Basic Thermodynamics Concepts

Elements of Biophysics

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Biomolecules
Folding and
Disease

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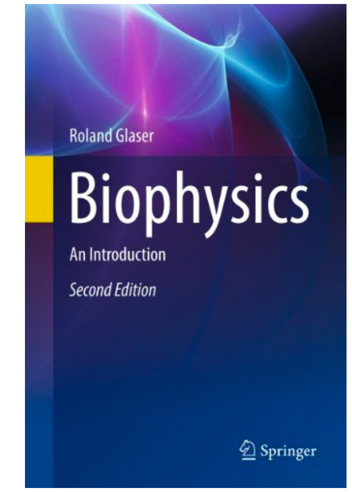
Main Topics

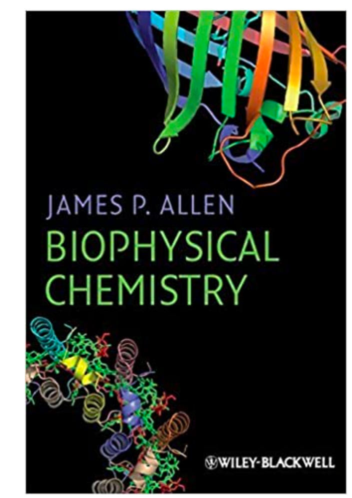
- Basic notions of thermodynamics and kinetics
- Basic elements of structural and functional biology.
- Basic elements of cell biology.

Suggested books

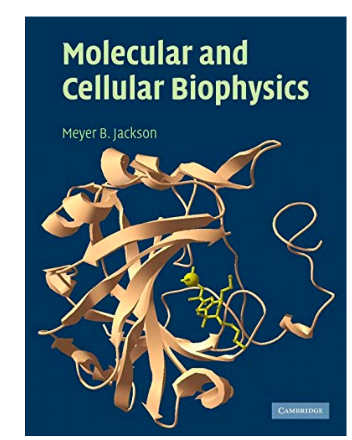
- **Biophysics: An Introduction** by Roland Glaser



- **Biophysical Chemistry** by James P. Allen



- **Molecular and Cellular Biophysics** by Meyer B. Jackson



What is Biophysics?

- The subjects of Biophysics are the physical principles underlying all processes of living systems.
- Biophysics is an interdisciplinary science which includes notions of biology and physics connected to other disciplines such as mathematics, physical chemistry, and biochemistry.
- Although not all biological reactions can be explained, there is no evidence that physical laws are no longer valid in biological systems.

Thermodynamics Concepts

- Definition: Thermodynamics is the characterization of the states of matter, namely gases, liquids, and solids, in terms of energetic quantities.
- Thermodynamic rules are very general and apply to all types of objects, ranging from gas molecules to cell membranes to the world.
- Fundamental thermodynamics state variables are: pressure, iemperature and volume

State variables

- A state variable is a property of a system that depends only on the current, equilibrium state of the system and thus do not depend on the path by which the system arrived at its present state.

- The state of an ideal gas can be characterized by:

  Pressure (P): is the force applied perpendicular to the surface of an object per unit area over which that force is distributed.
  Temperature (T): physical quantity that expresses the hotness of matter or radiation. It is related to the average kinetic energy of microscopic particle, such as atom, molecule, or electron.
  Volume (V): is a measure of the three-dimensional space occupied by an object.

- Relationships among the different properties of the system. For an ideal gas the relationship between state variable are described by the equation:

  $PV=nRT$ (van der Waals equation)

I Law of Thermodynamics

- The law of conservation of energy states that the total energy of any isolated system is constant; energy can be transformed from one form to another, but can be neither created nor destroyed.

$$\Delta U = q + w$$

ΔU is the change in internal energy, w is the work done on (or done by the system) and q is the transferred heat.

