Thermochemistry

Thermodynamics

All physical and chemical changes are accompanied by changes in energy.

Thermodynamics: **the study of energy and its interconversions**

Energy

Energy is the capacity to do work or produce heat

Some fundamentals

Mass (m)

Acceleration (a)

Force (F) = ma

Units of force: kg-m-s^{-2}

(derived term in SI is called a Newton)

Work

- the result of a force acting on a body and producing motion

Some fundamentals (Work)

Force (F)

Distance (*l*)

Units of force: kg-m-s^{-2}

Work = force x distance

Units of work: kg-m^2-s^{-2}

(derived term in SI is called a joule)

Some fundamentals (Heat)

symbol: q

the transfer of energy between two bodies that are at different temperatures

has same units (J) as work

Calorie

approximately 1 cal is required to increase the temperature of exactly 1 g of water by 1K or 1˚C

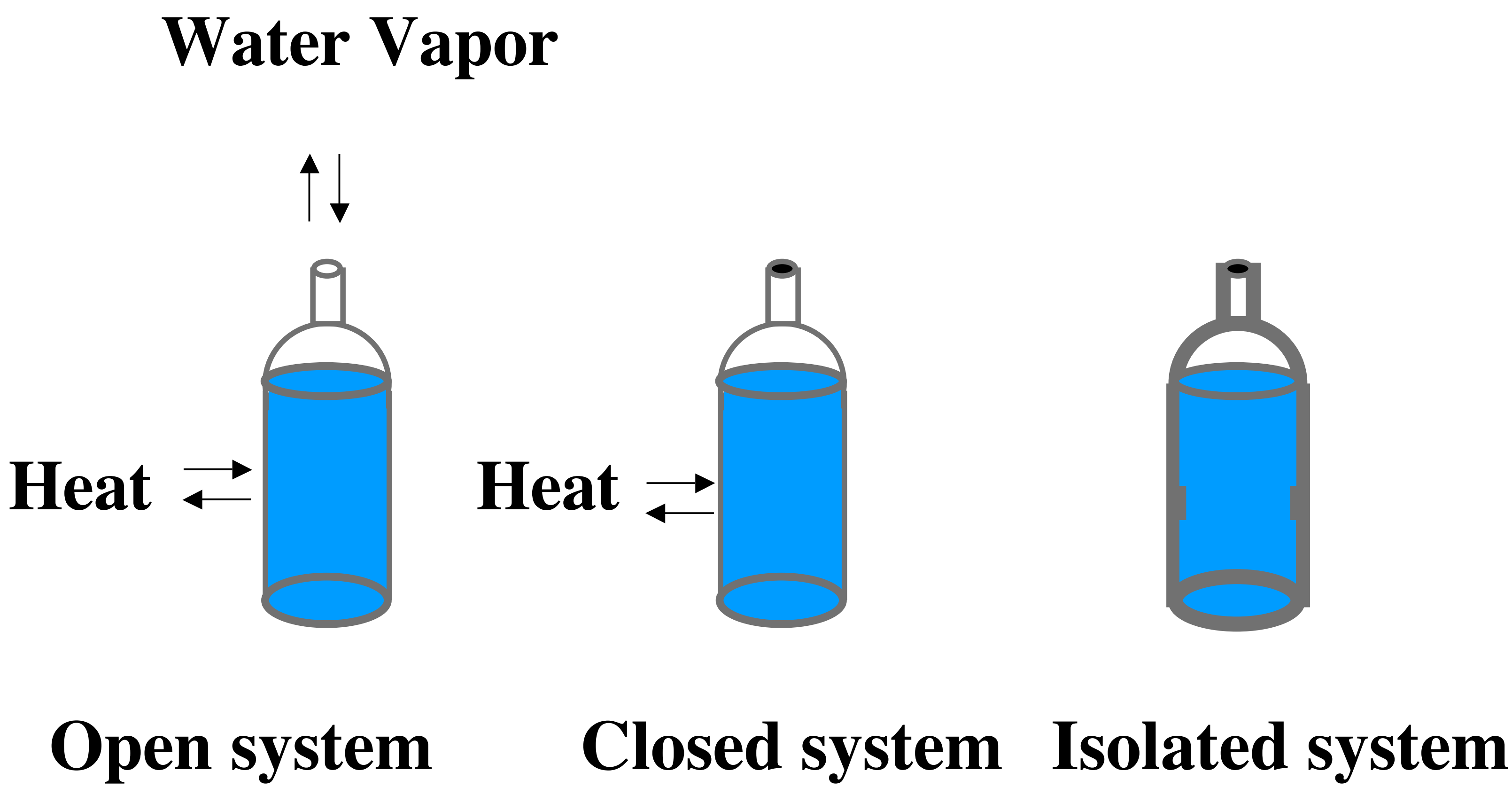
$$1 \text{ cal} = 4.184 \text{ J}$$

Some terminology

system + surroundings = universe

what we study

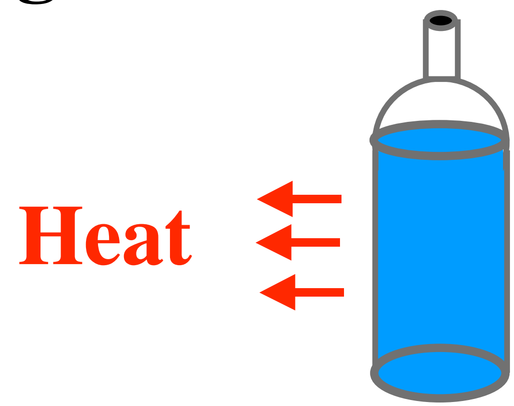
chemical reactions: reactants and products


Water Vapor
Heat
Heat
Open system
Closed system
Isolated system

Some terminology

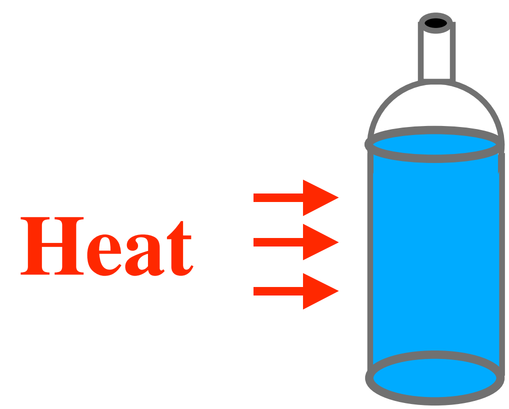
a reaction is exothermic if it gives off heat

energy flows from the system to the surroundings



a reaction is endothermic if it takes in heat

energy flows from the surroundings to the system



The heat released or absorbed during chemical reactions lies in the difference in potential energy between the products and the reactants

