Operation of molecular motors

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Properties of nanosystems

- Certain properties are quantized
- Gravity is negligible compared to the other forces
- Surface/mass ratio is very large
- Dissipation of heat is virtually instantaneous
- The role of different binding forces is large
- Molecular level recognition
- Self-organization
- The effect of inertia is negligible
- Increased role of viscosity and thermal movement

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Properties of biological motors

- Made of soft material (biopolymers)
- Function is governed by non-covalent forces
- There are no smooth frictionless surfaces
- Fuel: ATP (NADH), transmembrane gradient
- Work in solutions – high viscosity
- Their power is: 100-1000 ATP/s, i.e. 10^{-16} – 10^{-17} W
- The power of Brown motion is: 10^{-8} W
- The working principle uses Brown motion

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Can the role of the Brownian motion be eliminated?

The importance of the Brownian motion is the consequence of the size and not of the experimental conditions!

The effect of the Brownian motion can not be eliminated.
It does not help if:

- Pressure is decreased
  - (less frequent collisions, but smaller viscosity)
- Temperature is decreased
  - (the magnitude of the fluctuations is proportional to the square root of the absolute temperature)

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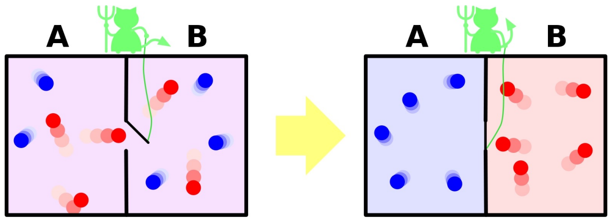
Maxwell demon



James Clerk Maxwell
(1871)

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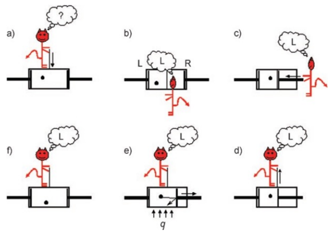
The Maxwell demon of Leó Szilárd



Leó Szilárd : The Maxwell demon has to store information and has to erase information if he wants to return in the initial state.

Rolf Landauer (1960): erasing information increases entropy:
- For every bit: $\Delta S = k_B \cdot \ln 2$

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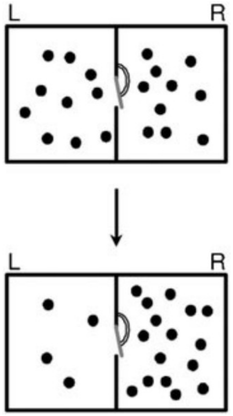
Smoluchowski's trapdoor Maxwell demon



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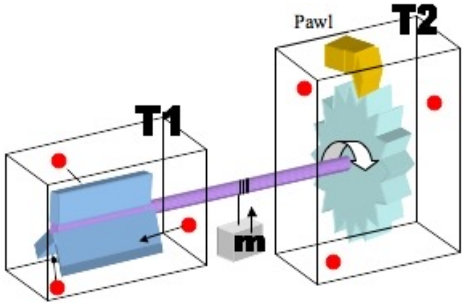
Brownian (Smoluchowski, Feynman) ratchet



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Function of the Brownian ratchet

- Random mixing
- Energy source
- Asymmetric energy surface along the reaction coordinate

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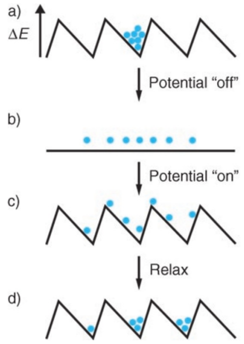
Pulsating ratchet

The potential should be turned of for a short time only, otherwise the transport happens with equal probabilities in both directions.



