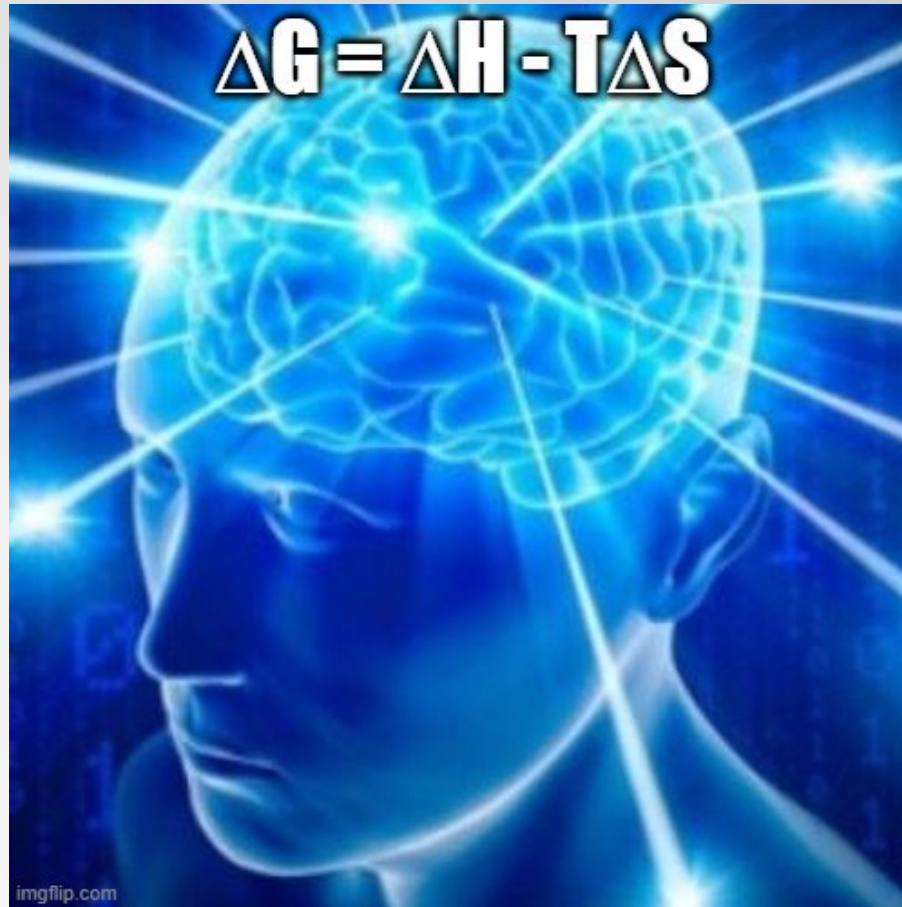


Seminar 1: Thermodynamics



Biophysics

Course 2023-2024

Alberto Meseguer
Irene Acero

The Gibbs free energy equation

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

The Gibbs free energy equation

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

This formula is assuming constant pressure and temperature

If $\Delta G < 0$ the reaction is spontaneous, and non spontaneous in the opposite direction

If $\Delta G = 0$ the reaction is at equilibrium

If $\Delta G > 0$ the reaction is not spontaneous, and spontaneous in the opposite direction

Entropy

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

Entropy is a measure of how dispersed energy is

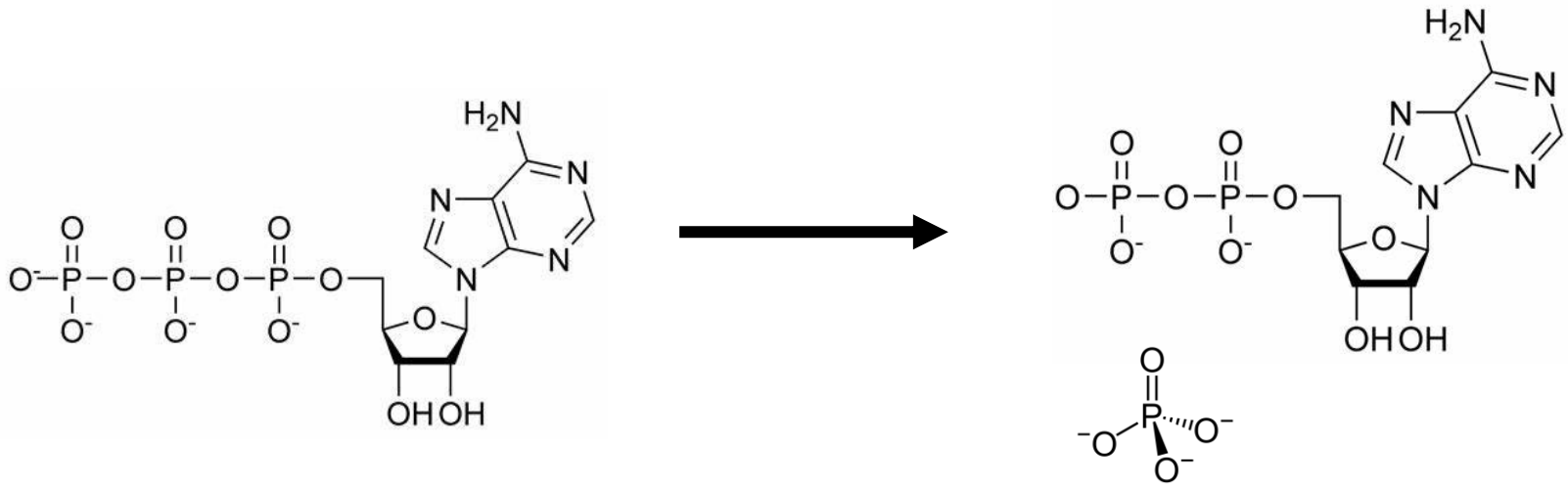
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$$\Delta G = \Delta H - T \cdot \Delta S$$

Entropy is a measure of how dispersed energy is

This definition can be applied to any type of energy, such as:

- Chemical energy



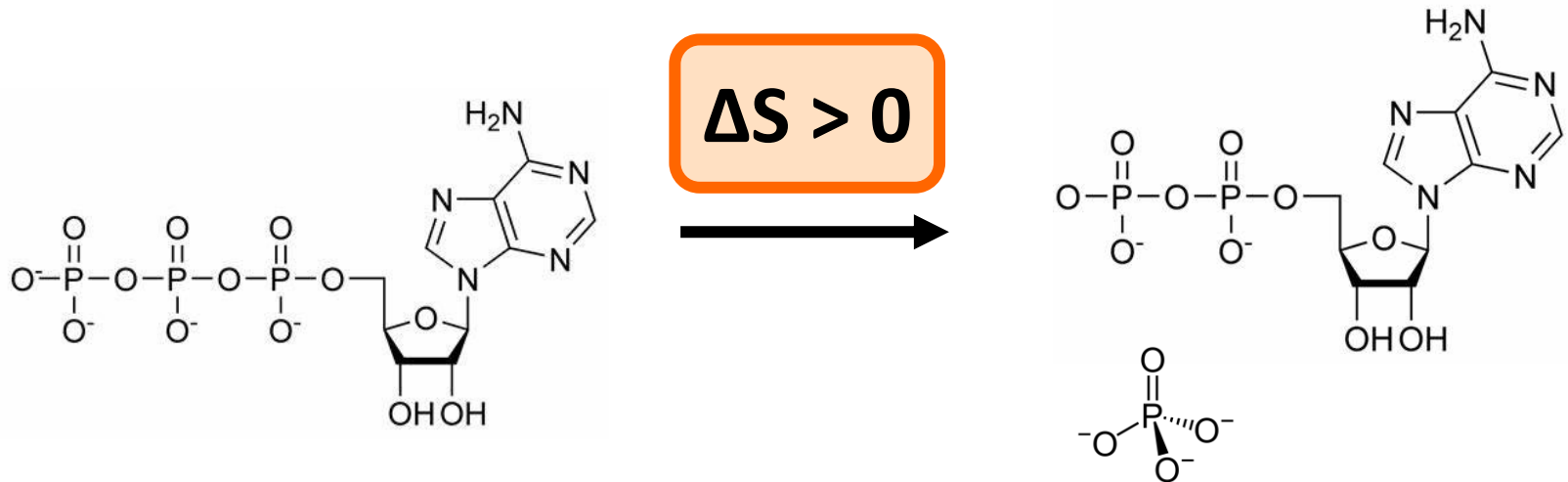
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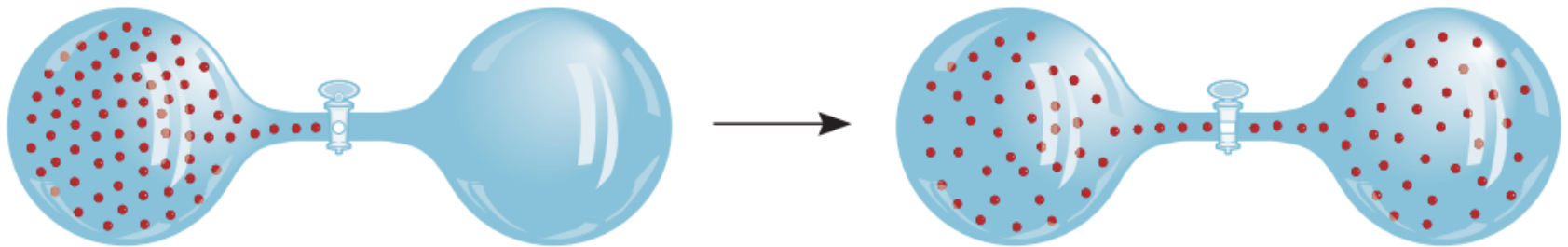
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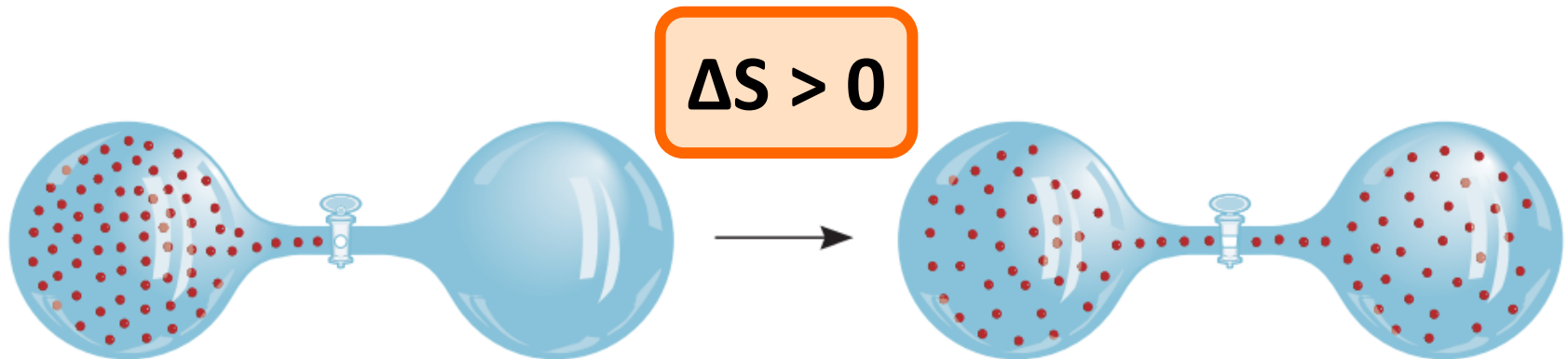
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Entropy


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

Entropy is a measure of how dispersed energy is

This definition can be applied to any type of energy, such as:

- Thermal energy



$$\Delta S > 0$$




Entropy

AC

**And to proof this I brought
you an
Stirling engine!!**



The Stirling engine

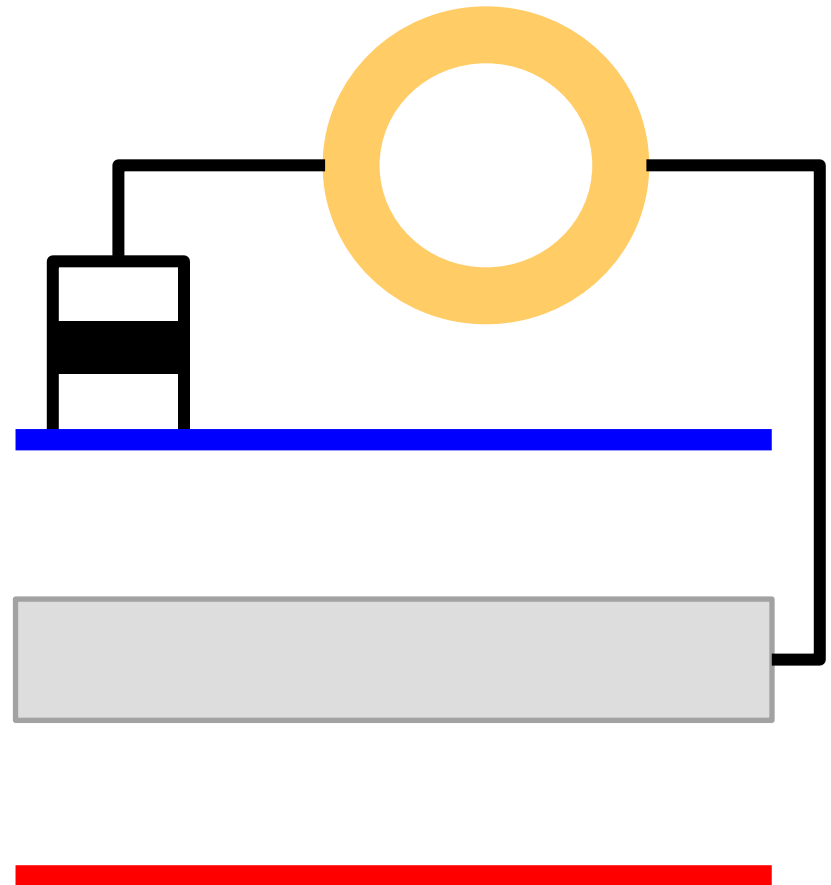
$$\Delta G = \Delta H - T \cdot \Delta S$$