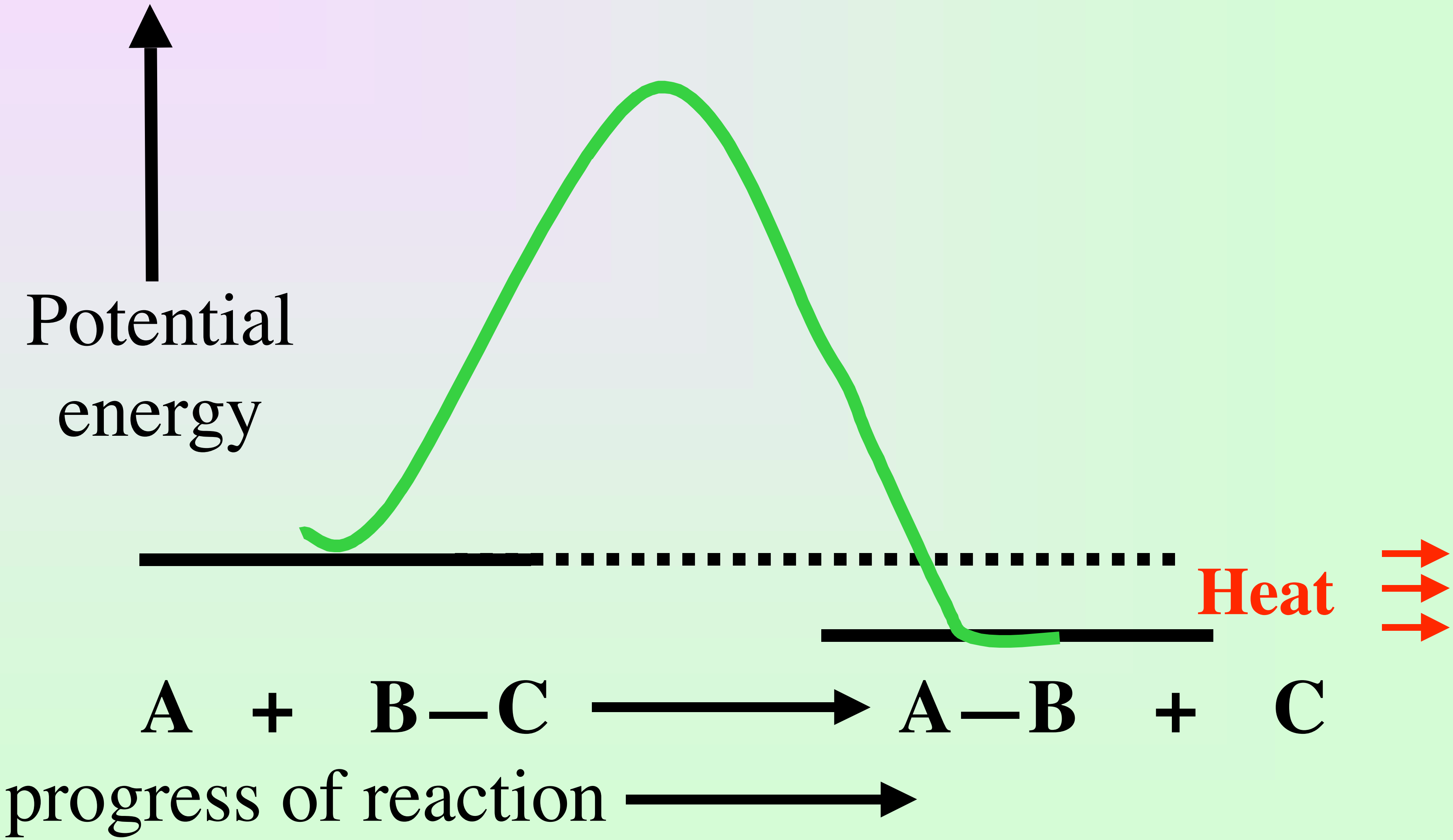
An exothermic reaction

$$2H_2(g) + 0_2(g) \longrightarrow 2H_2O(l) + \text{energy}$$

stronger chemical bonds in products than in reactants

less potential energy in products

