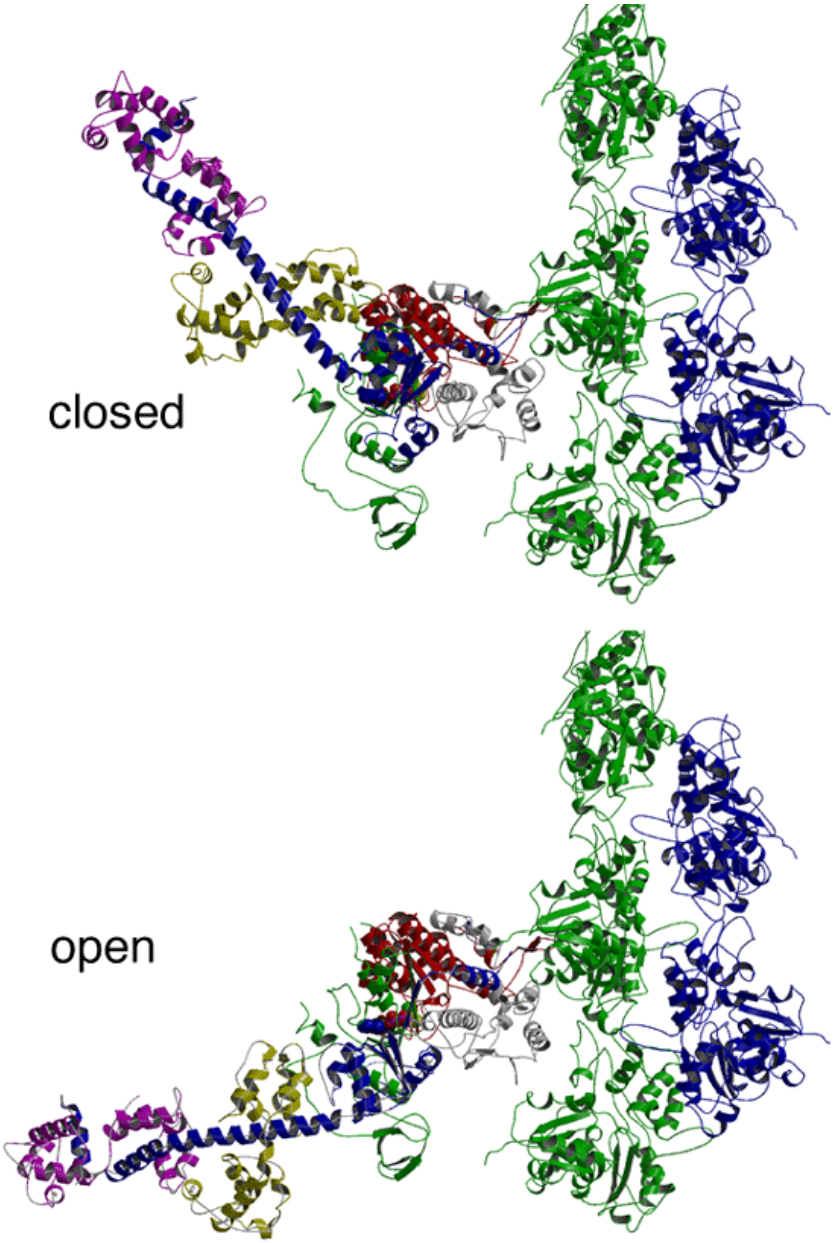
1st International Electronic Conference on Entropy and Its applications
3 – 21 November 2014

Maxwell's demons, protein molecular machines, and information processing in biophysic

Michal Kurzynski & Przemyslaw Chelminiak

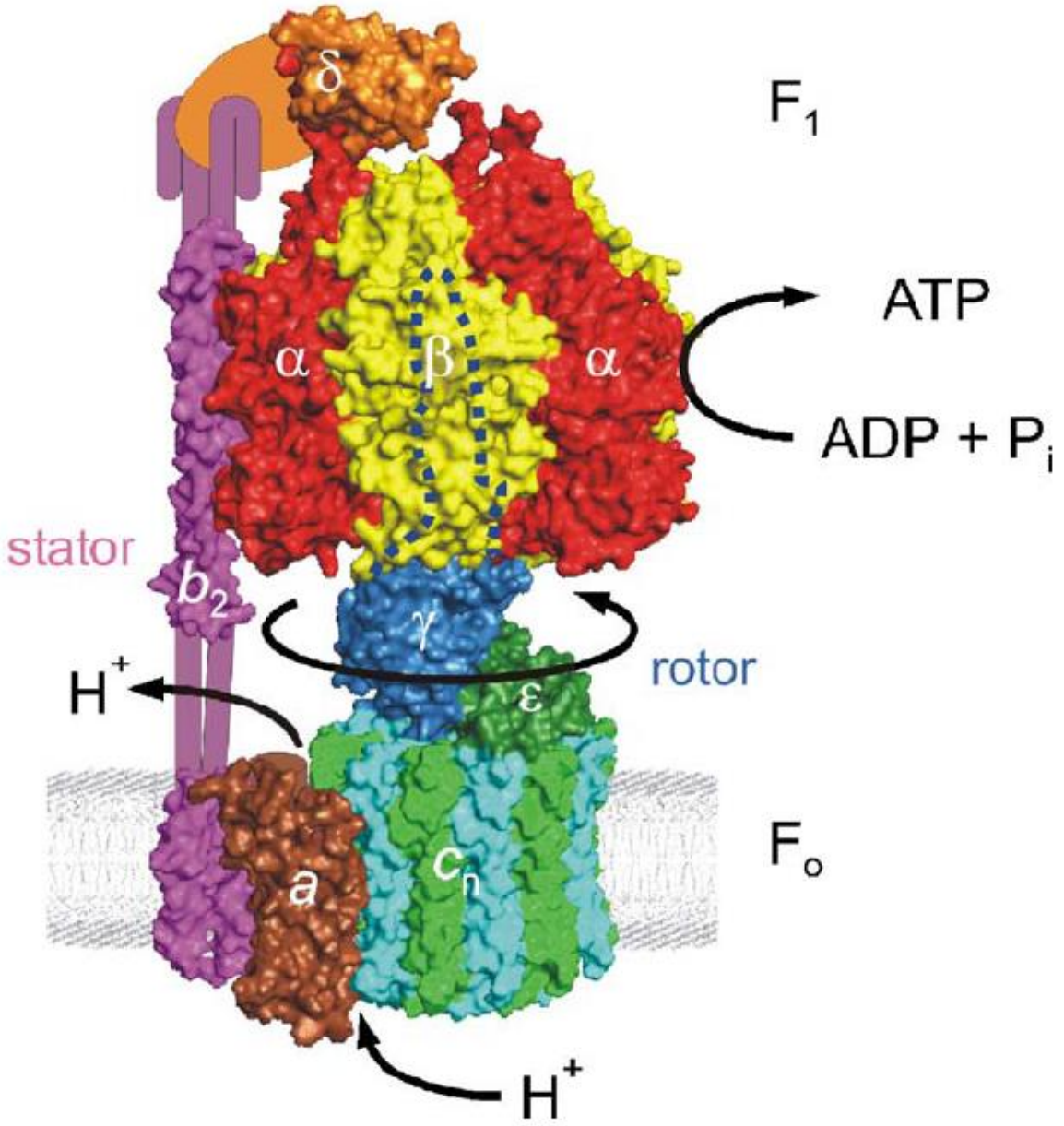
Faculty of Physics, A. Mickiewicz University, Poznan, Poland

