

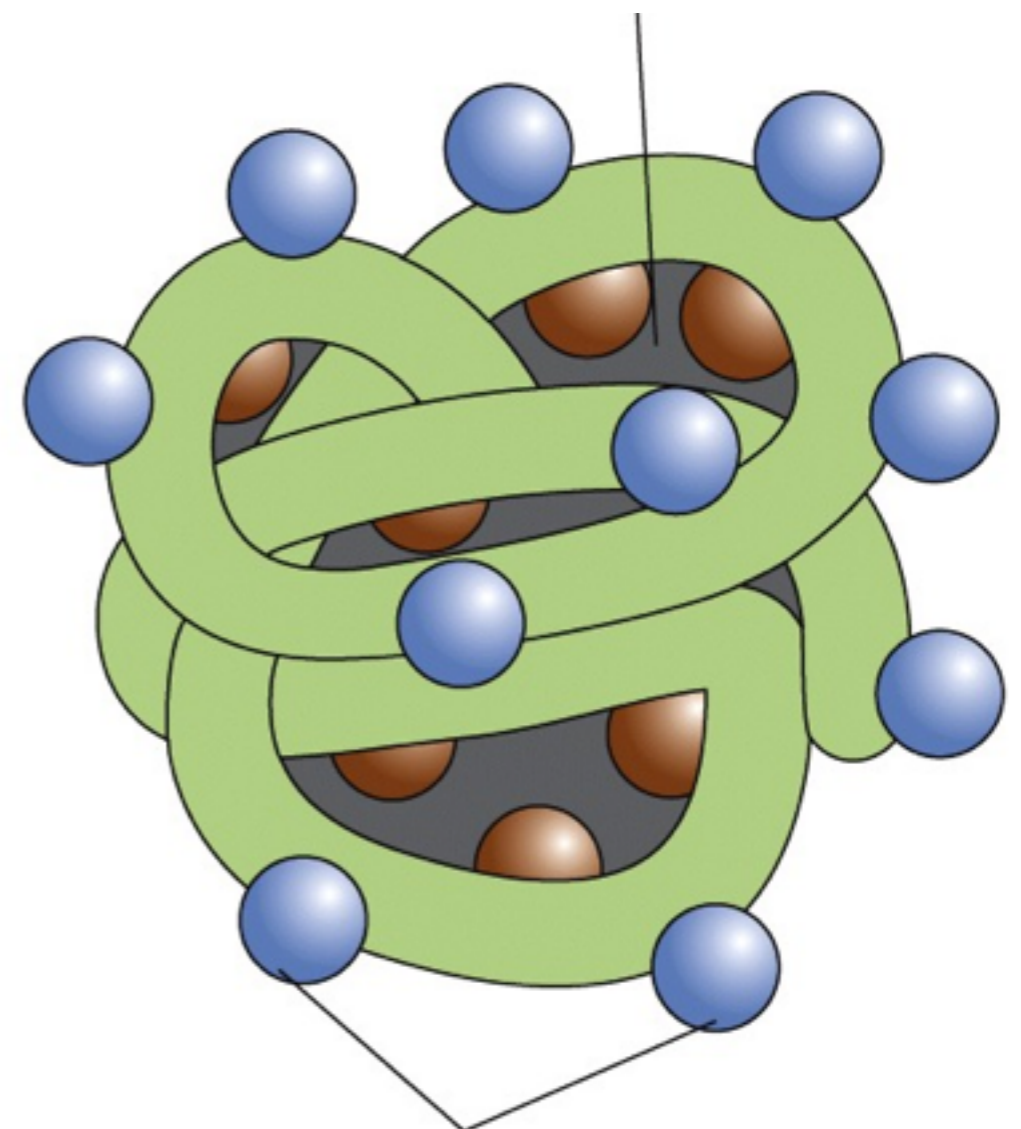
Física do Corpo Humano (4300325)



