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Minimum-dissipation protocol for F_1 -ATPase molecular motor

The event is part of the group seminar AG Klapp at TU Berlin and will take place via Zoom. For information on how to access the event, please contact: henning.reinken@itp.tu-berlin.de

Wednesday, 30.03.2022 · 16:00h · via Zoom

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Minimum-dissipation protocol for F_1 -ATPase molecular motor

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A biomolecular motor composed of protein complexes exchanges energy, matter, and information with its surrounding. Despite being in contact with a fluctuating environment, it performs (on average) a directed motion, in accordance with the second law, by transducing chemical energy stored in the surrounding environment¹. Among several biomolecular motors, F_0F_1 -ATP synthase has gained much attention due to its high efficiency². It produces $\sim 95\%$ of the cellular ATP (adenosine triphosphate) from ADP (adenosine diphosphate) and P_i (inorganic phosphate). The membrane-embedded F_0 -unit utilizes energy from proton flux to rotate F_1 -unit's γ -crankshaft and synthesizes ATP molecules. Since γ -crankshaft rotates as fast as ~ 350 revolutions per second, it remains a puzzle how F_0F_1 transduces energy with great efficiency. One possible way to investigate this is to uncover the functional principle of that particular unit where ATP is synthesized, i.e., F_1 -ATPase. To this end, we focus on an isolated F_1 -ATPase, which can also be controlled in an experimental setup³. We aim to design a control protocol (mimicking F_0 operation) by which the F_1 unit's γ -crankshaft can be rotated to synthesize ATP at low dissipation. We follow a theoretical method valid near-equilibrium⁴ to construct a non-trivial designed protocol. Then, we rotate the crankshaft with this designed protocol to compute dissipation. Our analysis reveals that the designed protocol dissipates a less amount of energy in comparison to a constant velocity protocol for a wide range of protocol durations⁵.

1 Mugnai, M. L., Hyeon, C., Hinczewski, M. & Thirumalai, D. Theoretical perspectives on biological machines. *Rev. Mod. Phys.* 92, 025001 (2020).

2 Soga, N., Kimura, K., Kinosita, K., Yoshida, M. & Suzuki, T. Perfect chemomechanical coupling of F_0F_1 -ATP synthase 114, 4960–4965 (2017).

3 Toyabe, S. et al. Nonequilibrium energetics of a single F_1 -ATPase molecule. *Phys. Rev. Lett.* 104, 198103 (2010).

4 Sivak, D. A. & Crooks, G. E. Thermodynamic metrics and optimal paths. *Phys. Rev. Lett.* 108, 190602 (2012).

5 Gupta, D. et al. Minimum-dissipation protocol for F_1 -ATPase molecular motor. Manuscript in preparation.