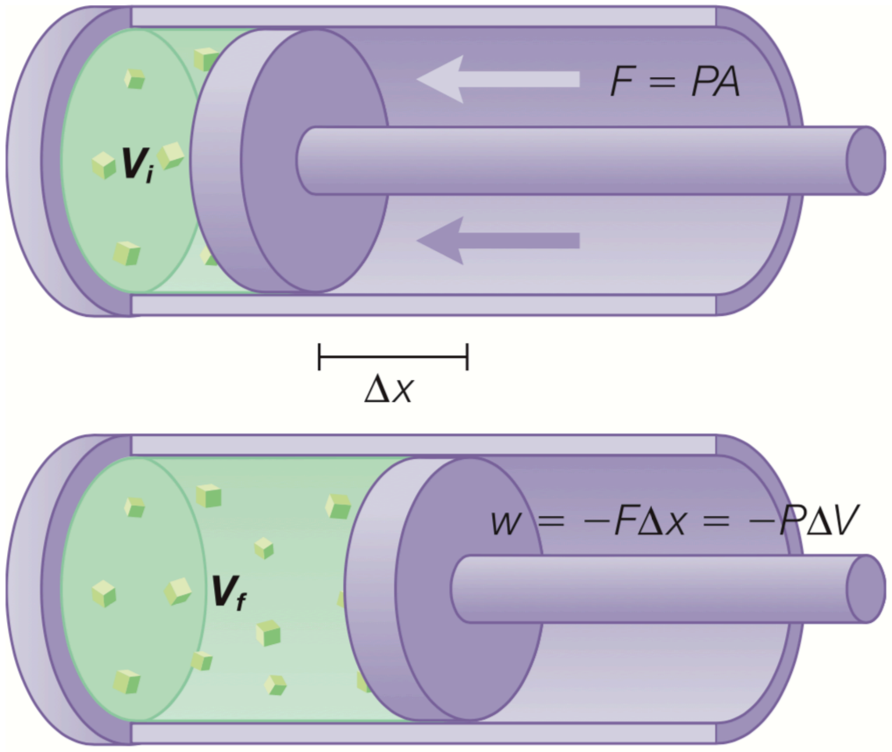
Work

The work is performed when a force (F) is used to move an object through a distance (Δx),

$$w = -F\Delta x$$

$$w = -F\Delta x = -(PA)\Delta x = -P\Delta V$$

$$w = -\int_{V_1}^{V_2} P\,\mathrm{d}V$$



$$w = -\int_{V_i}^{V_f} P\,\mathrm{d}V = -\int_{V_i}^{V_f}\left(\frac{nRT}{V}\right)\mathrm{d}V = -nRT\int_{V_i}^{V_f}\frac{\mathrm{d}V}{V} = -nRT\ln\frac{V_f}{V_i}$$

Enthalpy

Formally, enthalpy, H, is defined in terms of internal energy, U, and the product of pressure P and volume V according to:

$$H = U + PV$$

$$\Delta H = \Delta U + \Delta(PV) = \Delta U + P\Delta V \qquad P{=}constant$$

$$\Delta H = \Delta U + P\Delta V = (q - P\Delta V) + P\Delta V = q$$

At constant pressure, the change in enthalpy is equal to the heat transferred.

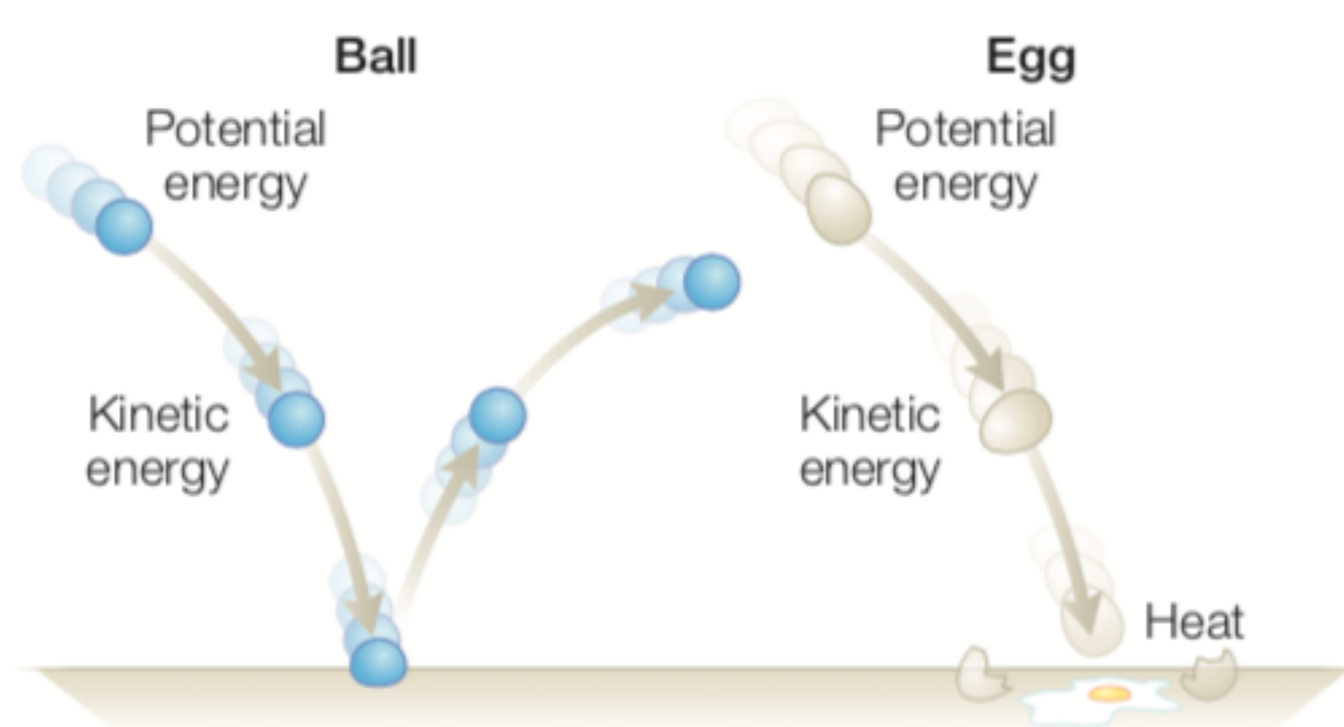
II Law of Thermodynamics

- The second law states that if the physical process is irreversible, the combined entropy of the system and the environment must increase.