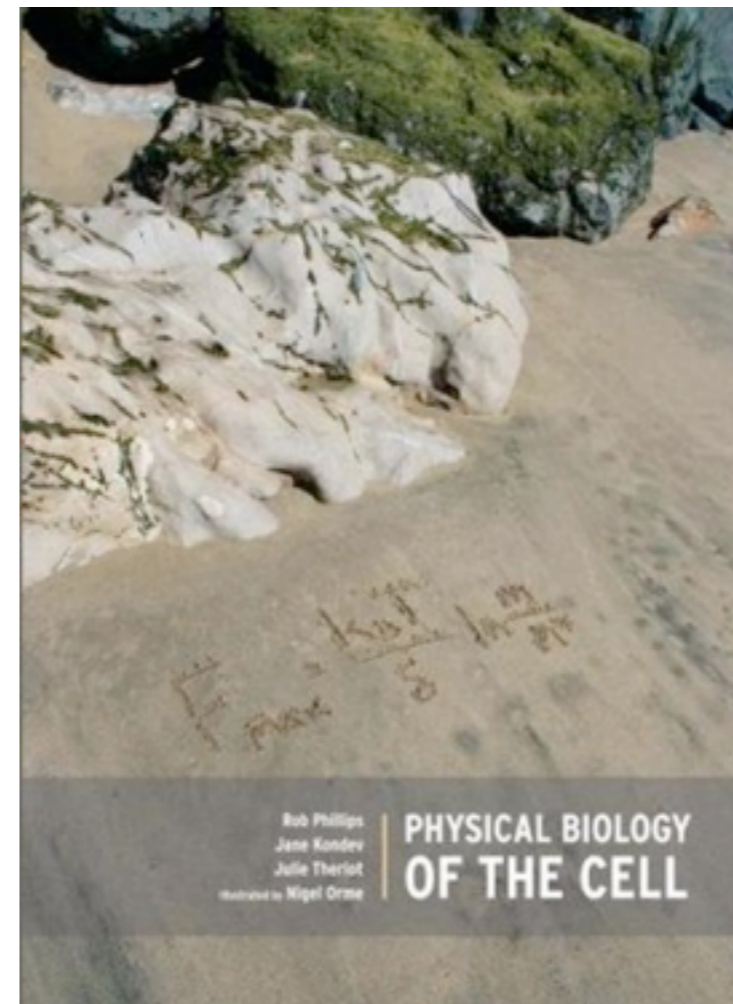
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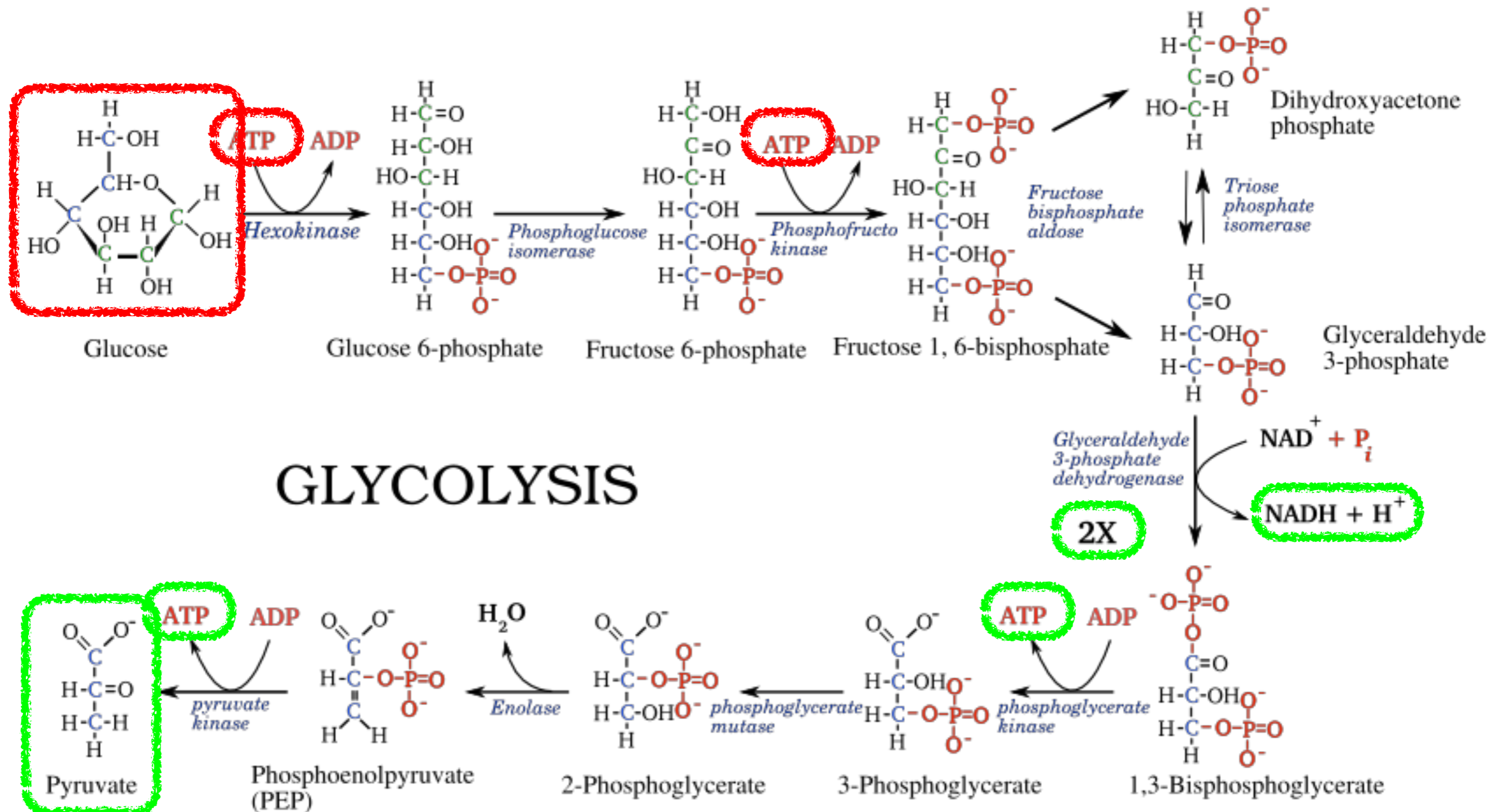
Equilíbrio Termodinâmico
Aula 7