Acto-myosin motor



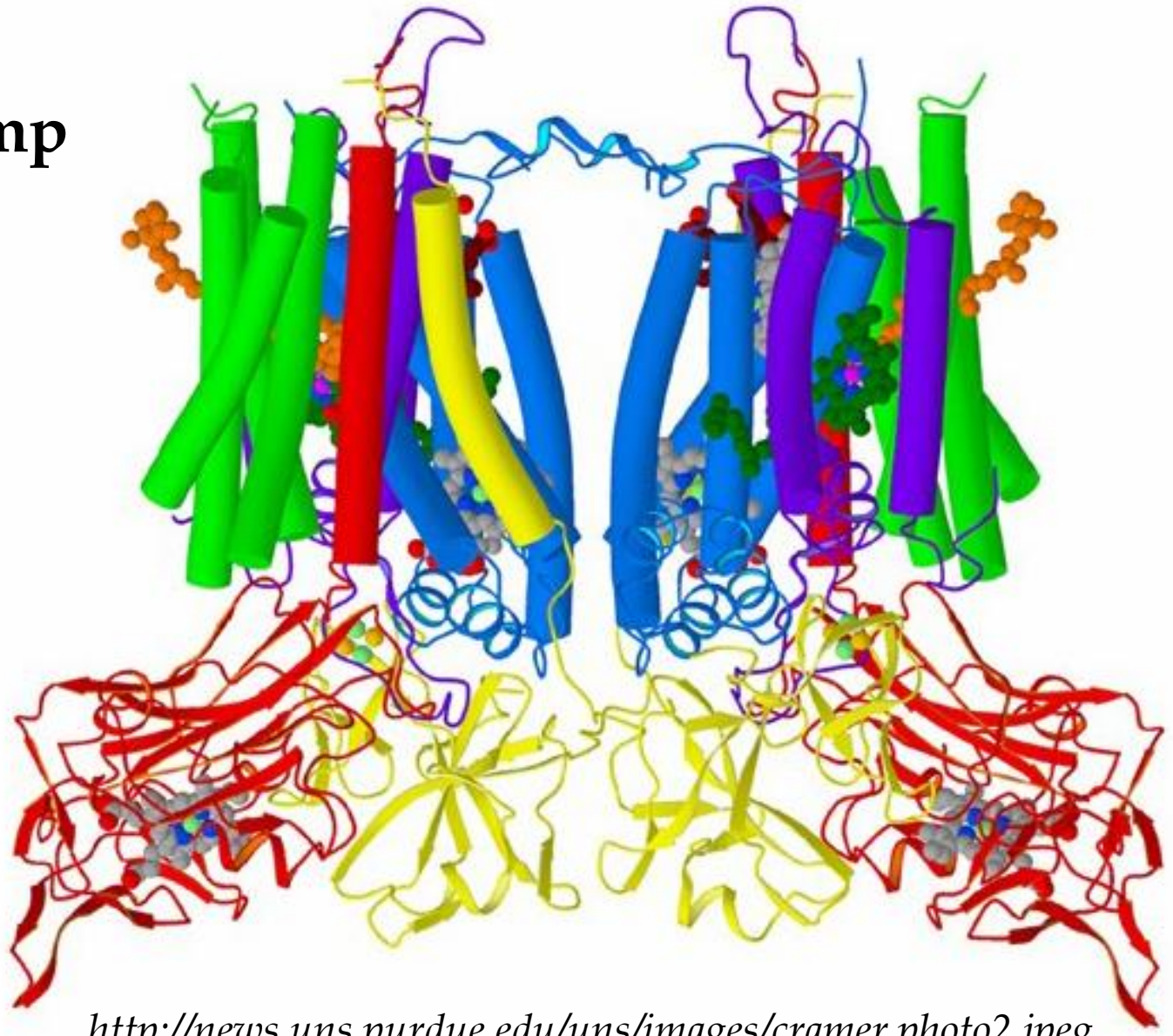
http://homes.mpimf-heidelberg.mpg.de/~holmes/newfigs/7+8.gif

ATP synthase



J. Weber, BBA **1757**, 1162 (2007)

Quinol : cytochrome c synthase
Proton pump



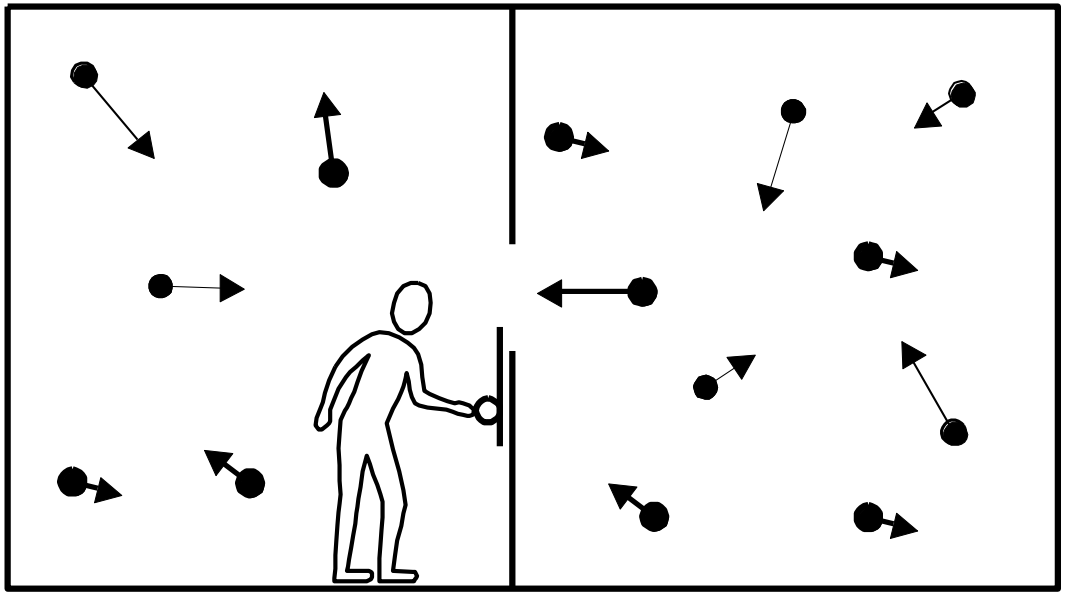
http://news.uns.purdue.edu/uns/images/cramer.photo2.jpeg

Machine: any physical system that enables two other systems to perform work on one another

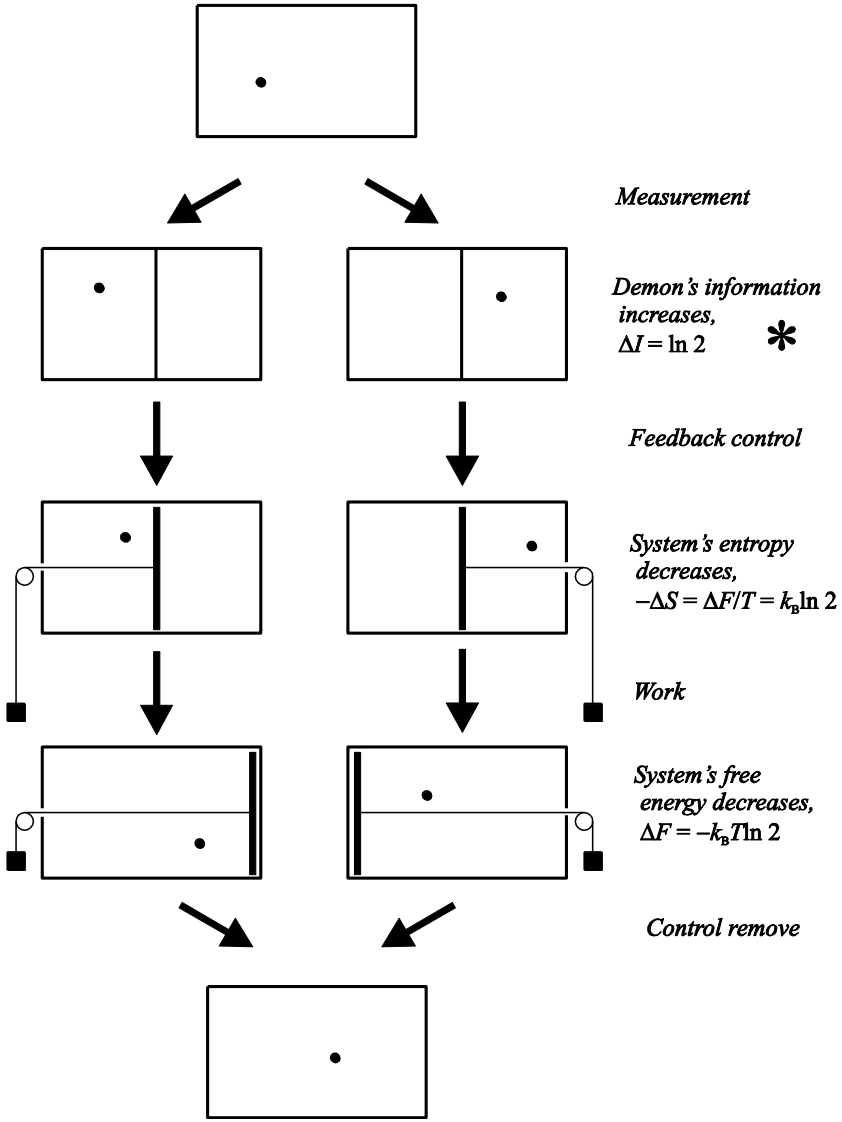
Molecular machines, like chemical reactions and Darwinian evolution, act due to **thermal fluctuations**

Maxwell's demon

Maxwell, 1871



Szilard engine with information processing



- *Szilard, 1929*
- *Brillouin, 1956*
- *Landauer, 1961*
- *Penrose, 1970*
- *Bennett, 1982*
- *Sagawa, Ueda, 2010*