Kay et al. (2007) Angev. Chem. 46: 72

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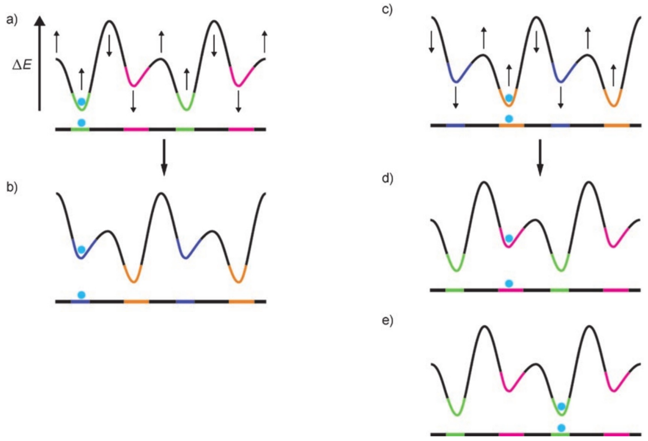
Flashing ratchet



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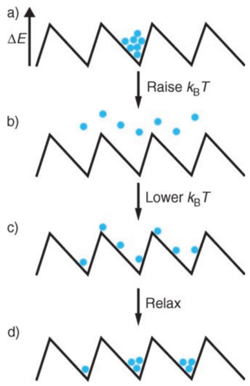
Temperature ratchet



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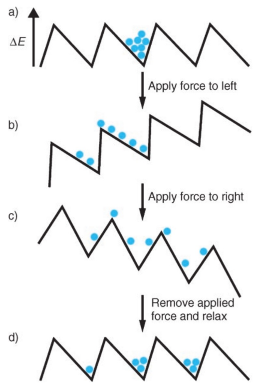
Tilting ratchet



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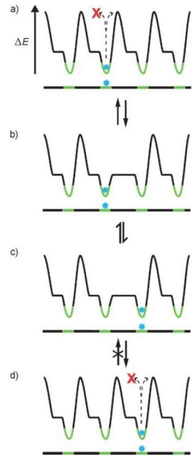
Information ratchet



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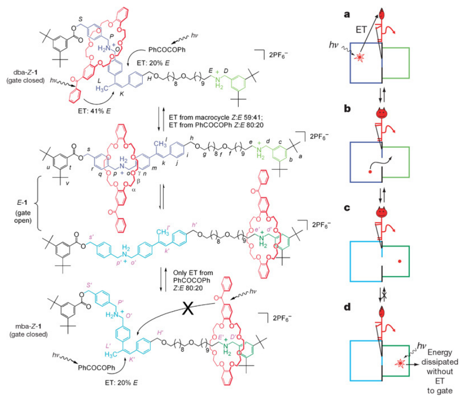
Experimental embodiment of the information ratchet



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The working principles of biological motors

- Break the isotropy of the transport resulting from fluctuations
- Kinetic coupling between substrate and motor
- Substrate movement is always localized
- Manipulating localization is important element of the transport
- Localization is the result of non-covalent interactions

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Biological application of Nonequilibrium thermodynamics

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Evans-Searles FT (revision)

Evans-Searles FT for the entropy production

$$\frac{P(\Omega = A)}{P(\Omega = -A)} = e^{A}$$

here Ω denotes entropy production

Evans and Searles (2002) Advances in Physics, 51: 1529

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Crooks FT (revision)

For a driven system in contact with thermostat:

$$\frac{P_F(A \rightarrow B)}{P_R(A \leftarrow B)} = e^{\frac{W-\Delta G}{k_B T}}$$

W is the work done when the system is driven from the state described by the value A of the control parameter into B

ΔG is the free enthalpy difference between states A and B

G. E. Crooks, J. Stat. Phys. (1998) 90: 1481

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Jarzynski equality (revision)

Connects the work measured during non-equilibrium measurements to the free enthalpy difference between the initial and final states.

$$\left\langle e^{\frac{-W}{k_B T}} \right\rangle = e^{\frac{-\Delta G}{k_B T}}$$

W is the work done when the system is driven from the state described by the value A of the control parameter into B.

The transition between the initial and final states need not happen through equilibrium states.

