mode. In a model system consisting of the central stalk and a single β- subunit, steered molecular dynamics transforms an isolated β-subunit from an half-closed state to a closed state, while the central stalk is constrained to rotate on the pseudo-symmetry axis. We describe how central stalk rotation proceeds as closing is enforced, and how several β-subunit structures effect the force transfer.

AKB 55.4 Di 15:15 TU H2013

Random walks and traffic of molecular motors — •Stefan Klumpp and Reinhard Lipowsky — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam-Golm

Molecular motors exhibit movements on various length scales. Movements on large scales are characterized by the binding to and unbinding from the filaments along which the motors move, and can be described by a class of lattice models [1]. In addition to providing a description of the random walks which arise from many diffusive encounters of motors with filaments, these models allow us to study motor-motor interactions.

The simplest and most obvious such interaction is the hard core repulsion or mutual exclusion of motors, in particular the mutual exclusion from the filament sites, which leads to a variety of cooperative phenomena such as traffic jams, the formation of density patterns and boundary-induced phase transitions [1,2].

In addition, we studied the case where two species of motors moving into opposite directions compete for the filament sites. For sufficiently strong motor–motor interactions, spontaneous symmetry breaking is observed [3]: One motor species occupies the filament while the other one is largely excluded from it. This symmetry breaking provides a mechanism for the formation of traffic lanes.

[1] R. Lipowsky, S. Klumpp, and Th. M. Nieuwenhuizen, Phys. Rev. Lett. **87**, 108101 (2001).
[2] S. Klumpp and R. Lipowsky, J. Stat. Phys. **133**, 233 (2003).
[3] S. Klumpp and R. Lipowsky, Europhys. Lett. **66**, 90 (2004).

AKB 55.5 Di 15:30 TU H2013

Filament depolymerisation by motor proteins — •Gernot Klein, Karsten Kruse, and Frank Jülicher — MPIPKS, Noethnitzerstr. 38, 01187 Dresden

Many active processes in cells are driven by highly specialized motor proteins, which interact with filaments of the cytoskeleton. Members of the Kin-13 kinesin subfamily are able to interact specifically with filament ends and induce depolymerisation of the filaments ends. Recent in vitro assays and single molecule studies have shown, that MCAK accumulates at both ends of stabilized microtubules and induces depolymerisation while at the same time MCAK molecules do not generate directed motion along the microtubules [1].

We analyse both, a stochastic model and a generic mean-field description of this process. We discuss conditions under which motors dynamically accumulate at the filament end. Such a dynamic accumulation occurs for processive cutting, which implies, that the motor can remain attached to the shrinking edge after subunit removal. For processive cutting, the depolymerisation speed as a function of the bulk motor concentration can exhibit several different types of behaviour, including the possibility of a dynamic instability. We discuss our results in relation to recent experiments.

[1]A.W. Hunter, et al., Mol. Cell 11, 445 (2003)