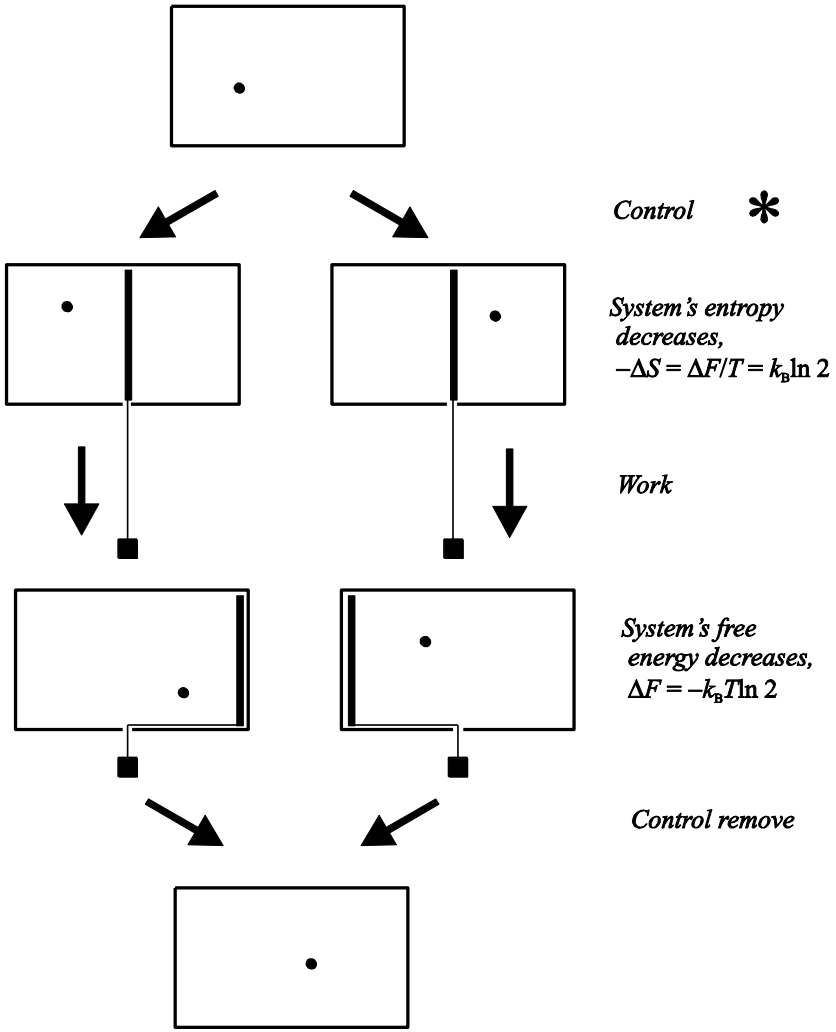
isothermal gas decompression

$\Delta E = \Delta F + T\Delta S$

$= W + Q = 0$

no dissipation

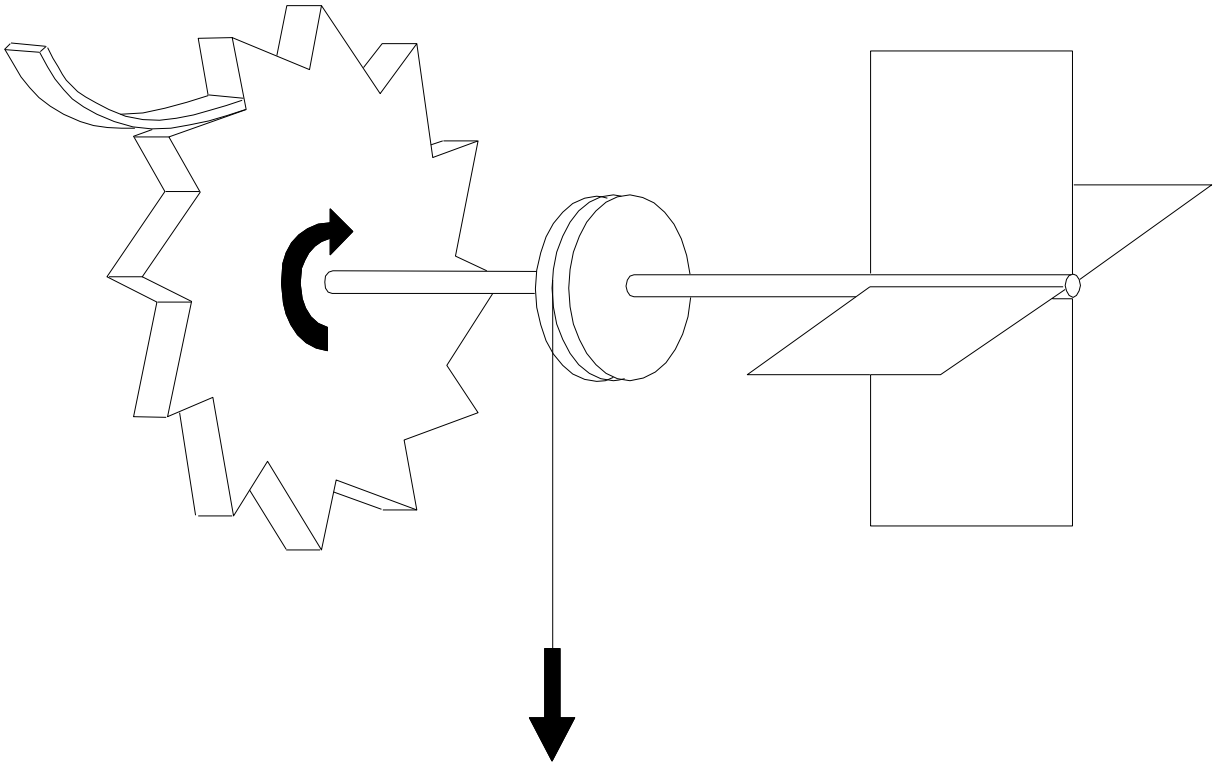
Szilard engine without information processing



- *Popper, Feyerabend, 1966*
- *Alicki, 2014*

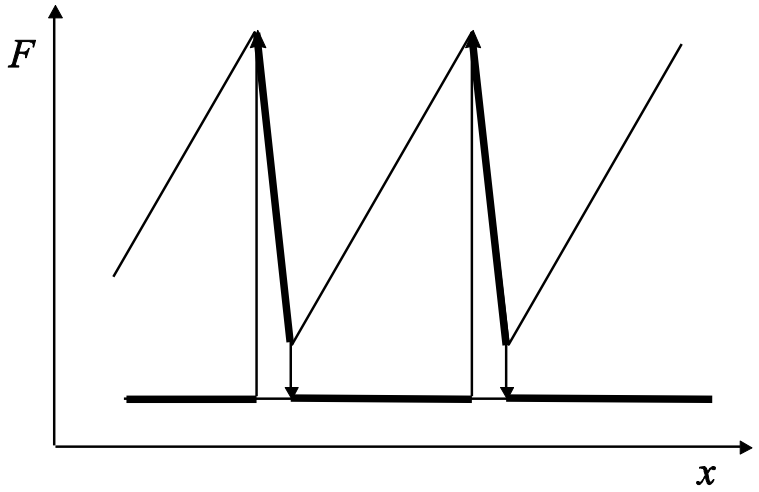
Ratchet and pawl machine

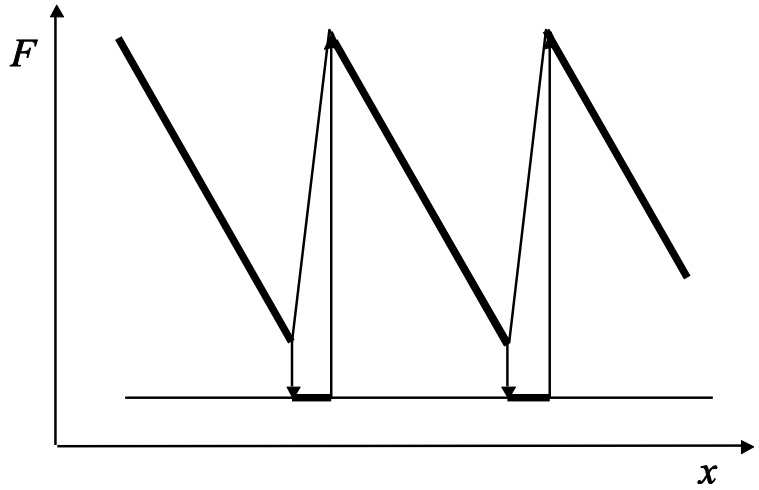
- *Smoluchowski, 1912*
- *Feynman, 1966*