An Stirling engine is an external combustion engine



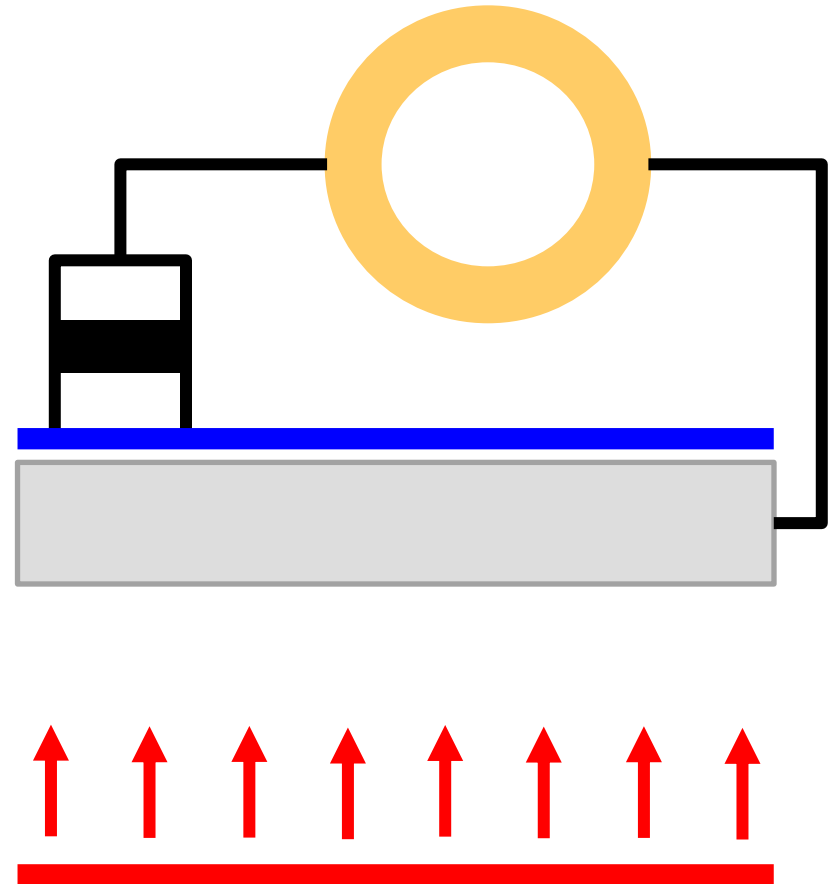
The Stirling engine

This is an scheme of the Stirling engine with all its important parts



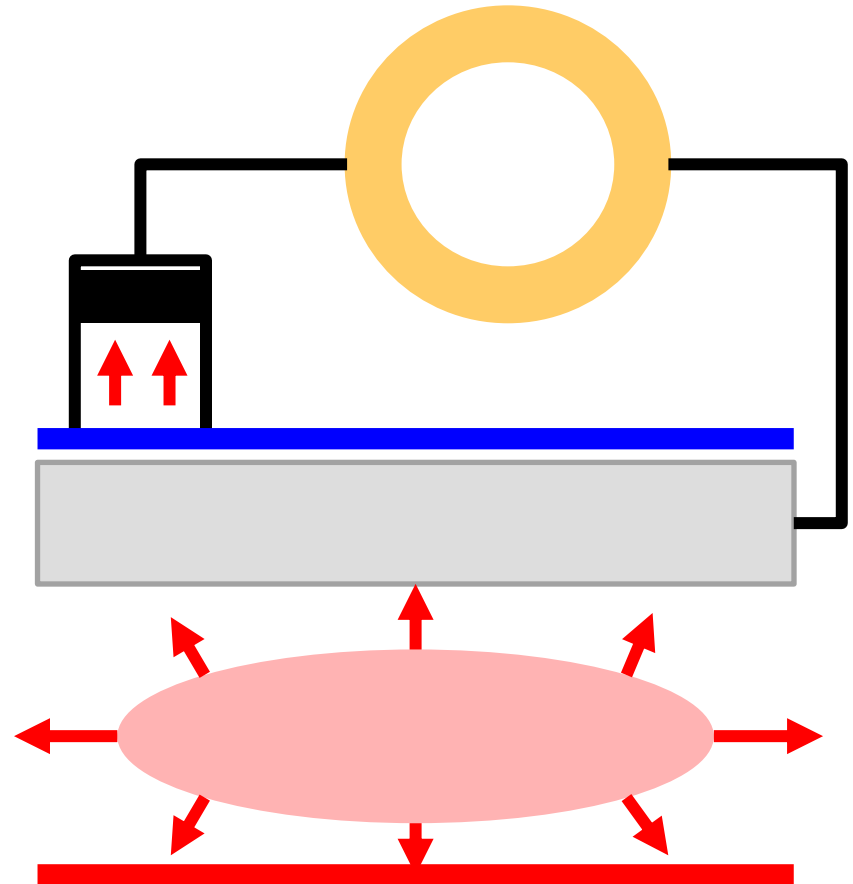
The Stirling engine

When we start the engine we make the foam go up. The air in the chamber gets in contact with the hot plate and gets warmed up.