Consider a hypothetical one-step reaction (exothermic)



An endothermic reaction

$$2H_2O(l) + \text{energy} \longrightarrow 2H_2(g) + 0_2(g)$$

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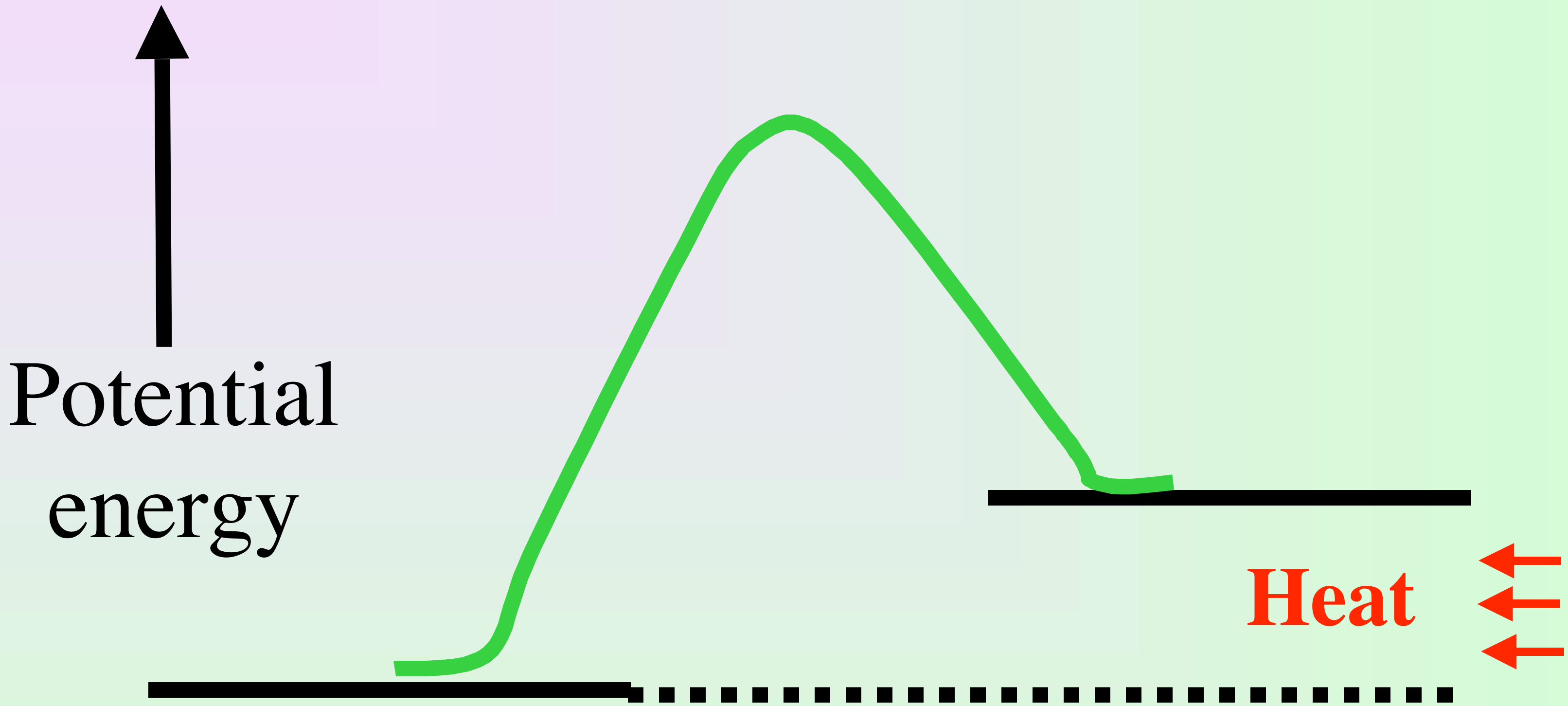