Flashing ratchet

Random versus controlled transitions





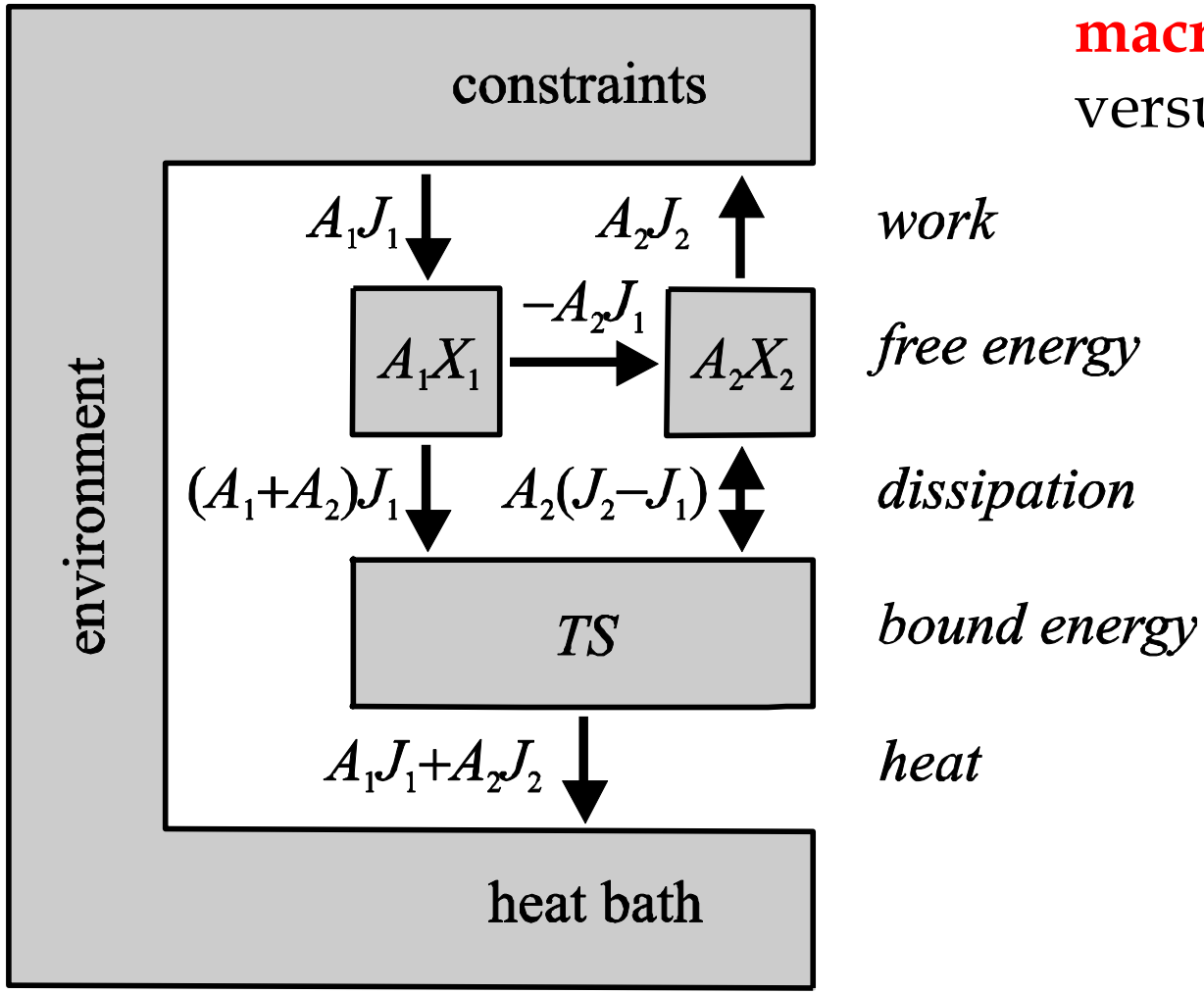
- *A. F. Huxley, 1957, 1971*
- *Cordova, Ermentrout, Oster, 1992*
- *Astumian, Bier, 1994*
- *Prost, Chauwin, Peliti, Ajdari, 1994*
- *Cao, Dinis, Parrondo, 2004*
- *Howard, 2001, 2006*

Brownian ratchet

Power stroke

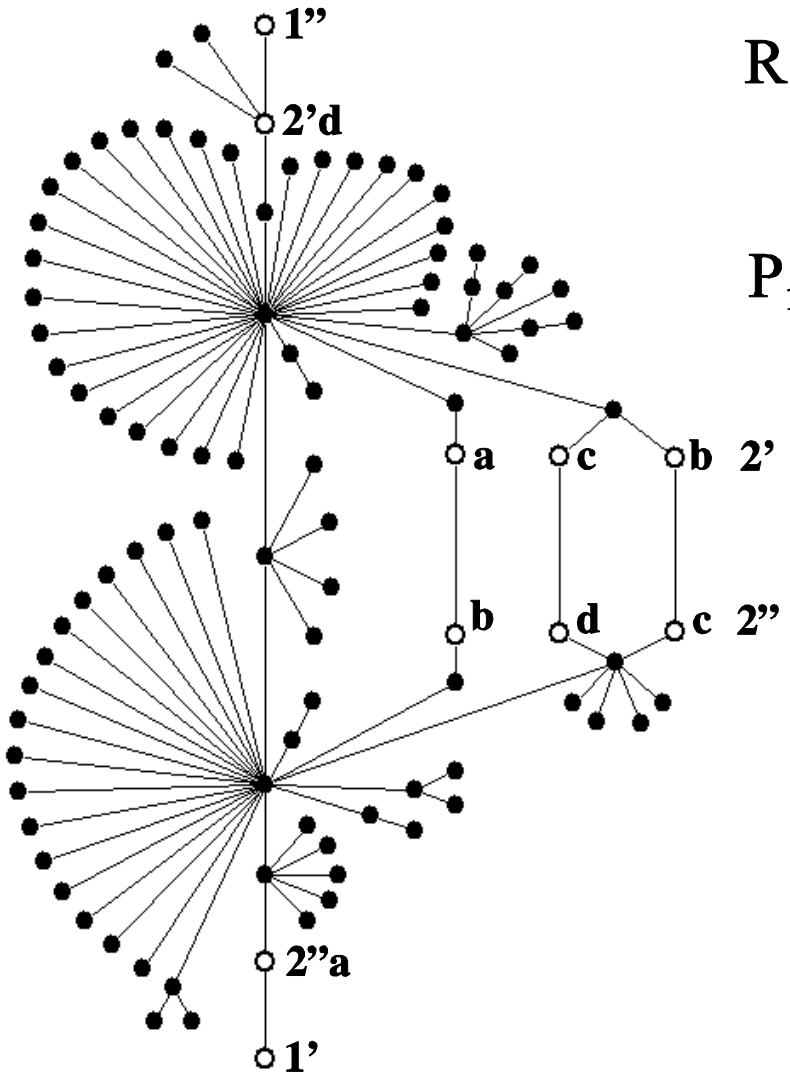
Friction (**energy dissipation**)
is necessary for any machine
to be controlled

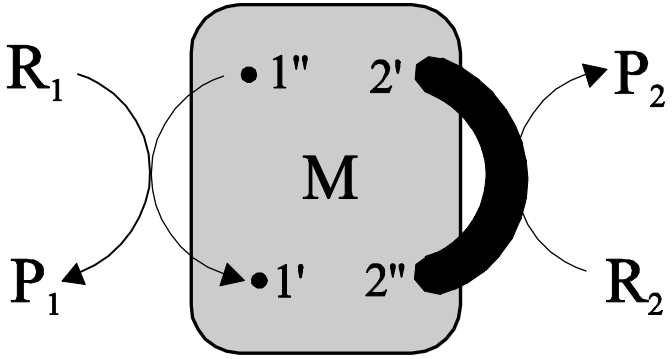
Stationary isothermal machine (free energy trasducer)



macroscopic
versus **nanoscopic**

Biological chemo-chemical machine





PHYSICAL REVIEW E **89**, 012722 (2014)

Output-input ratio in thermally fluctuating biomolecular machines

Michal Kurzynski,[1,*] Mieczyslaw Torchala,[1,2] and Przemyslaw Chelminiak[1]
[1]*Faculty of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland*
[2]*BioInfoBank Institute, Limanowskiego 24A, 60-744 Poznan, Poland*

Torchala *et al. BMC Systems Biology* 2013, **7**:130
http://www.biomedcentral.com/1752-0509/7/130