Princípios Físicos Aplicados à Fisiologia (PGF5306-I)



Geração de Energias



ATP-ADP ~ varias tipos de reações bioquímicas

ATP-ADP ~ 20 kBT

Ligação covalente típica ~ 150 kBT

NADH ~ 2 ATP

NADPH ~ 2 ATP

Custo de Sínteses

Amino acid	Abundance (molecules per cell)	Glucose equivalents	ATP equivalents (aerobic)	ATP equivalents (anaerobic)
Alanine (A)	2.9×10^8	0.5	-1	1
Arginine (R)	1.7×10^8	0.5	5	13
Asparagine (N)	1.4×10^8	0.5	3	5
Aspartate (D)	1.4×10^8	0.5	0	2
Cysteine (C)	5.2×10^7	0.5	11	15
Glutamate (E)	1.5×10^8	0.5	-7	-1
Glutamine (Q)	1.5×10^8	0.5	-6	0
Glycine (G)	3.5×10^8	0.5	-2	2
Histidine (H)	5.4×10^7	1	1	7
Isoleucine (I)	1.7×10^8	1	7	11
Leucine (L)	2.6×10^8	1.5	-9	1
Lysine (K)	2.0×10^8	1	5	9
Methionine (M)	8.8×10^7	1	21	23
Phenylalanine (F)	1.1×10^8	2	-6	2
Proline (P)	1.3×10^8	0.5	-2	4
Serine (S)	1.2×10^8	0.5	-2	2
Threonine (T)	1.5×10^8	0.5	6	8
Tryptophan (W)	3.3×10^7	2.5	-7	7
Tyrosine (Y)	7.9×10^7	2	-8	2
Valine (V)	2.4×10^8	1	-2	2

Após um aminoácido ser sintetizado (custo médio ~ 1.2 ATP equivalente), ele deve ser colocado junto para formar uma proteína (4 ATP equivalente).
Número médio de aminoácidos por proteína = 300.

Proteínas em uma bactéria

$$\begin{aligned} \text{Custo da Proteína} &\approx 5.2 \text{ ATP} \times 300 \times 3 \times 10^6 \\ &\approx 4.5 \times 10^9 \text{ ATP equivalentes} \end{aligned}$$

Termodinâmica no Equilíbrio

Visto que organismos vivos são exemplos típicos de sistemas fora do equilíbrio, é possível utilizar as ferramentas da física para o equilíbrio?

Modelos no equilíbrio podem ser utilizados para problemas fora do equilíbrio se certos processos acontecem mais rápidos que outros.