$$A \quad + \quad B{-}C \longrightarrow A{-}B \quad + \quad C$$

progress of reaction ⟶

First Law of Thermodynamics

energy can not be created or destroyed

types of energy

Kinetic (thermal) energy

energy associated with motion

Potential energy

energy available by an object by virtue of its position

Kinetic energy

Energy an object possesses because of its motion

$$\text{kinetic energy} = \frac{1}{2}\,mu^2$$

Units: kg-m^2-s^{-2} (joules)

Potential energy

energy an object has because of position

an example is potential energy of an object with the potential to fall

gravitational potential energy = mass x height x gravitational constant

Units: kg-m^2-s^{-2} (joules)

Chemical Potential Energy

due to the attractive and repulsive forces between protons and electrons

Ionic Compounds

Coulomb's Law

the potential energy between two ions in an ionic solid is directly proportional to the product of their charges and inversely proportional to the distance between them

Charge on Li^+

Charge on F^-

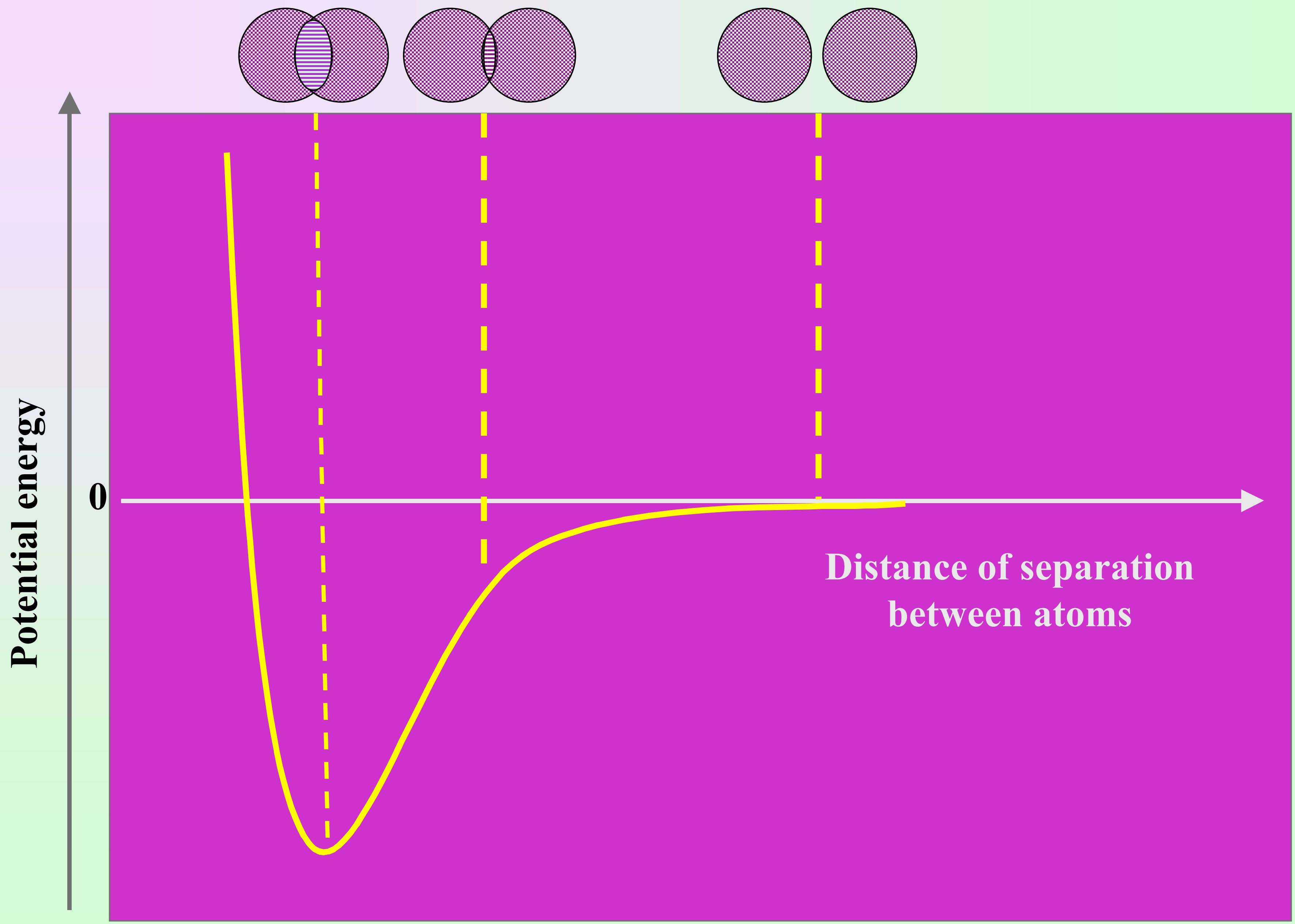
$$E = k \frac{Q_{Li^+} Q_{F^-}}{r}$$

The distance between the ions

Covalent Compounds

Compounds containing covalent bonds

(electrons shared by two atoms)


Potential energy
0
Distance of separation
between atoms

First Law of Thermodynamics

Energy can be converted from one form to another but can neither be created nor destroyed

Energy = Heat + Work

$$\boxed{\mathrm{E} = q + w}$$

Example : kinetic energy to potential energy

Internal Energy (E)

$$\mathbf{E} = q + w$$

Internal Energy (E)

The sum of the kinetic and potential energies of all the particles in a system

$$\boxed{E} = q + w$$

Change Internal Energy (ΔE)

The energy entering or leaving the system