BMC
Systems Biology

SOFTWARE Open Access

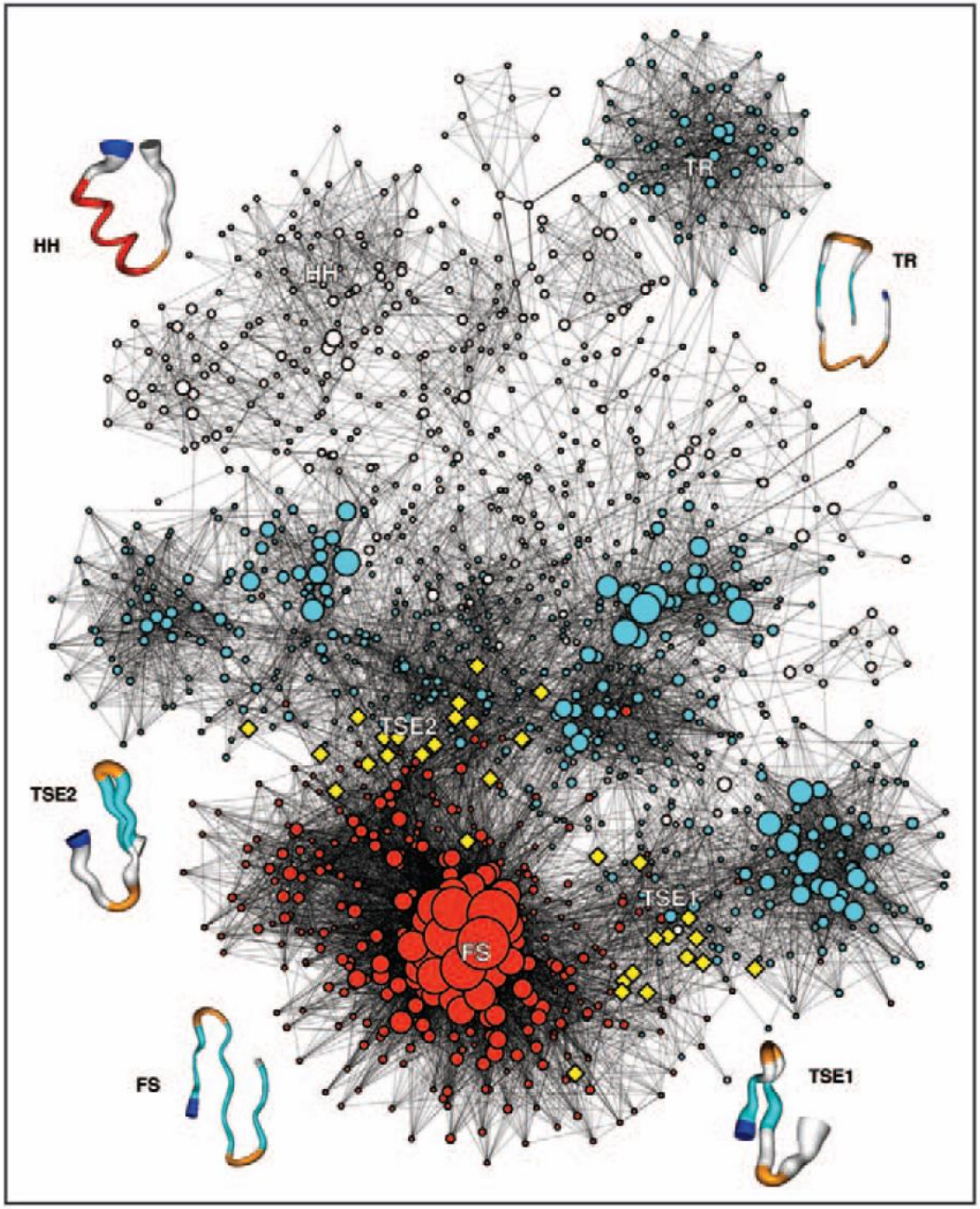
RaTrav: a tool for calculating mean first-passage times on biochemical networks

Mieczyslaw Torchala[1], Przemyslaw Chelminiak[2], Michal Kurzynski[2] and Paul A Bates[1*]

Peptide β3s

20 residues
1 μs MD trajectory
at 330 K (melt. temp.)

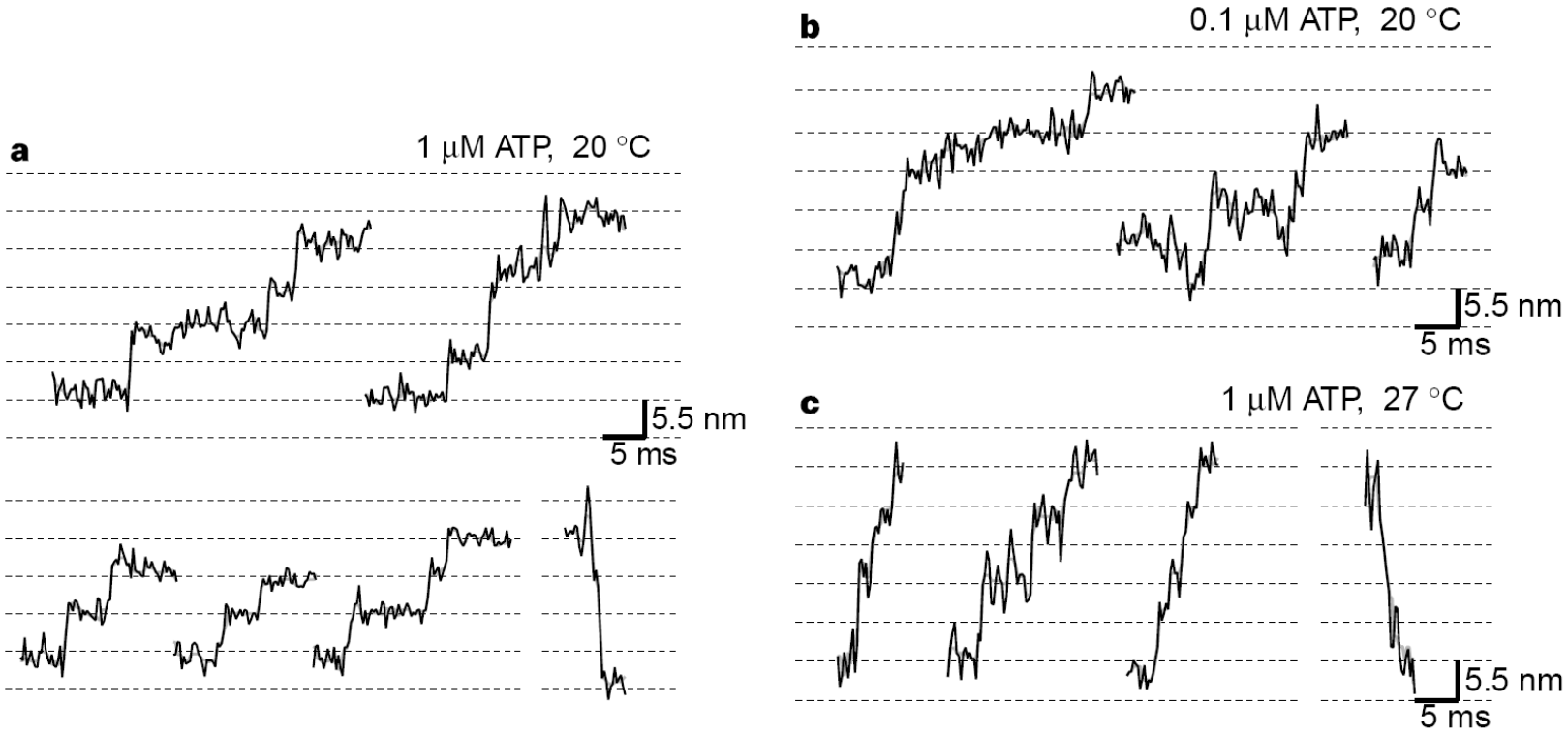
HH – helical
TR - trap
TSE – trans. state
FS – folded state



Rao, Caflisch (2004)

Can the value of $\varepsilon = J_2/J_1$ be higher than unity?