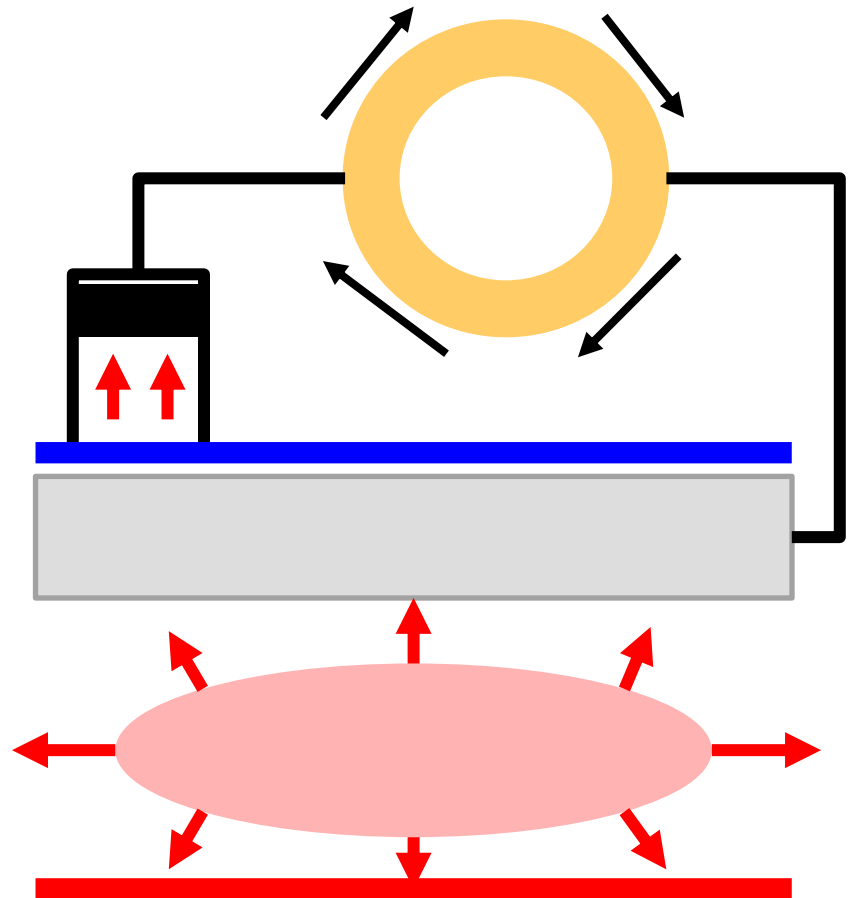
The Stirling engine

As the air in the chamber gets hot, it expands itself. This moves the piston up.



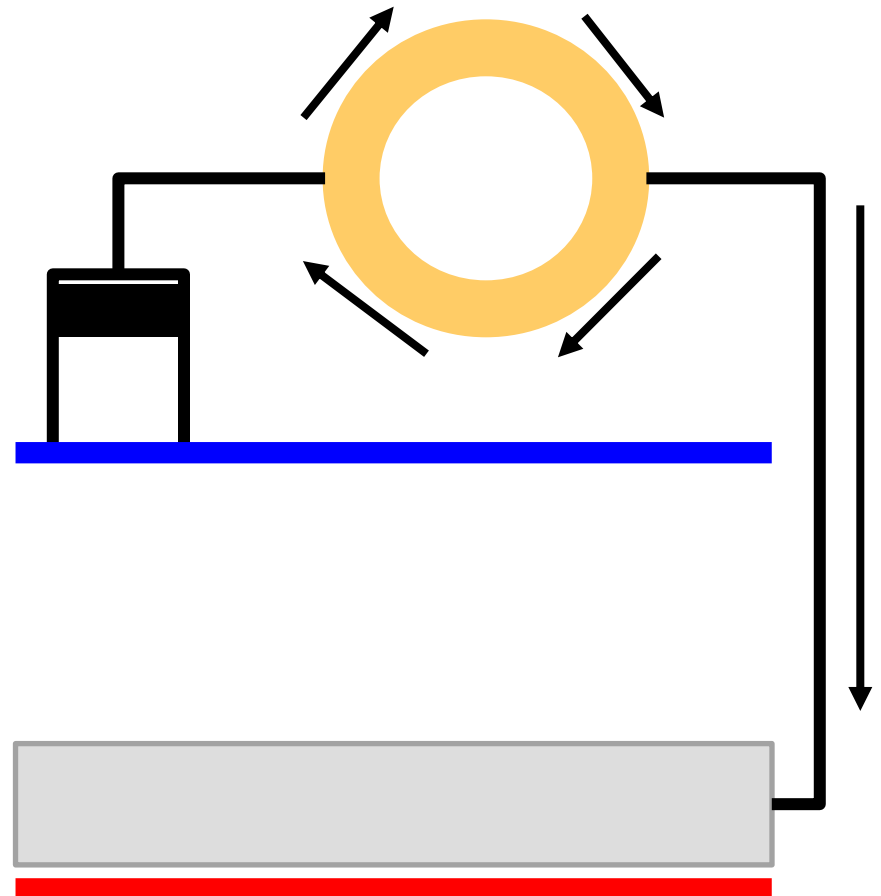
The Stirling engine

The piston is connected to the wheel, which starts turning.



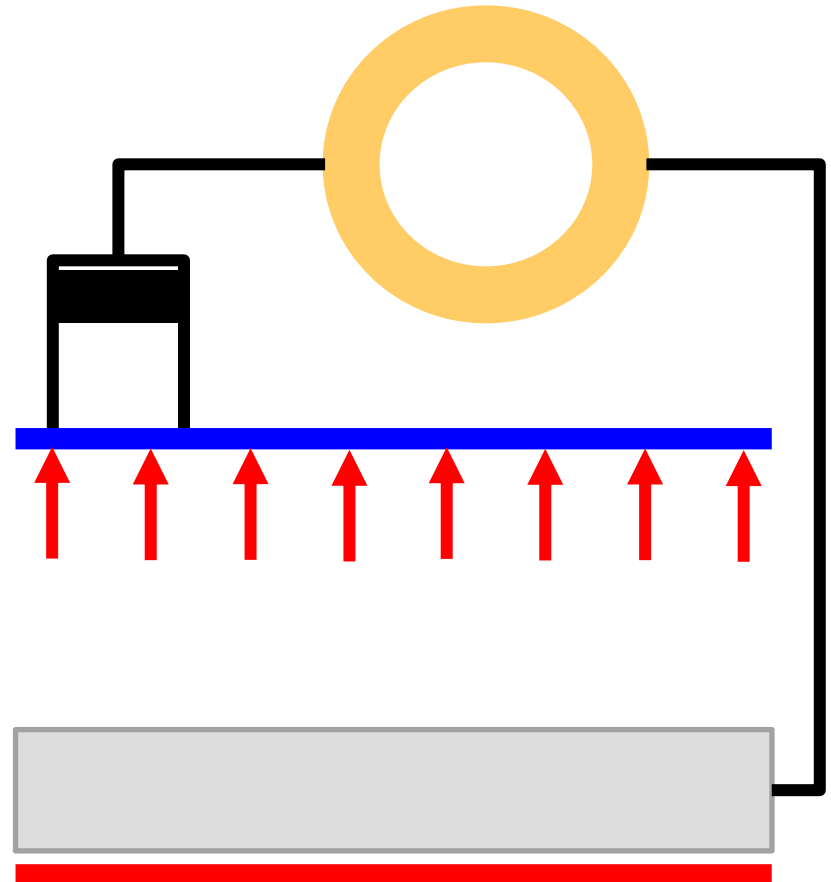
The Stirling engine

The wheel is connected to the block of foam, when it moves it pushes the foam down.