$$\boxed{\Delta E} = q + w$$

A common type of work associated with chemical processes is the expansion and compression of a gas.

$$\text{Pressure} = \frac{\text{Force}}{\text{Area}}$$

$$\boxed{F = P\,A}$$

$$\text{work} = F \times d$$

A common type of work associated with chemical processes is the expansion and compression of a gas.

$$\text{Pressure} = \frac{\text{Force}}{\text{Area}}$$

$$\boxed{F = P\,A}$$

$$\text{work} = \underset{}{P\overset{m^2}{A}} \times \overset{m}{d}$$

the work done by an expanding gas against pressure P

W is negative because work is leaving the system during an expansion

$$m^3$$

$$\textbf{work} = -P\Delta V$$

Example

A balloons volume changes from $4.0x10^6$L to $4.5x10^6$L by the addition of $1.3x10^8$J of heat energy.Assuming a constant pressure of 1.0atm,calculate □*E* for the process.

$$\square E = q + w$$

$$w = -P\square V = (-1.0\text{atm})(4.5\text{x}10^6\text{L} - 4.0\text{x}10^6\text{L})$$

$$= -5.0\text{x}10^5\ \text{atmL} \times \frac{101.3\ \text{J}}{\text{atmL}} = -5.1\text{x}10^7\ \text{J}$$

$$\frac{R' \quad (8.314\text{J}/\cancel{\text{mol}}\cancel{\text{K}})}{R \quad (0.08206\text{atmL}/\cancel{\text{mol}}\,\cancel{\text{K}})} = \frac{101.3\ \text{J}}{\text{atmL}}$$

Example

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$$\boxed{\Delta E = q + w}$$

$$w = - 5.1x10^7 \text{ J}$$

$$\Delta E = q + w = 1.3x10^8\text{J} + (- 5.1x10^7 \text{ J})$$

$$\Delta E = 8 x10^7\text{J}$$

Enthalpy

Enthalpy（H）

Used to describe heat changes taking place at a constant pressure (q_p)

$$\Delta E = q_p + w$$

$$\Delta E = q_p - P\Delta V$$

$$q_p = \Delta E + P\Delta V$$

$$q_p = \Delta H$$

$$\Delta H = \Delta E + P\Delta V$$