C. Jarzynski, Phys. Rev. Lett. (1997) 78: 2690

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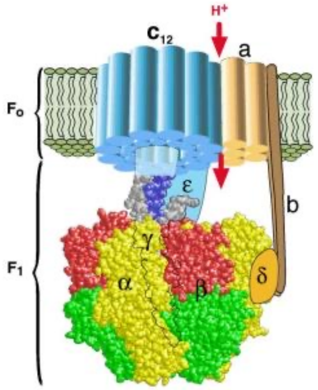
Structure of the F_1-ATP-ase motor



H. Wang and G. Oster (1998). Nature 396:279-282.

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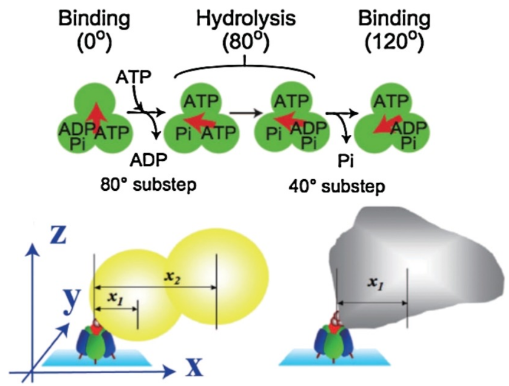
Rotation of F_1-ATP-ase motor



Hayashi et al. (2010) Phys. Rev. Lett. 104: 218103

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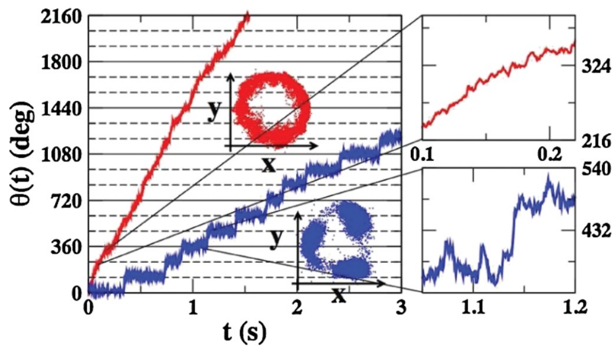
Rotation of F_1-ATP-ase motor (experiment)



Hayashi et al. (2010) Phys. Rev. Lett. 104: 218103

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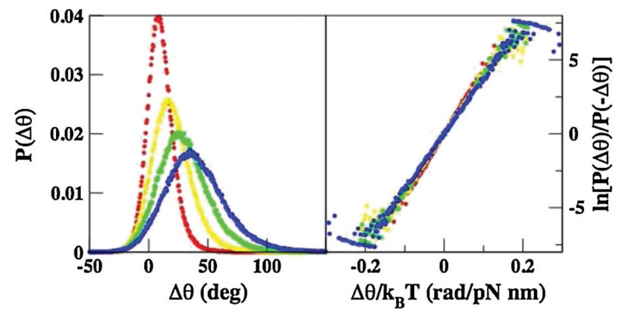
Fluctuation theorem for the F_1-ATP-ase motor



red: 2.5 ms; yellow: 5.0 ms; green: 7.5 ms; blue: 10 ms

Hayashi et al. (2010) Phys. Rev. Lett. 104: 218103

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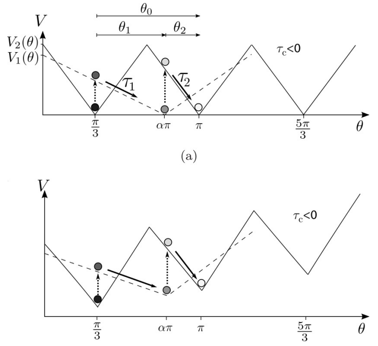
F_1-ATP-ase flashing ratchet mechanism

Rotation mechanism of the free-rotating and the loaded F_1-ATP-ase motor.

relaxed state: continuous line

nucleotide binding state: dashed line



Sancho and Perez-Carrasco (2010) Fluct. Noise. Lett. 11: 1240003

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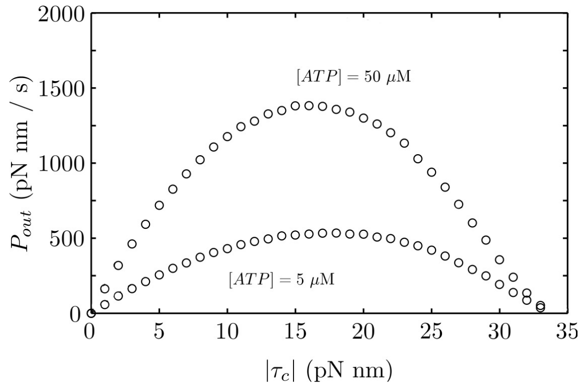
Power release of the F_1-ATP-ase