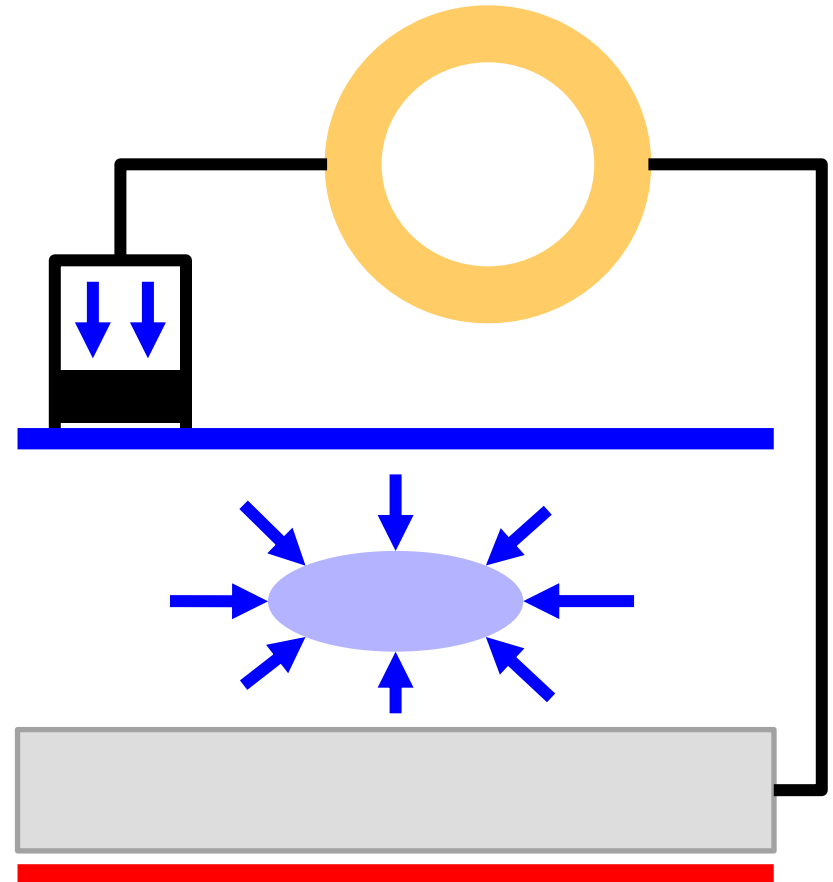
The Stirling engine

The hot air in the chamber transfers heat to the cold plate.



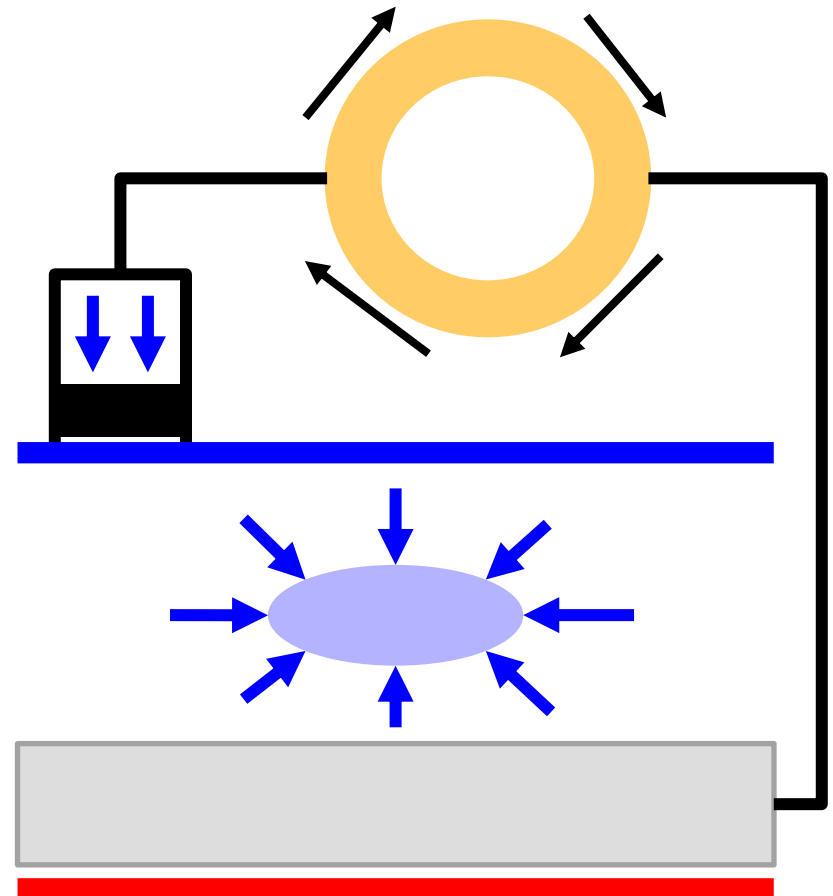
The Stirling engine

As the air in the chamber gets cold, it compresses itself. This moves the piston down.



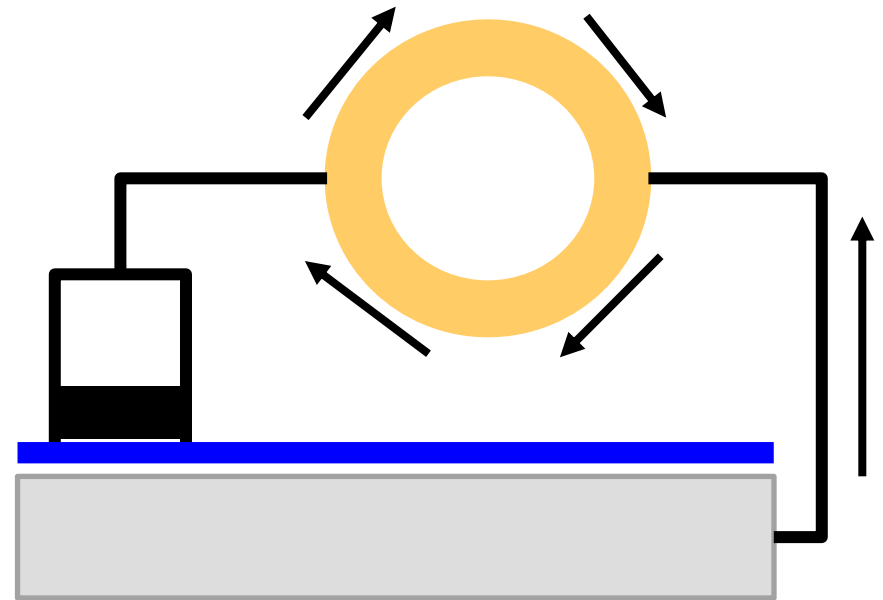
The Stirling engine

The piston is connected to the wheel, which starts turning.



