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Energy and information flows in biological systems: Bioenergy transduction of V_1-ATPase rotary motor and dynamics of thermodynamic entropy in information flows

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ABSTRACT

We classify research fields in biology with respect to flows of materials, energy, and information. We investigate energy transducing mechanisms in biology, using as a representative the typical molecular rotary motor V_1-ATPase from a bacterium *Enterococcus hirae*. The structures of several intermediates of the rotary motor are described and the molecular mechanism of the motor converting chemical energy into mechanical energy is discussed. Comments and considerations on the information flows in biology, especially on the thermodynamic entropy in quantum physical and biological systems, are presented in section 3 in a biologist friendly manner.

Contents

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1. Classification of research fields: flows of materials, energy, and information (Asano et al., 2015b)

Buddha advocated Buddhism containing the concepts of reincarnation and causation. People developed modern natural sciences including physics, chemistry, and biology. Now we know that everything (not only living organisms) recycles in our universe as symbolically suggested by "reincarnation". Thus everything cannot be steady but changes form constantly.

When we think of materials, it is easy to imagine such recycling, because we learned many such examples from a chemistry class. Living organisms do not reincarnate by themselves but their constituents actually recycle. The concepts of energy and information are rather new in the course of establishment of modern sciences. Energy and information also flow and change their forms. In this note an example of typical energy flow in living organisms from chemical to mechanical energy is introduced and discussed using our recent achievement on the structural studies of V-type ATPase from a bacterium (Arai et al., 2013; Suzuki et al., 2016; Yamato et al., 2016).

Information flow in living organisms has been studied in molecular biology and also, as a signal transduction, in biochemistry. The main flow from DNA sequences to proteins has been established as the central dogma. Many biological signal transduction systems, such as the hormone and nervous systems, have been studied extensively. The results of such studies in molecular biology and biochemistry are used to understand our life and have practical importance in medicine.

Now that many such information flows are known, attempts to understand living systems as a whole using a unified concept of information flow have been undertaken to give birth of the establishment of quantum bioinformatics (Asano et al., 2015a, 2015b), which is supposed to be a major theme of this special issue. Two-body systems with interaction can be solved analytically but systems with more than two bodies cannot, in general, be solved analytically. They usually do not evolve according to the classical probability conservation law but rather behave in a non-Kolmogorovian or quantum-like way (Asano et al., 2016). In many cases, such complex systems may be ergodic, presumably producing an entropy increase, which is the origin of the time arrow; see Section 3 for more detail.

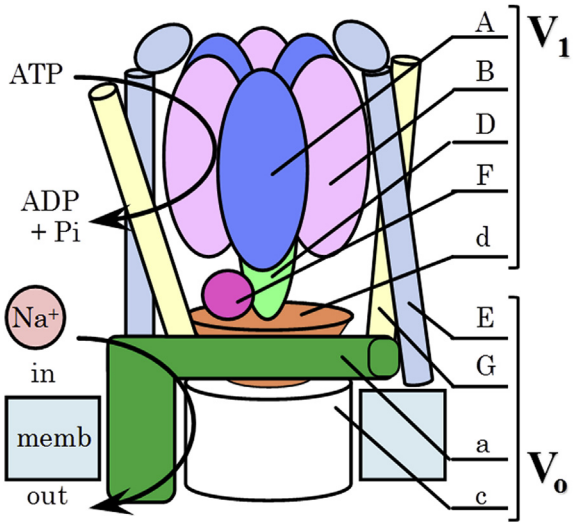

Fig. 1. A model of V-ATPase from *E. hirae*. V_1 indicates catalytic domain (consisting of A_3B_3DF) and V_o indicates membrane domain (consisting of a-c_{10}). Peripheral stalk consists of E and G subunits and the central stalk consists of d, D, and F subunits.

Biological information transfer systems are consisted of complex networks having a large number of interacting members: Molecules including DNA/RNA and proteins; organelles; cells (including the whole nervous system as studied in psychology); organs; individual organisms; ecosystems; societies; and even economics. Complex interacting network systems such as biological systems can be understood to behave quantum-like (Asano et al., 2015a, 2015b) and can be easily imagined to bring about the "causation" in our universe; everything is interconnected, nothing is isolated. In the quantum formalism, one form of the interconnection is entanglement which is often treated as an exhibition of quantum nonlocality. The main distinguishing feature of the state of entanglement for a composite system $S = S_1 + \ldots + S_n$ is that any modification of the state of any subsystem S_j induces modification of the "global state", the state of S. In this formalism, for example, expression of some concrete gene in the genome generates update of the state of the whole genome (or epigenome; see Asano et al., 2013). Therefore, everything effects the meaning of its existence by the existence itself.

2. Bioenergy transduction of a molecular rotary motor, V_1-ATPase

2.1. Introduction

F-ATPases working as ATP synthases in mitochondria, chloroplasts, and bacterial membranes and V-ATPases working as H^+ pumps in eukaryotic acidic organelles and certain bacterial membranes are the relatives functioning as rotary motors (Forgac, 2007; Mulkidjanian et al., 2007): Hydrolysis energy of ATP at the catalytic hydrophilic domain ($\alpha_3\beta_3$ in F_1 or A_3B_3 in V_1) drives the three step rotation of its axis (γ in F_1 or DF in V_1) connected to the membrane hydrophobic rotor ring (oligomer of c in F_o or V_o), which in turn results in the ion translocation through the interface between the rotor ring and the hydrophobic stator subunit (a in F_o or V_o) (Fig. 1). The three dimensional structures of F_1 (Abrahams et al., 1994) or V_1 (Arai et al., 2013) have been obtained and the single-molecule analysis of the rotation revealed important facets of the rotation mechanism (Adachi et al., 2007; Minagawa et al., 2013); the correlation of the nucleotide binding with the (sub)steps of rotation (Adachi et al., 2007). However, the basic mechanism of energy transduction, chemical energy of ATP hydrolysis converted to rotational motion, has not been fully elucidated; especially, how the hydrolysis of ATP resulting in the conformational change of A_3B_3 brings about the rotation of the DF axis is unclear.

We have been studying V-ATPase of *Enterococcus hirae*, which acts as a primary ion pump similar to eukaryotic V-ATPases but uniquely transports Na^+ or Li^+ instead of H^+ (Mizutani et al., 2011). The enzyme is thought to be a bacterial homologue of eukaryotic V-ATPase (Zhou et al., 2011). We have determined its crystal structures (Arai et al., 2013; Suzuki et al., 2016), finding the asymmetrical structures of A_3B_3 or supposedly intermediate structures during rotation driven by ATP hydrolysis.

2.2. Several structures of V_1-ATPase and A_3B_3 complexes showing intermediate states of the chemomechanical energy transduction

We have obtained several intermediate structures of the rotary motor as published (Arai et al., 2013; Suzuki et al., 2016). Fig. 2 shows the schematic representation of the rotational conformational changes deduced from the obtained structures (Suzuki et al., 2016).

Crystal structure of A_3B_3 showed asymmetry without nucleotide (bound, bindable and empty forms) and that of V_1 showed a