Sancho and Perez-Carrasco (2010) Fluct. Noise. Lett. 11: 1240003

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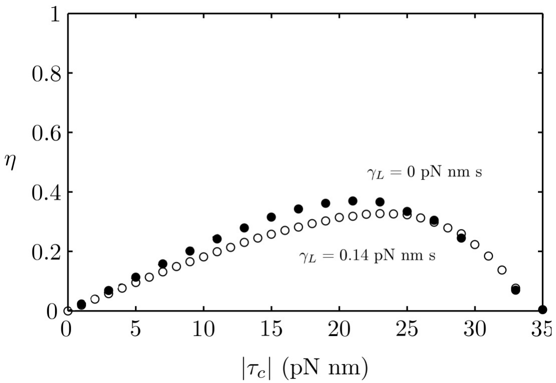
Efficiency of the F_1-ATP-ase



Sancho and Perez-Carrasco (2010) Fluct. Noise. Lett. 11: 1240003

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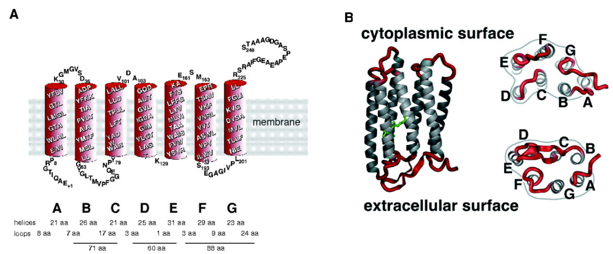
Structure of bacteriorhodopsin



Oesterhelt et al. (2000) Science 288: 143

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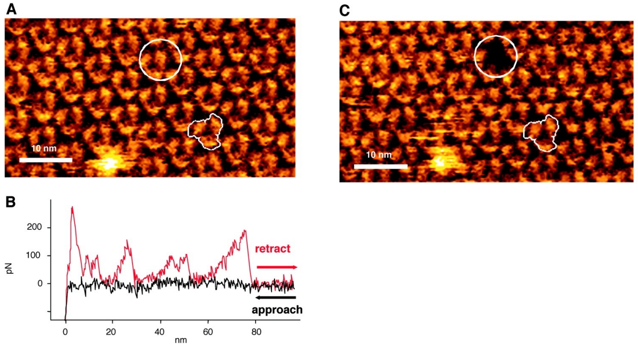
Mechanical unfolding of bacteriorhodopsin



Oesterhelt et al. (2000) Science 288: 143

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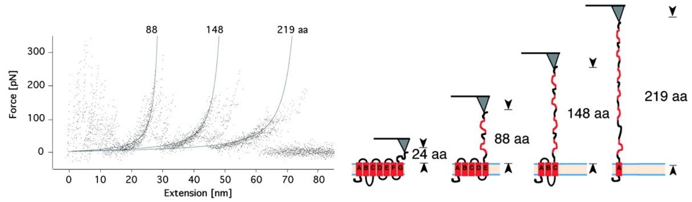
Mechanical unfolding of bacteriorhodopsin



Oesterhelt et al. (2000) Science 288: 143

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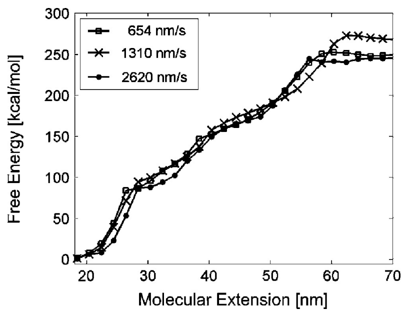
Free enthalpy surface of bacteriorhodopsin



Preiner et al. (2007) Biophys. J. 93: 930

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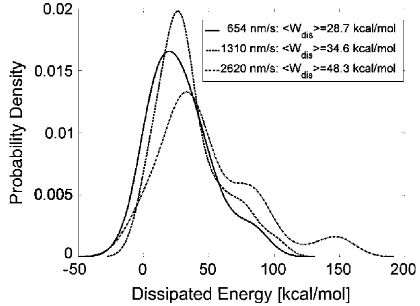
Free enthalpy surface of bacteriorhodopsin



Preiner et al. (2007) Biophys. J. 93: 930

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