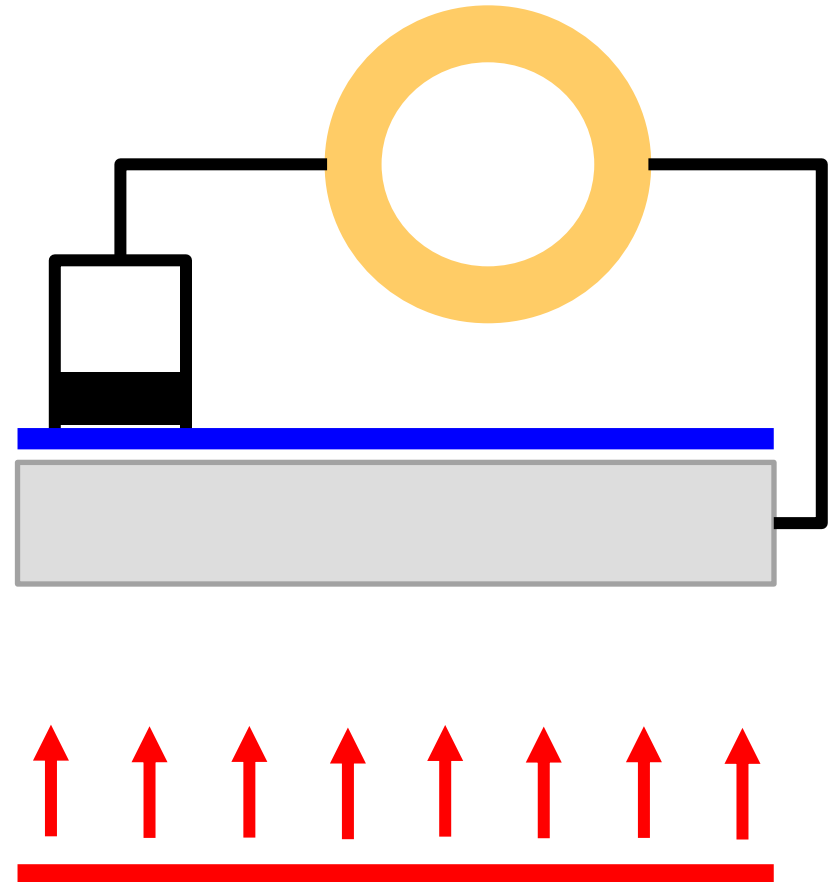
The Stirling engine

The wheel is connected to the block of foam, when it moves it pushes the foam up.



The Stirling engine

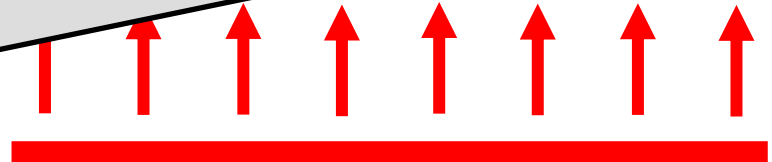
This is where we were at the beginning. The air in the chamber gets in contact with the hot plate and gets warmed up.



The Stirling engine

This is where we were at
gets it

**And this process repeats
again and again**



The Stirling engine

Some questions for you to answer

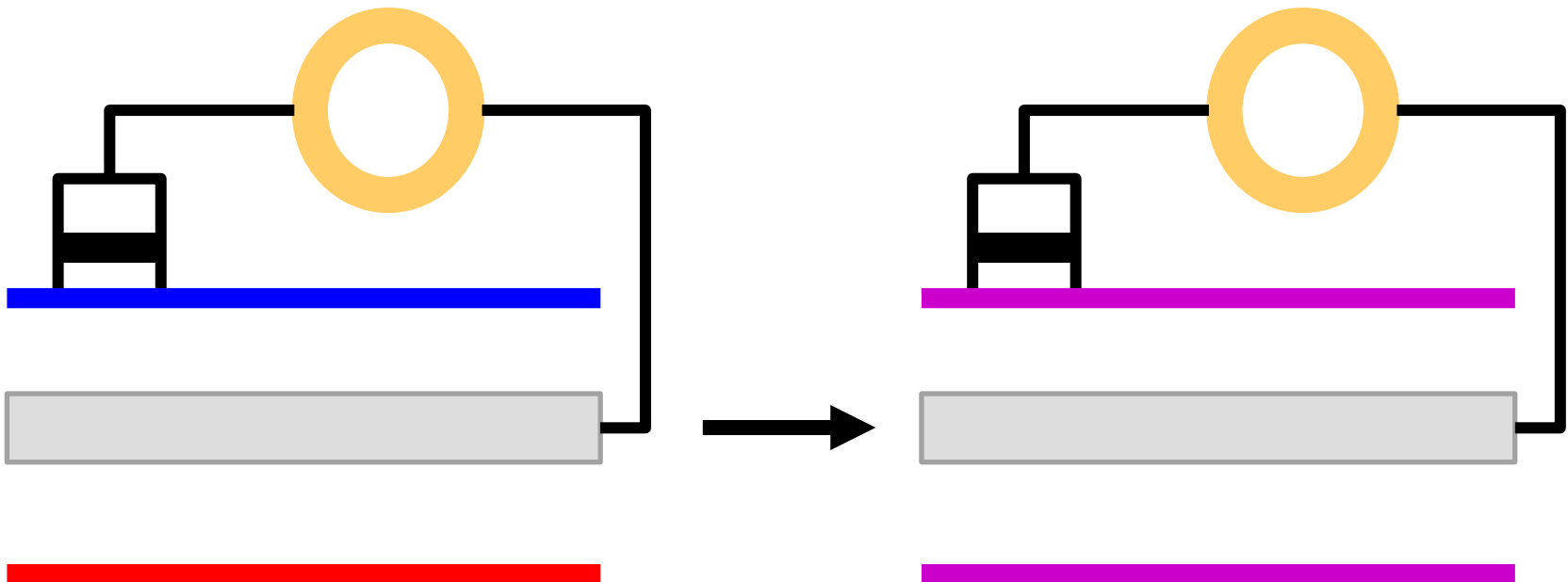


1. What is the role of entropy in the functioning of an Stirling engine?
2. Do you think this engine can run forever from the heat of a cup of hot water? Why?
3. If we put the engine in a very hot room, do you think it will be able to run using the heat of a cup of hot water? Why?
4. Do you think this engine can run using a source of cold instead of a source of heat? Why?