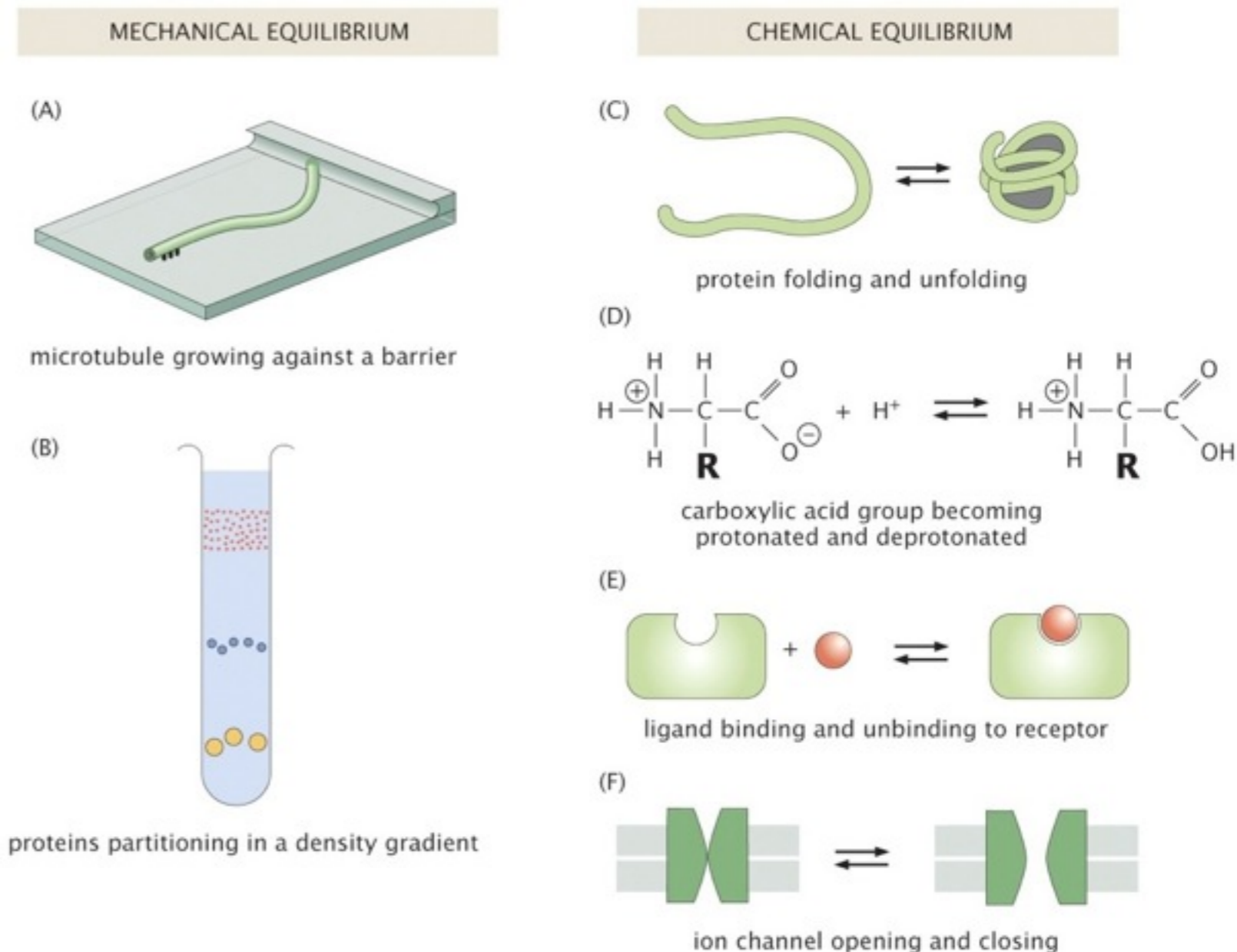


Figure 5.7 Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Cell movements

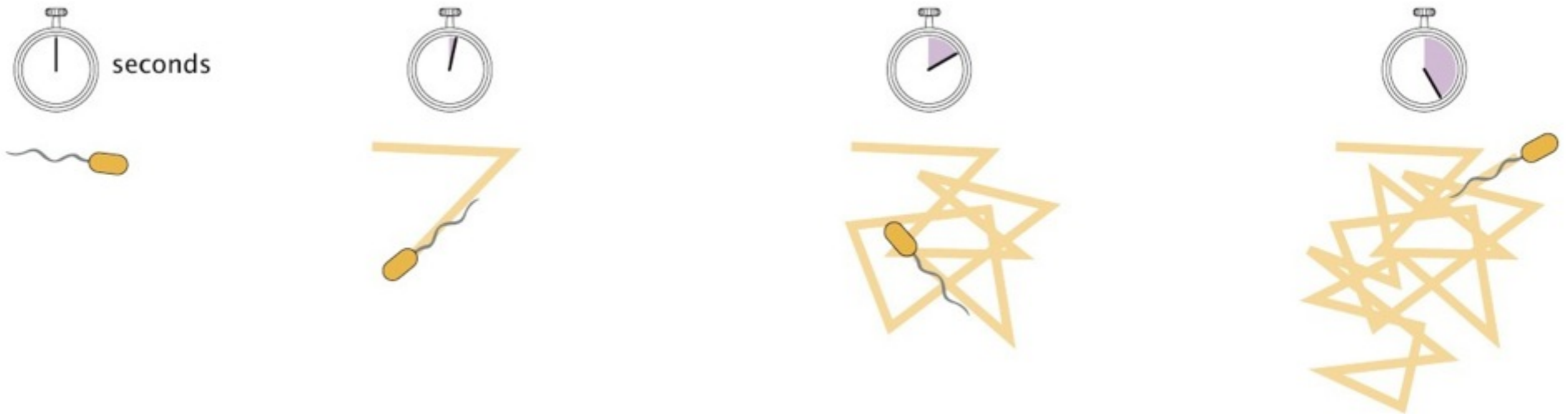


Figure 3.2d Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Protein synthesis