Ball vs Egg

For the ball the kinetic energy is transformed in potential energy.

For the egg the kinetic energy is converted in to heat bu the egg is in a more disordered state

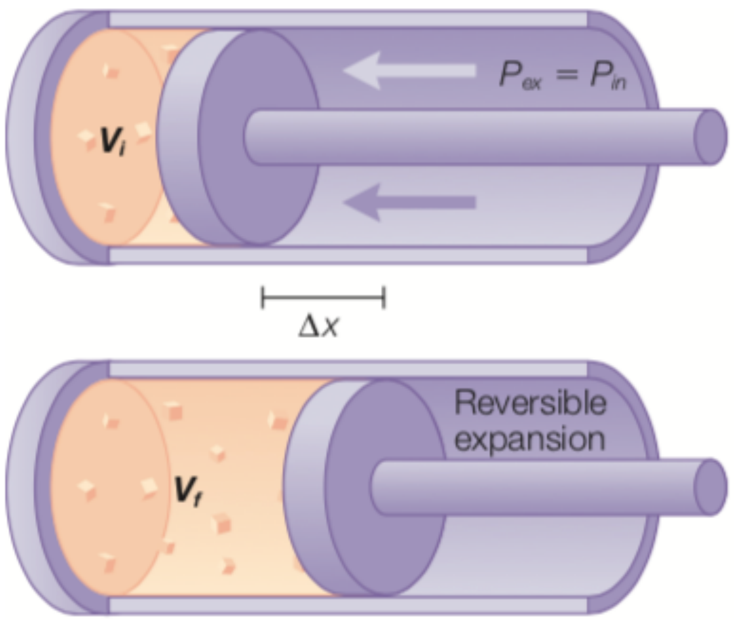


Entropy

The entropy represents the molecular disorder of a system. The concept of entropy is explicitly defined in terms of the heat and temperature of a system. In an isothermal process, the change in entropy is

$$\Delta S = \frac{q}{T}$$

For an ideal gas, when temperature is fixed, internal energy does not change and the heat flow balances the work, yielding:



$$q = -w = nRT \ln\frac{V_f}{V_i} = T\left(nR\ln\frac{V_f}{V_i}\right)$$

$$\Delta S = \frac{q}{T} = \left(nR\ln\frac{V_f}{V_i}\right)$$

III Law of Thermodynamics

- The third law of thermodynamics states that the entropy of all perfectly crystalline substances is zero at a temperature of zero Kelvin.

  In general, as temperature is decreased, random motion due to thermal motion is quenched. For a crystal, all of the atoms or molecules are located in well-defined, regular arrays and hence spatial disorder is absent.

  From a molecular viewpoint, the entropy can also be viewed as being zero as the arrangement of molecules is uniquely defined.

Gibbs energy

- The Gibbs energy is a quantity that is used to measure the maximum amount of work done in a thermodynamic system when the temperature and pressure are kept constant.

$$\Delta G = \Delta H - T\Delta S$$

$\Delta G = 0$	Equilibrium
$\Delta G < 0$	Spontaneous process
$\Delta G > 0$	Unfavorable process

Gibbs energy for ideal gas

For an ideal gas, the change in the Gibbs energy can be directly related to its thermodynamic parameters

$$dG = dH - d(TS)$$

$$dH = dU + PdV + VdP$$

$$dU = TdS - PdV \qquad with \quad q{=}TdS \;\; and \;\; w{=}\,{-}PdV$$

$$dG = TdS - PdV + PdV + VdP - TdS - SdT$$

$$dG = VdP - SdT$$

$$dG = VdP \qquad\qquad T{=}constant$$

$$\Delta G = \int_{P_i}^{P_f} \frac{nRTdP}{P} = nRT \ln \frac{P_f}{P_i}$$

Equilibrium Constant

For any given reaction A → B with an equilibrium constant K, the value of the equilibrium constant can be written in terms of the change in the Gibbs energy:

$$K = \frac{[B]}{[A]} = e^{-\Delta G/kT}$$

The equilibrium constant for a reaction is simply an alternative representation of the Gibbs energy change.

$K=1 \rightarrow \Delta G = 0$		Equilibrium
$K>0 \rightarrow \Delta G < 0$		Proceeds forward
$K<0 \rightarrow \Delta G > 0$		Proceeds backward