Number of actomyosin motor steps per ATP molecule hydrolyzed



Kitamura, Tokunaga, Iwane, Yanagida, 1999

Fluctuation theorem

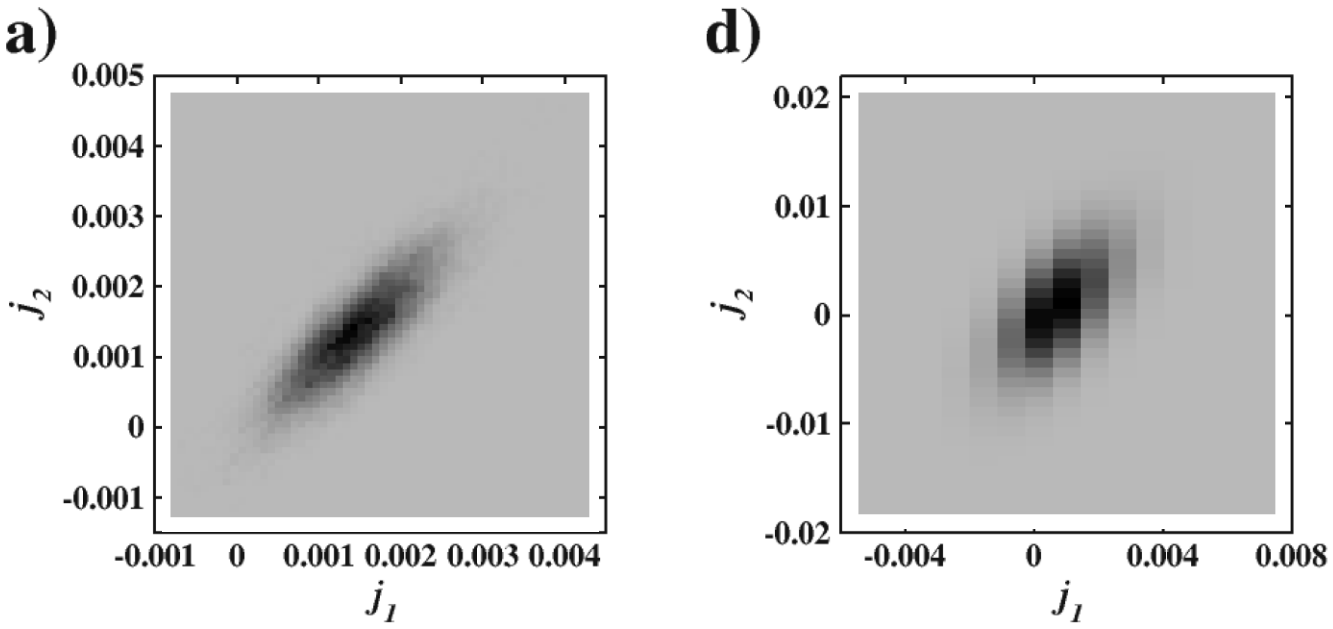
Jarzynski,1997
Crooks, 1999
Searles, Evans, 1999
Andrieux, Gaspard, 2007
Sagawa, Ueda, 2010

$$p(j_1(t), j_2(t))/p(-j_1(t), -j_2(t)) = \exp \beta \left[A_1 j_1(t) + A_2 j_2(t)\right] t$$

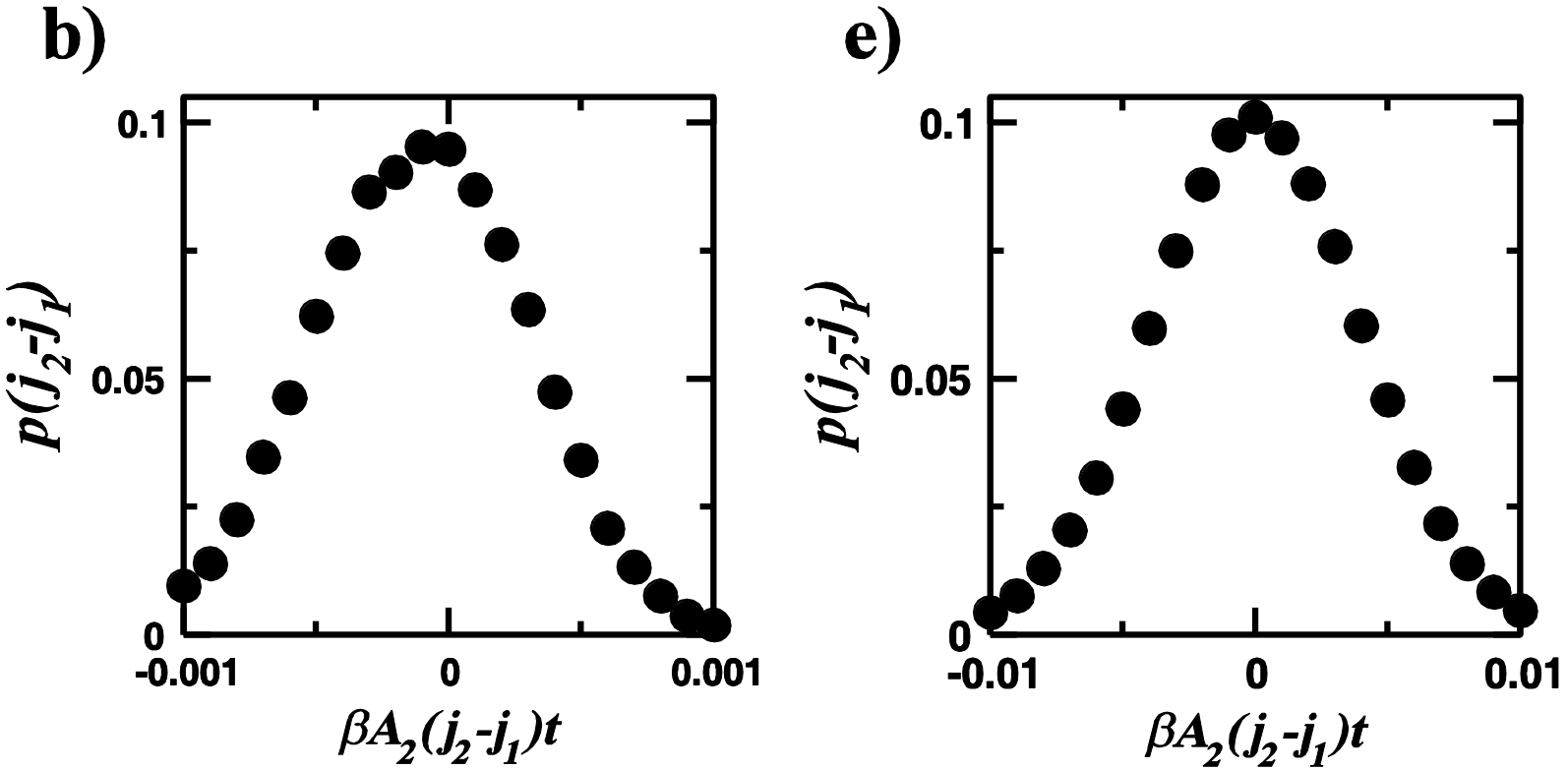
$$\langle \exp(-\sum_i \beta A_i \mathcal{J}_i(t) t) \rangle = \langle \exp(-\sigma) \rangle = 1$$