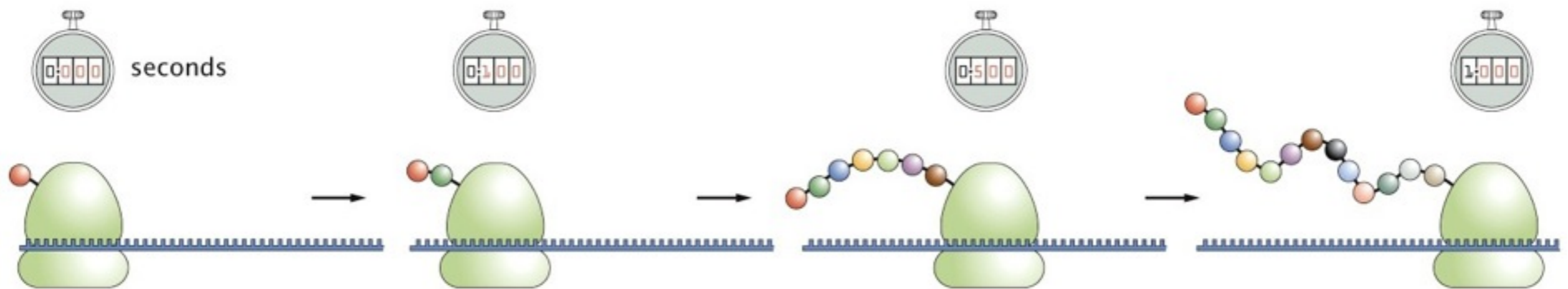


Figure 3.2e Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Transcription

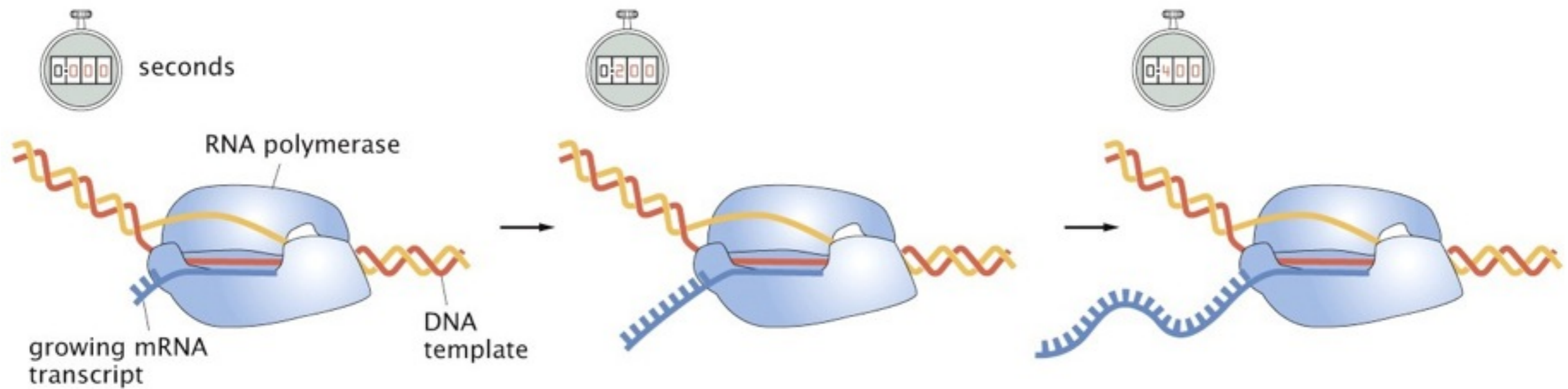


Figure 3.2f Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Gating of ion channels

