halved torque were now under analysis. The effect of torque decrease upon the energy coupling of F_0F_1 will be discussed in this presentation.

1L1536 イースト F1-ATPase の 16° 回転に伴う水のエントロピー変化の理論解析

A theoretical analysis on water-entropy change in yeast F1-ATPase during 16 degrees rotation of gamma subunit

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We have recently proposed a novel rotation mechanism of F1-ATPase [1] in which the key factor is the water entropy. As part of the demonstration of the validity of our rotation mechanism, we analyze the water-entropy change of yeast F1-ATPase during the 16 degrees rotation of the gamma subunit. The structures before and after the 16 degrees rotation are taken from the crystal structures. For each of them, we calculate the hydration entropies of three different sub-complexes comprising the gamma subunit, one of the beta subunits, and two alpha subunits adjacent to them. The beta_E, beta_TP, and beta_DP subunits are involved in the sub-complexes I, II, and III, respectively. The calculation is performed by a hybrid of the integral equation theory of molecular liquids and the morphometric approach [2]. It follows that due to an asymmetric packing of F1-ATPase, the absolute of the hydration entropy is in the order, sub-complex I > sub-complex II > sub-complex III. Namely, the packing is the tightest in the sub-complex III. When the 16 degrees rotation occurs, the packing of the sub-complex III becomes less tight, leading to a water-entropy loss. However, the loss is almost compensated by water-entropy gains of the other two sub-complexes. The compensation is required for the smooth rotation of the gamma subunit. These results are consistent with the mechanism we have proposed [1].

[1] T. Yoshidome, Y. Ito, M. Ikeguchi, and M. Kinoshita, *J. Am. Chem. Soc.* 133, 4030 (2011).

[2] M. Kinoshita, *Front. Biosci.* 14, 3419 (2009).

1L1548 分子モーターの 1 分子非平衡熱力学

P05 Single-molecule nonequilibrium thermodynamics of molecular 1YE1000 motor

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Molecular motor is a chemical engine that converts chemical potential to mechanical motion. Therefore, it is crucial to reveal the energetics for better understanding of the design principle. However, information about the energetics has remained limited due to lack of methodology. We developed a novel methodology to measure thermodynamic quantities of molecular motors by single-molecule experiments on the basis of nonequilibrium physics. We also developed a novel analytical method to extract information regarding the mechanical potentials at each chemical state and the transition positions between states only from the single-molecule trajectories.

For a single rotary molecular motor F1-ATPase, we measured the "output" of the free-energy transduction, that is, the work performed by the motor and the heat through rotations for the first time under the precise control of the free energy change of ATP hydrolysis. We demonstrated that F1-ATPase has a "thermodynamic" efficiency of nearly 100%.

Furthermore, to understand the mechanism to achieve such a high efficiency, on the basis of a novel analytical method, we evaluated the mechanical potential profiles at each chemical state and the transition angular positions from only the probe's trajectory. We demonstrated that the position-dependent transition of the chemical states is the key feature for the highly efficient free-energy transduction by F1-ATPase. It is suggested that Maxwell's demon resides inside the motor. Our simple and powerful method is applicable to other molecular motors.

1L1612 F1 で見る拡散の Giant Acceleration

Giant Acceleration of Diffusion in F1-motors

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A diffusion coefficient (D), which quantitatively characterizes fluctuation of a small system (nano- or micro-sized system), has been measured frequently in single molecule observations. Applying a constant external force (f) to a small system, we investigate the force dependence of a diffusion coefficient (D(f)),

and introduce the phenomena called "the giant acceleration of diffusion" [1-2]. We show a force-dependent diffusion coefficient (D(f)) provides energetic information of the system. As an example, we first observe the giant acceleration of diffusion in F1-motors which are rotary motor proteins. We succeeded in applying a constant force (f) to F1 by using high-frequency rotating electric field [3]. According to the theories [1-2], D(f) measured in F1 should have a maximum at $f=f^*$ which corresponds to the force exerted by its rotary potential. Noting that a diffusion coefficient is one of useful measurable quantities in single molecule experiments, in future, the giant acceleration of diffusion will be widely observed in biological systems *in vitro* and *in vivo*. We hope our application will be a good example to show the availability of a diffusion coefficient measured in a non-equilibrium state achieved by an external operation.

[1] P. Reinmann et al., *Phys. Rev. Lett.* 87, 010602 (2001).

[2] K. Hayashi and S. Sasa, *Phys. Rev. E* 69, 066119 (2004).

[3] M. Washizu et al., *IEEE Trans. Industry Appl.* 29, 286 (1993).

1L1624 粗視化シミュレーションによるリボソームトランスロケーション機構の研究

Coarse-grained molecular simulation study of ribosomal translocation dynamics

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In the final step of the translation-elongation cycle, the complex of two tRNA and mRNA needs to be advanced by exactly one codon in the ribosome. To realize it, the two ribosomal subunits are thought to be largely rearranged as the so-called ratchet-like rotation. This dynamic behavior, translocation, must be essential for the sequential and accurate translation. Although many experiments including high-resolution structural study have been performed, it is still unclear how the ribosome achieves the movement dynamically.

The molecular dynamics simulation is a good tool to investigate such biological phenomena at atomic resolution. To overcome the limitation of system size and long-time scale, we have developed a coarse-grained (CG) simulation model of RNA and RNP. In the model, each nucleotide is represented as three CG beads and interactions are modeled with structure-based potential, parameters of which were determined by fluctuation matching method to achieve higher accuracy.

Then we employed the CG model to study dynamic behavior of ribosome complex. We focused on especially the relationship among the inter-subunit motion, fluctuation of the tRNAs in the bindings sites, and tRNA-mRNA movement. Some experiments have suggested that tRNAs make hybrid states in the translocation phase, and we were motivated to examine whether it is realized or not in our CG simulations.

1L1636 マイコプラズマのあしが認識するシアル酸オリゴ糖の構造

The structure of sialylated oligosaccharide recognized by mycoplasma leg

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Mycoplasmas, known as the cause of human pneumonia bind to solid surfaces and glide to one direction. Mycoplasmas catch sialylated oligosaccharides, the target of many pathogens, including influenza virus and botulinum toxin. However, there is no information on the structures of sialylated oligosaccharide recognized by mycoplasmas. In the present study, we studied the structure recognized by *Mycoplasma mobile*, using 17 sialylated compounds chemically synthesized. *M. mobile*, the fastest species, glides at 2.5-4 μm per second with the maximum force of 27 pN.

We examined the inhibitory effects of those 17 compounds by counting the number of cells bound to glass surface. The inhibitory effects showed cooperativity, where the Hill coefficient ranged 2 to 4. The most effective structure was N-acetylneuraminic acid alpha-(2,6)-galactose, whose Kd was 0.1 μM . The inhibitory effects changed significantly with the small structural modifications, suggesting that the binding is "lock and key". Next, we examined the inhibitory effects by tracing the number of cells released from glass surface after those compounds were added to gliding cells. The inhibition also showed cooperativity and similar dependency on the chemical structure. The analyses of movements before the detach from glass showed reduction of gliding speed, suggesting that the resting legs generate the drag force. The cells also showed pivoting around the subcellular position of gliding machinery, suggesting the cooperativity of leg movements.