The Stirling engine and entropy

With the Stirling engine we can see how energy that is clumped together can be used to do work

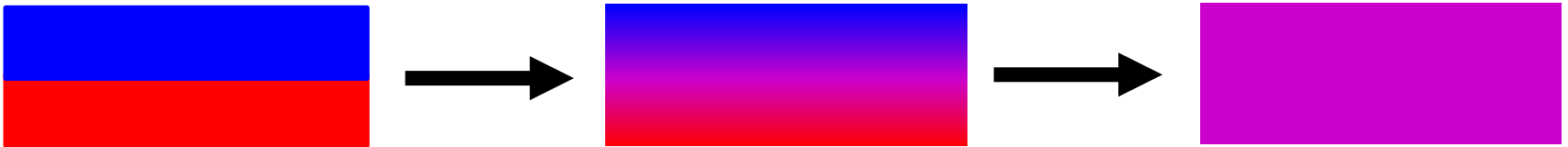
But after this energy is used to do work it is dispersed, and it cannot be used back again



The Stirling engine and entropy

With the Stirling engine we can see how energy that is clumped together can be used to do work

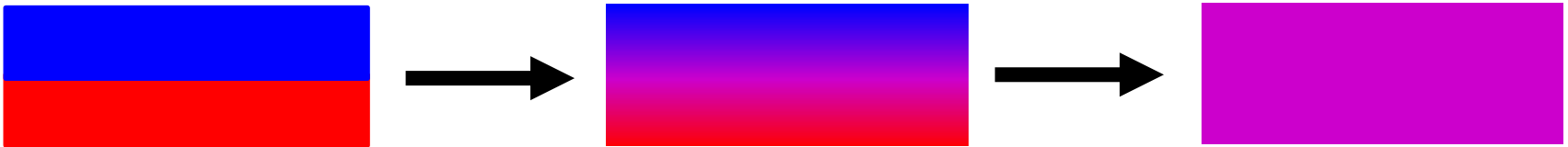
But after this energy is used to do work it is dispersed, and it cannot be used back again



The Stirling engine and entropy

With the Stirling engine we can see how energy that is clumped together can be used to do work

But after this energy is used to do work it is dispersed, and it cannot be used back again



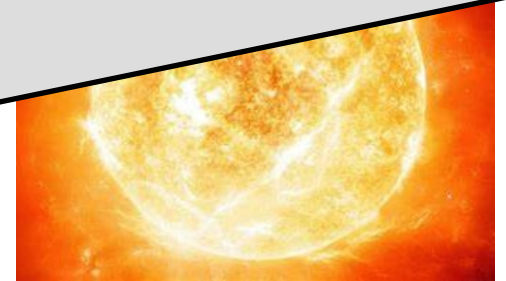
And this happens with everything:



The Stirling engine and entropy

With the Stirling engine

**And this may be the reason
why the universe ends!!
(Check the heat death of the
universe)**



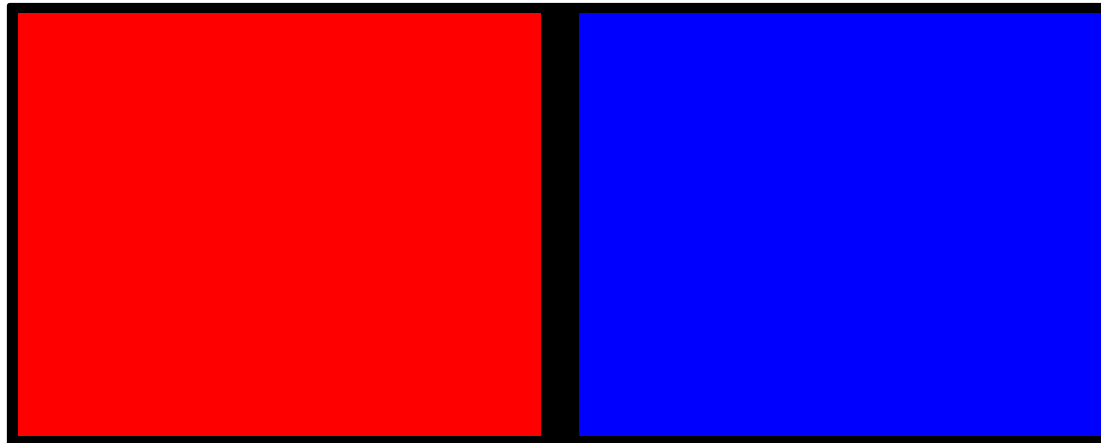
Why is entropy always increasing?

Entropy is always increasing because it is always the most likely situation from an statistical point of view

Imagine the following situation:

Hot water

Cold water



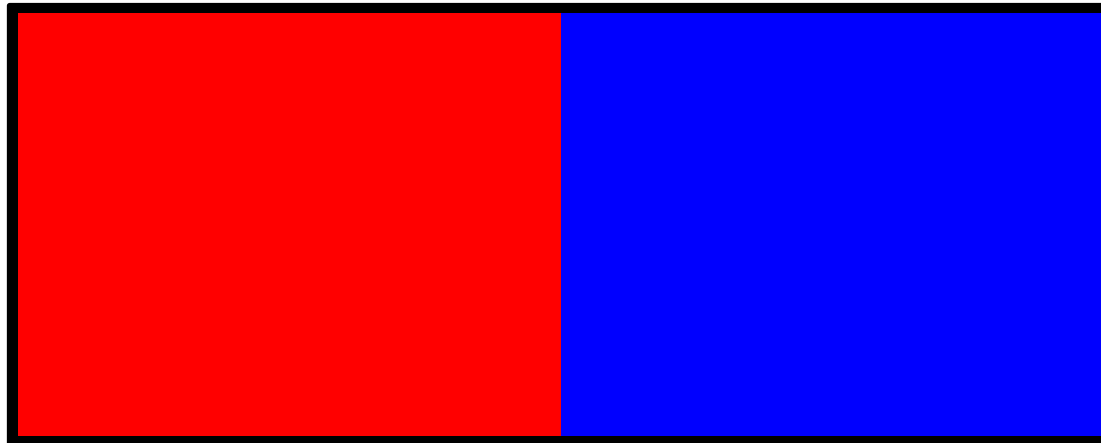
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Imagine the following situation:

Hot water

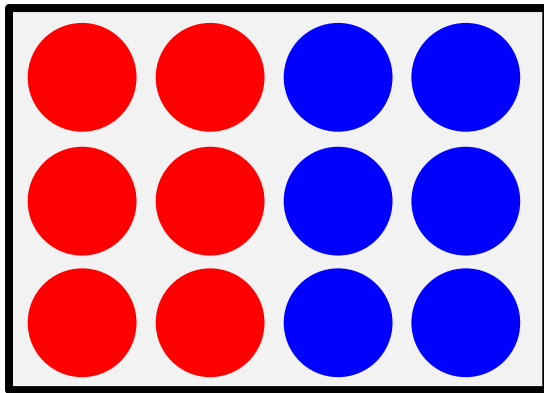
Cold water



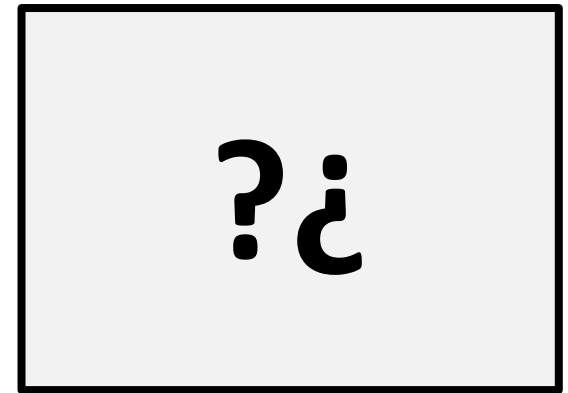
Why is entropy always increasing?