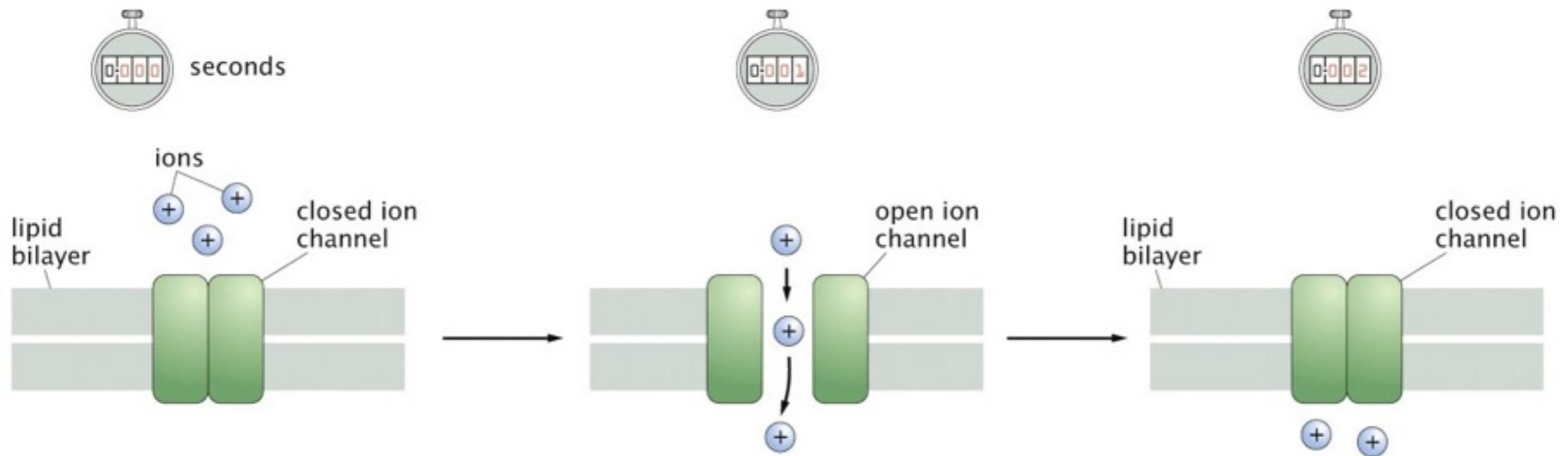


Figure 3.2g Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Enzyme catalysis

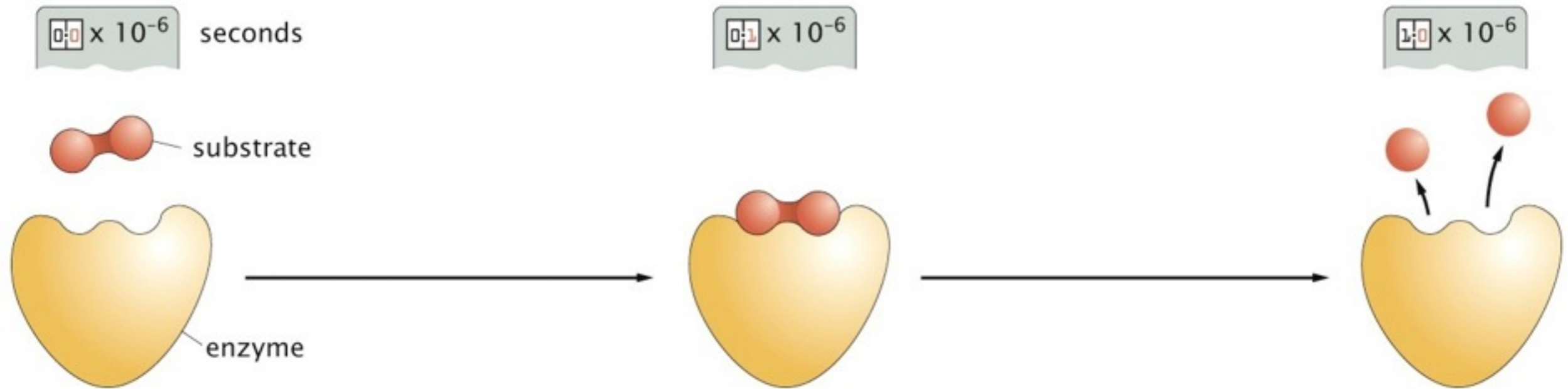


Figure 3.2h Physical Biology of the Cell, 2ed. (© Garland Science 2013)

Termodinâmica no Equilíbrio

Proteína no equilíbrio: o estado “empacotado” da proteína é um estado que minimiza a energia livre