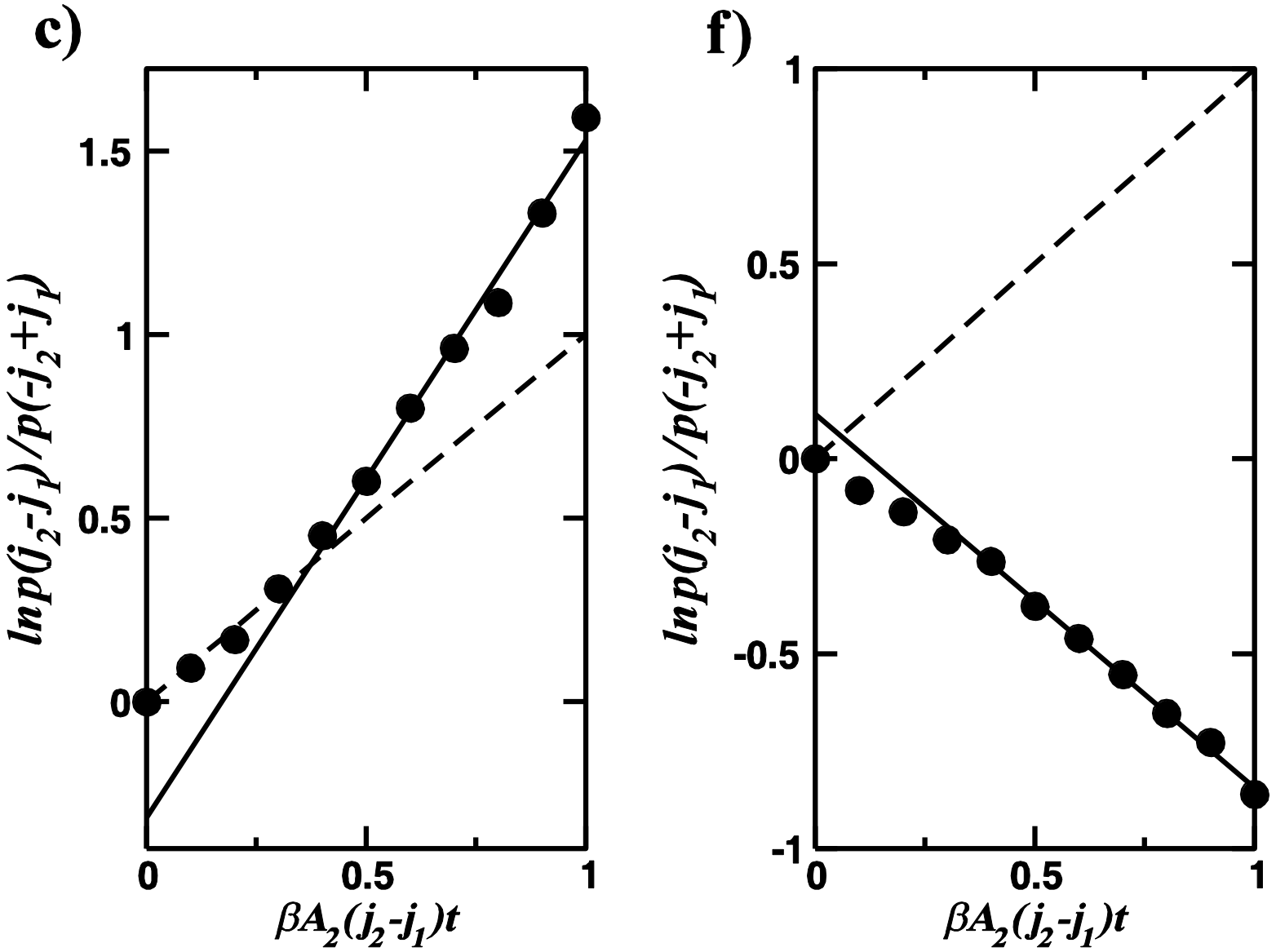
$$\begin{aligned} \ln p(j_2 - j_1)/p(-j_2 + j_1) &= \beta A_2 (j_2 - j_1) t \\ &+ \beta (A_1 + A_2) j_1 t + \ln p(-j_1 | -j_1 + j_2)/p(j_1 | j_1 - j_2) \end{aligned}$$

$$\langle \exp(-\sigma + I) \rangle = 1$$

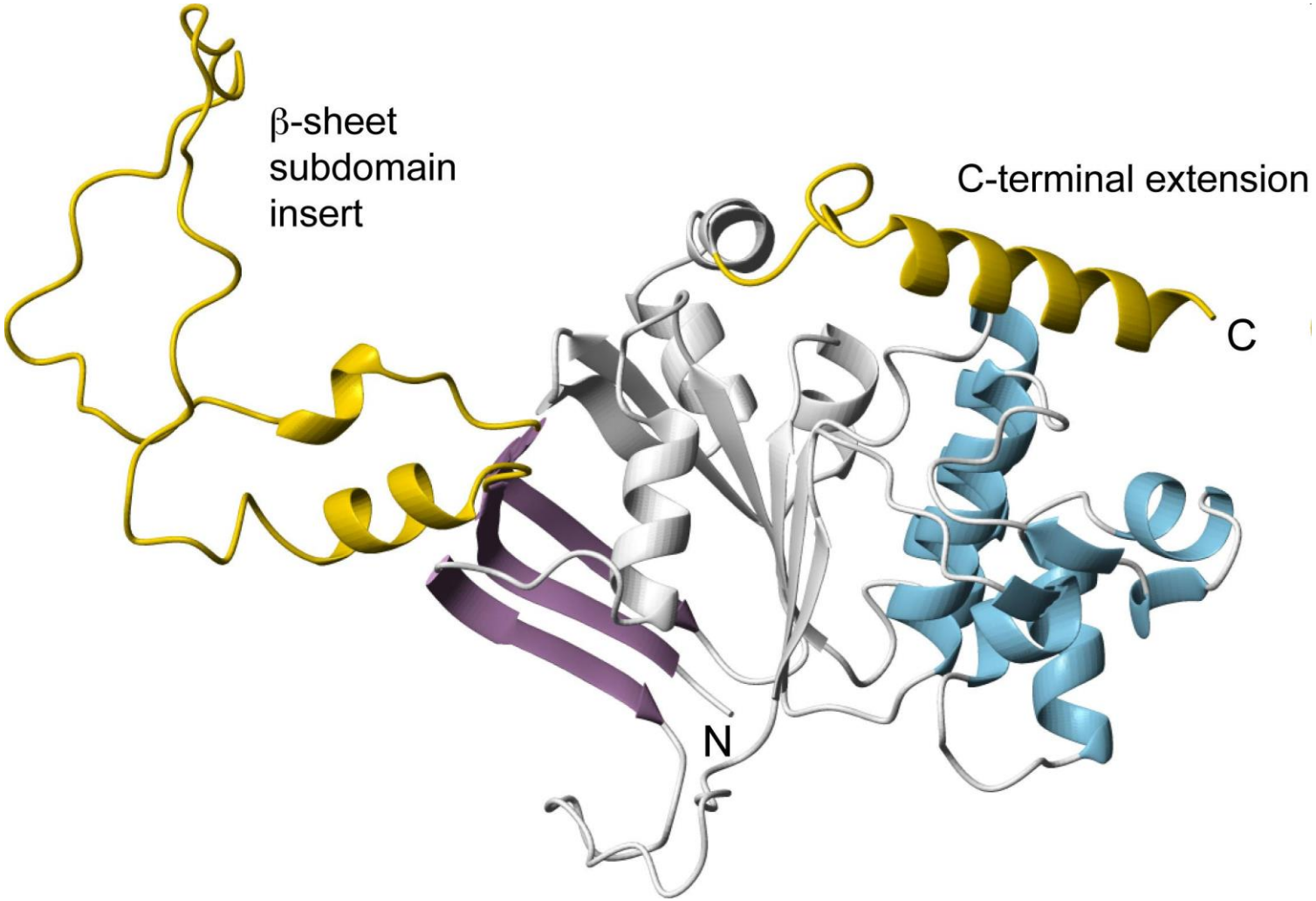


- The fluctuation theorem for ($j1$, $j2$) is satisfied
- Degree of coupling higher than unity, $J_2 > J_1$, is possible
- For $J_2 - J_1$, the generalized fluctuation theorem is satisfied


b)
e)
0.1
0.05
0
-0.001
0
0.001
-0.01
0.01
$p(j_2\text{-}j_1)$
$\beta A_2(j_2\text{-}j_1)t$


c)
f)
1.5
1
0.5
0
-0.5
-1
0
0.5
1
$ln p(j_2-j_1)/p(-j_2+j_1)$
$\beta A_2(j_2-j_1)t$

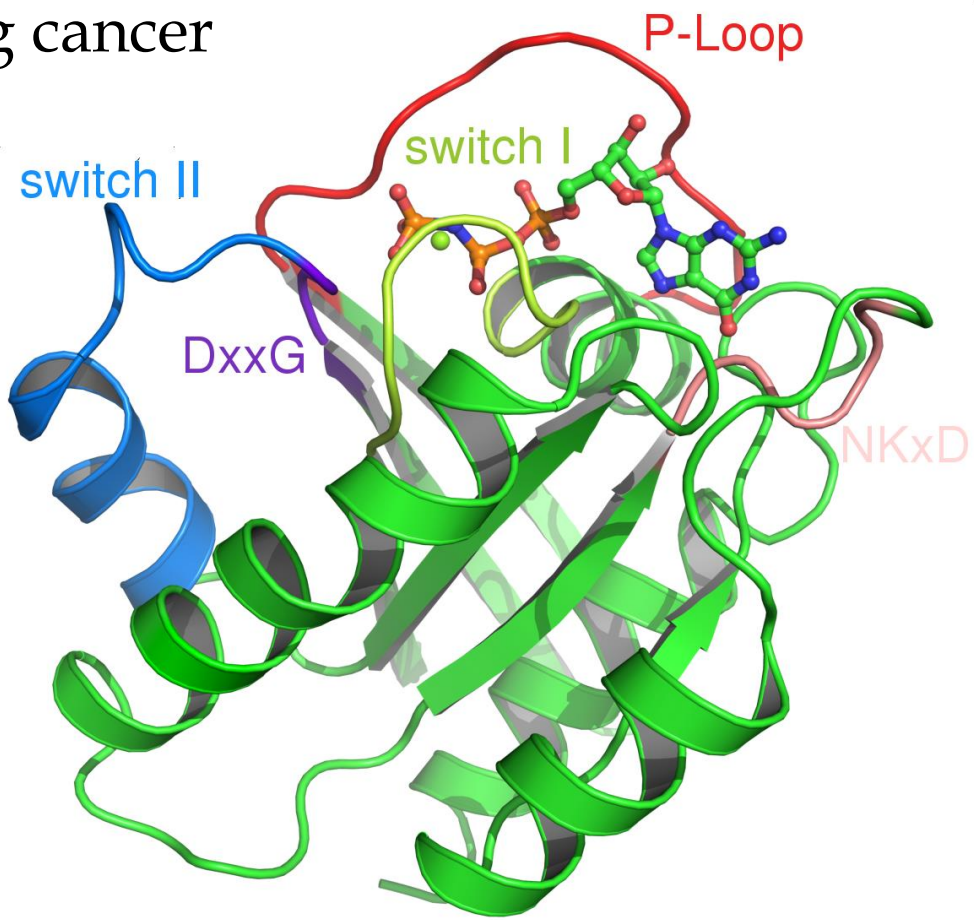
Myosin II – partly unfolded after ATP binding



