Session 2SDA—Nonequilibrium energetics of biological molecular machines

Shoichi Toyabe¹ · Chun-Biu Li² · Kazushi Kinbara³

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Biological molecular motors can operate robustly and efficiently in highly fluctuating nano-scale environments. How these molecules achieve such remarkable functions is an intriguing question that requires the understanding of the general principles of structural design, enzymatic kinetics, and nonequilibrium dynamics of the biological machineries. By bringing together both experimental and theoretical experts from interdisciplinary fields (Fig. 1), this symposium aimed to explore (A) the novel experimental techniques in probing the energetic efficiencies at the single-molecule level; (B) the recent theoretical methods in explaining the biophysical principles of molecular energetics; and (C) the common strategies shared among different bio-molecular machines in achieving high efficiencies.

This symposium was motivated and co-sponsored by the collaborative project “Molecular Engine” (a Grant-in Aid for Scientific Research on Innovative Areas, JSPS KAKENHI Grant No. JP18H05427) led by Kazushi Kinbara (Tokyo Inst. of Tech.). The goal of the project is to design molecules with autonomous functions resembling those in biological molecular motors, especially focusing on the functions associated with energy conversions.

The symposium started with a brief remark by Chun-Biu Li (Stockholm Univ.). Shoichi Toyabe (Tohoku Univ.) introduced basic concepts of energetics in the context of molecular motors, including efficiencies and precision.

Takayuki Ariga (Yamaguchi Univ.) introduced their recent single-molecule assay of energetics in kinesin molecules, which combined a force-clamp experiment with high-speed feedback and a nonequilibrium relation to determine the heat dissipation (Ariga et al. 2018). They found that kinesin has a large internal dissipation, implying a low energetic efficiency.

Toshiharu Suzuki (Tokyo Inst. of Tech.) showed their works on the ATP synthase with a novel crystallographic technique. They visualized the structural rearrangements in elementary chemical steps, leading to an understanding of the highly efficient energy conversion by the ATP synthase (Soga et al. 2017; Guo et al. 2019).

Holger Flechsig (Kanazawa Univ.) presented their theoretical model describing the walking motions of myosin V along actin filaments to understand its dynamics and energetics. Their model successfully reproduced and explained the recent observations from interactive high-speed AFM experiments, showing that stimulations by the AFM tip can trigger the myosin walking in the absence of chemical energy supply from ATP.

Jin Yu (UC Irvine) discussed the energetics and structural dynamics of a viral RNA polymerase to understand its mechano-chemical coupling and fidelity (Long et al. 2019). Their massive molecular-dynamics simulations quantitatively characterized the Brownian-ratchet working scenario of the polymerase.

Simone Pigolotti (Okinawa Inst of Sci. and Tech.) discussed their theoretical finding on the trade-off between the error and speed in the biopolymer synthesis process (Sartori and Pigolotti 2013). He also discussed the intriguing correlation between fluctuations in the error and speed (Chiuchiú et al. 2019).

Kei-ichi Okazaki (Inst. for Mol. Sci.) presented a novel approach to extract the energy landscape of a linear motor

✉ Shoichi Toyabe
toyabe@tohoku.ac.jp

Chun-Biu Li
cbli@math.su.se

Kazushi Kinbara
kkinbara@bio.titech.ac.jp

¹ Department of Applied Physics, Grad. Sch. of Engineering, Tohoku University, Aoba 6-6-05, Sendai, 980-8579, Japan

² Department of Mathematics, Stockholm University, 106 91, Stockholm, Sweden

³ School of Life Science and Technology, Tokyo Institute of Technology, Nagatsuda-cho 4259 B58, Midori-ku, Yokohama, 226-8501, Japan

Fig. 1 This symposium brings together experts in experiment, simulation, and theory of the field to explore the nonequilibrium energetics of biological molecular motors

chitinase from single-molecule trajectories based on hidden Markov model to estimate parameters of a diffusion model on discrete potential surfaces (Okazaki et al. 2019). Their

work revealed the dynamic burnt-bridge Brownian-ratchet mechanism of the chitinase motor.

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