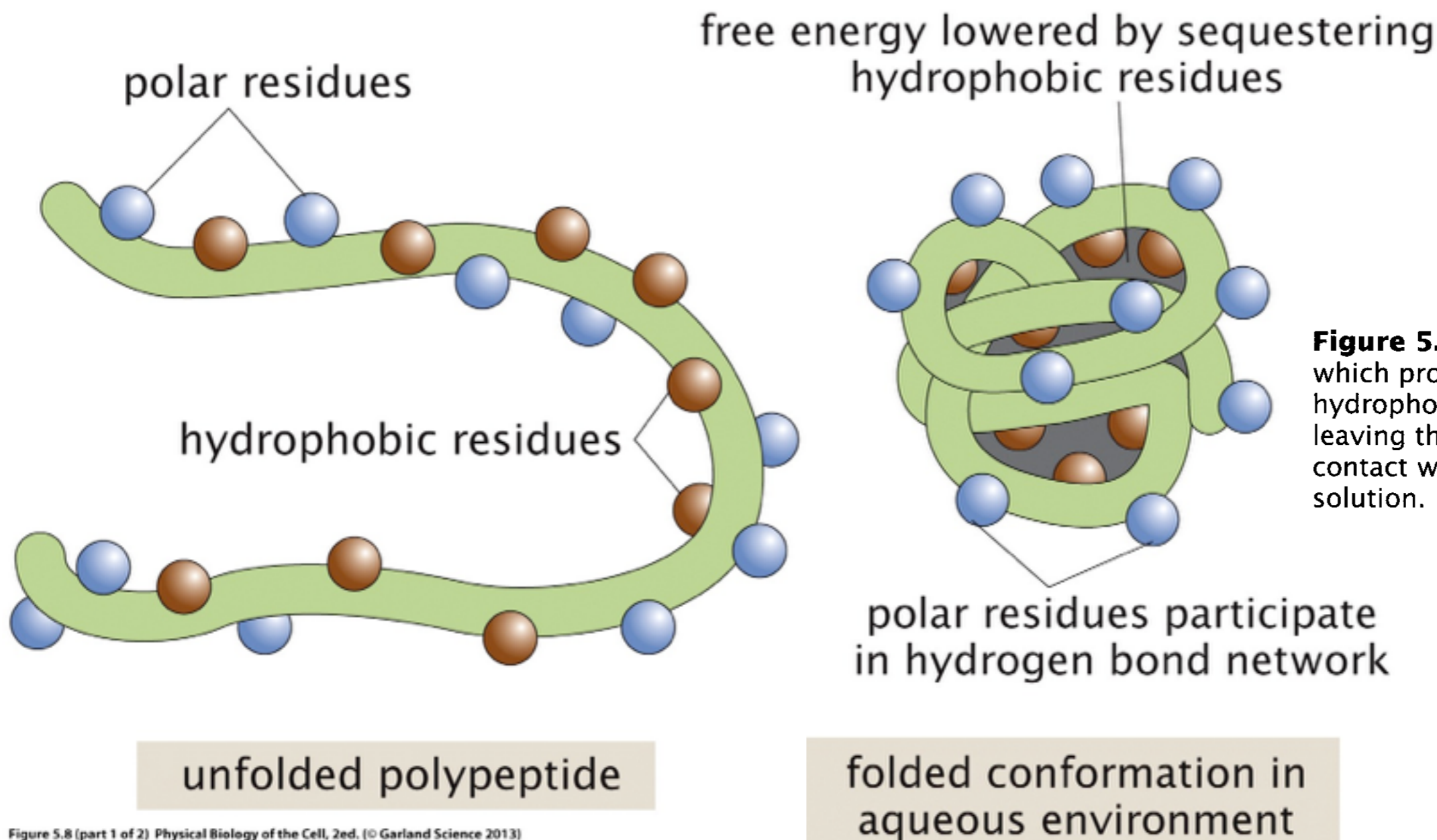


Figure 5.8 Schematic of the way in which protein folding sequesters hydrophobic amino acids while leaving their polar counterparts in contact with the surrounding solution.

Proteína no Equilíbrio

Encontrar o mínimo implica buscar:

$$\frac{\partial F}{\partial u_i} = 0 \quad (i = 1, 2, 3, \dots, N)$$

JOURNAL OF CHEMICAL PHYSICS

VOLUME 116, NUMBER 19

15 MAY 2002

**Foldability and the funnel of HP-36 protein sequence:
Use of hydrophathy scale in protein folding**

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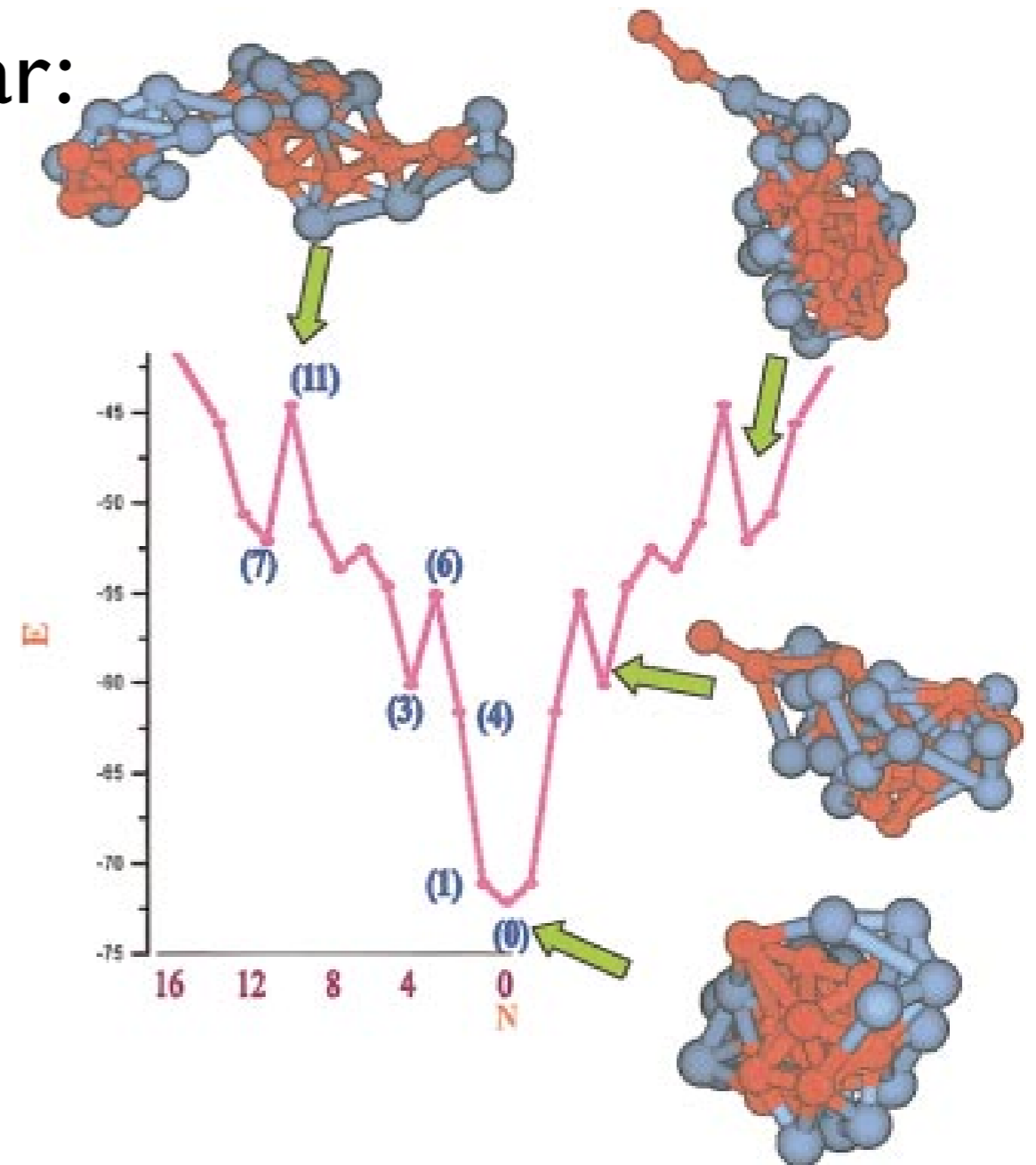
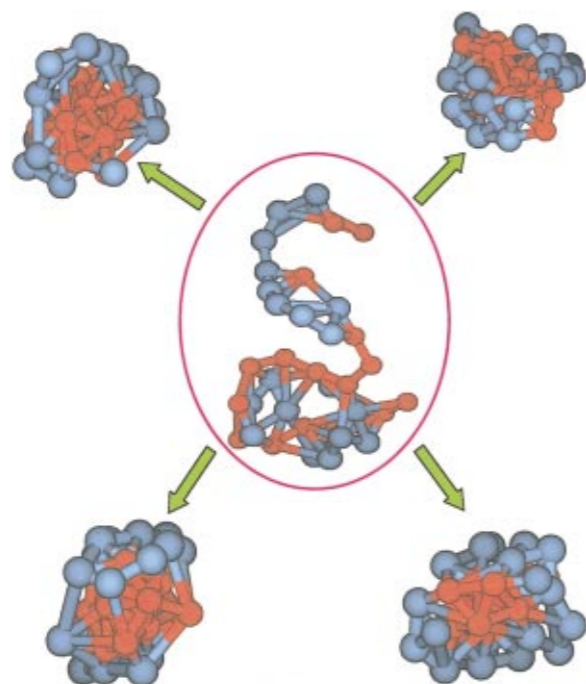


FIG. 5. (Color) Energy landscape (the funnel) for the model HP-36 protein obtained from BD simulations is shown. The distance from the native state Q in terms of topological contacts is indicated for different energy states. Configurations corresponding to various energy states (given in parentheses) (unfolded, transition, and native state) are also shown. The X axis denotes the number of configurations at energy E .