http://meds.queensu.ca/biochem/assets/kanelis.jpg

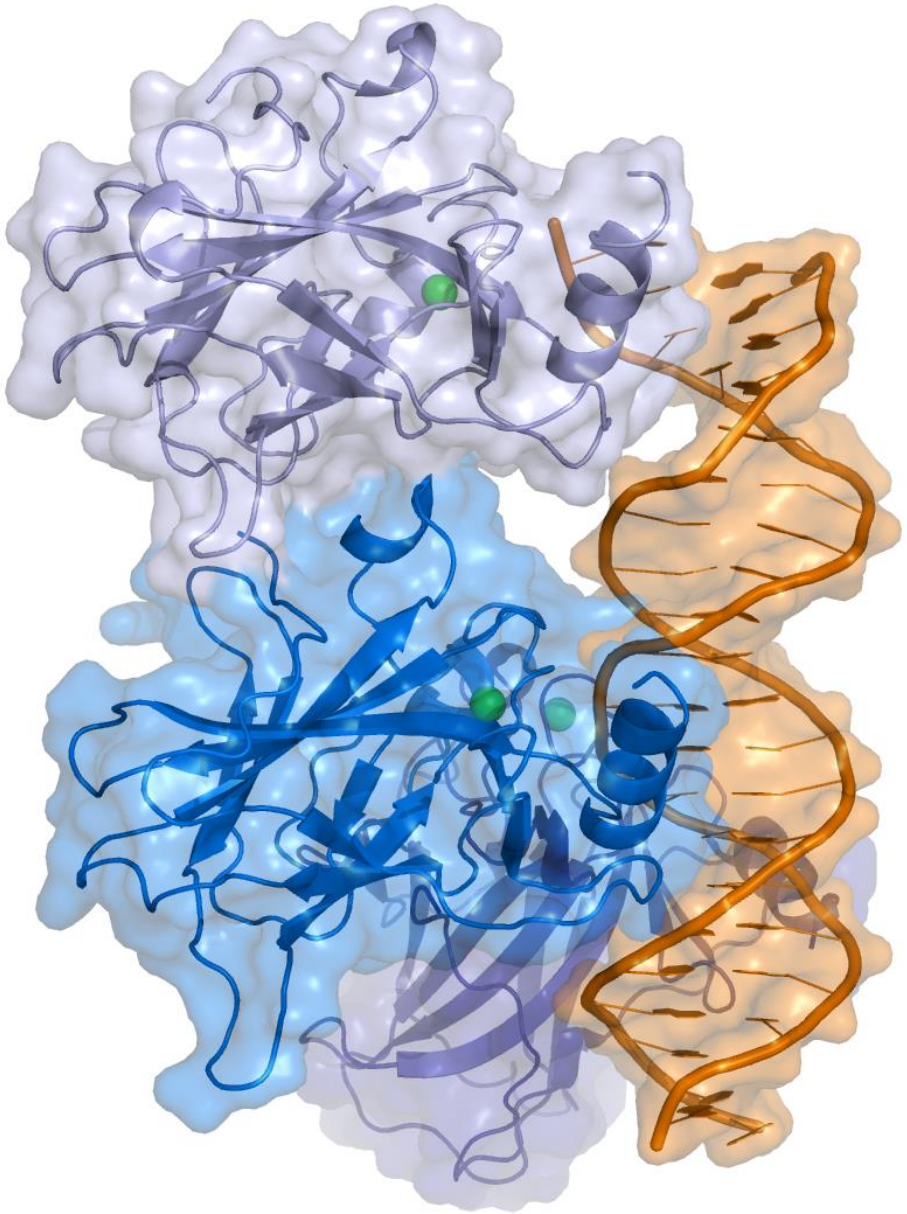
Ras: G-protein signal transducer

activation of transcription factors
proto-oncogene of lung cancer

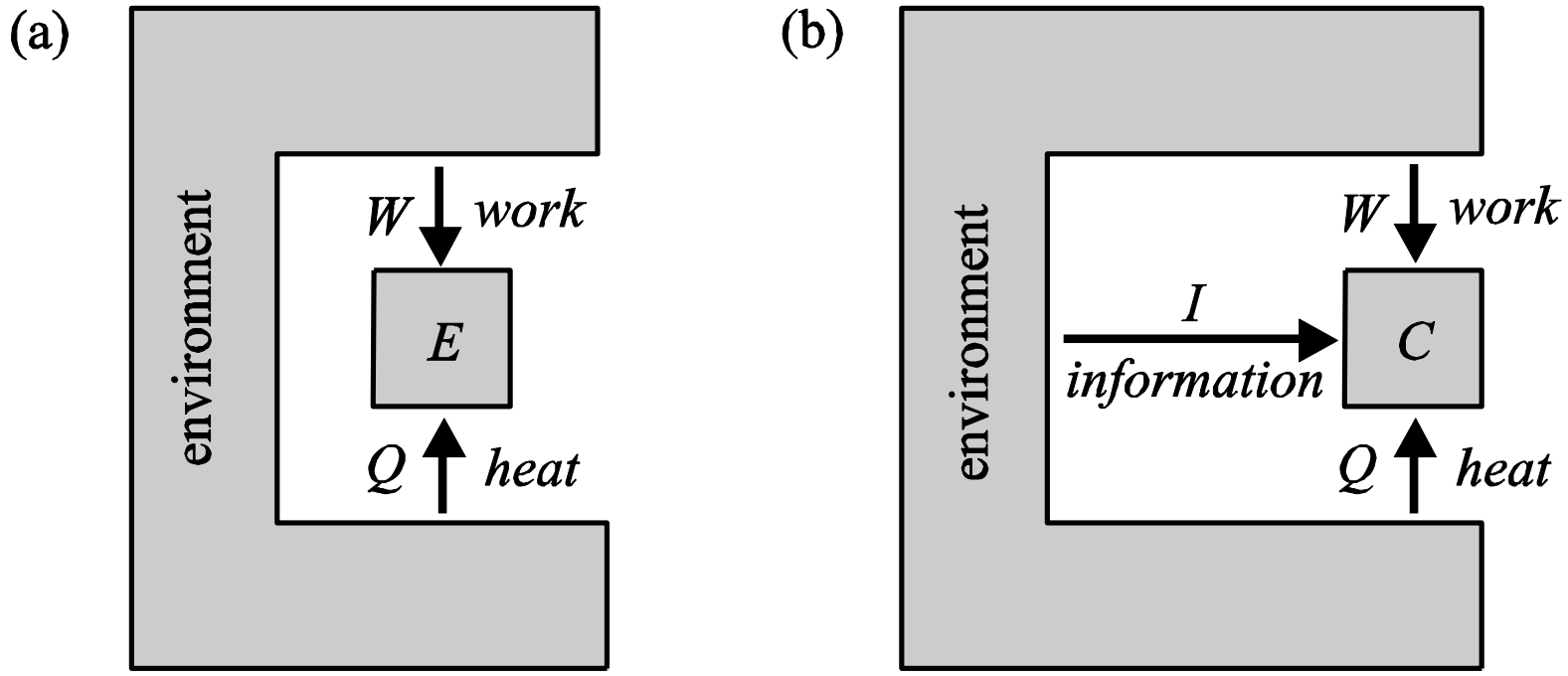


http://upload.wikimedia.org/wikipedia/commons/2/26/Ras-Structure.png

Transcription factor p53 (tumor supressor)



http://upload.wikimedia.org/wikipedia/commons/b/bb/P53.png


(a)
environment
W
work
E
Q
heat
(b)
environment
W
work
I
information
C
Q
heat