Entropy is always increasing because it is always the most likely situation from an statistical point of view

Since atoms have a lot of freedom of movement, this situation is equivalent to have ping pong balls of different colors in a box and shaking that box.



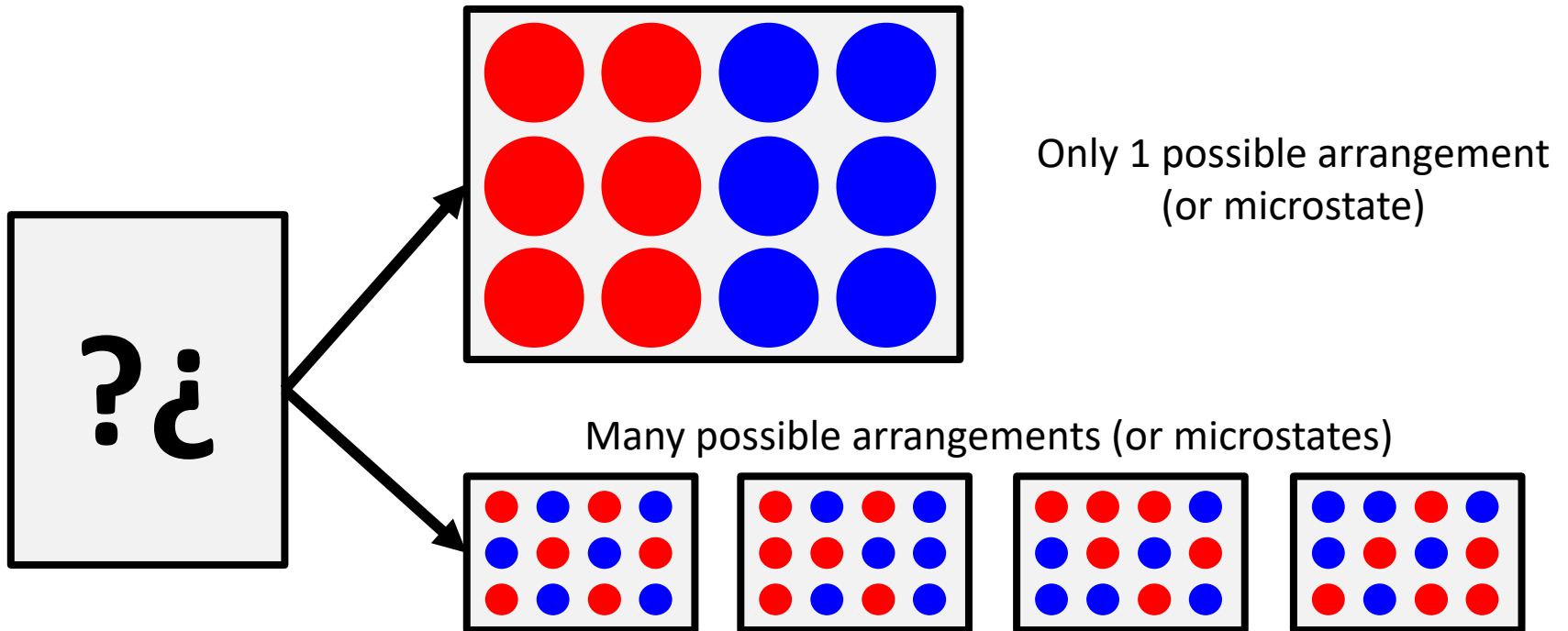
Shaking



Why is entropy always increasing?

Entropy is always increasing because it is always the most likely situation from an statistical point of view

Since atoms have a lot of freedom of movement, this situation is equivalent to have ping pong balls of different colors in a box and shaking that box.



Why is entropy always increasing?

Entropy is always increasing because it is always the most likely situation from an statistical point of view

Also, keep in mind that molecules can clash with each other, then transferring part of their energy to other molecules




Why is entropy always increasing?

Entropy is always increasing because it is always the most likely situation from an statistical point of view

It is something similar to what happens with the probabilities of having a number when rolling a dice

The number you get is the macrostate

Each combination of dices is a microstate



2	3	4	5	6	7
3	4	5	6	7	8
4	5	6	7	8	9
5	6	7	8	9	10
6	7	8	9	10	11
7	8	9	10	11	12

Number	Probability
2	1/36
3	2/36
4	3/36
5	4/36
6	5/36
7	6/36
8	5/36
9	4/36
10	3/36
11	2/36
12	1/36

Why is entropy always increasing?

Some questions for you



	2	3	4	5	6	7
	3	4	5	6	7	8
	4	5	6	7	8	9
	5	6	7	8	9	10
	6	7	8	9	10	11
	7	8	9	10	11	12

1. What number is the most likely when rolling two dice? Why?
2. How many microstates are available for that number?
3. What number is the most unlikely when rolling two dice? Why?
4. How many microstates are available for that number?

Why is entropy always increasing?

Think about this the next time you play Catan



The Stirling engine

This part of the class was inspired by this youtube video by Steve Mould: <https://www.youtube.com/watch?v=w2iTCm0xpDc&t=261s>

If you like science divulgation I really recommend you his channel



A better description of entropy

The Gibbs free energy equation

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

Enthalpy

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

At constant pressure, the change in enthalpy (ΔH) equals heat

Enthalpy

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

At constant pressure, enthalpy can also be understood as the change in energy that comes from breaking and creating bonds in a reaction

When bonds are created, energy is released as heat

When bonds are broken, energy is taken as heat

Enthalpy

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

At constant pressure, enthalpy can also be understood as the change in energy that comes from breaking and creating bonds in a reaction

When bonds are created, energy is released as heat

$$\Delta H < 0$$

When bonds are broken, energy is taken as heat

$$\Delta H > 0$$

Enthalpy

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

At constant pressure, enthalpy can also be understood as the change in energy that comes from breaking and creating bonds in a reaction

When bonds are created, energy is released as heat

$$\Delta H < 0$$

Processes with $\Delta H < 0$ are exothermic

When bonds are broken, energy is taken as heat

$$\Delta H > 0$$

Processes with $\Delta H > 0$ are endothermic

Bond energy and enthalpy

Chemical bonds are related to energy called bond energy

At constant pressure:

The energy that is released when a bond is made is the bond energy

The energy you have to give to break a bond is the bond energy

Bond energy and enthalpy

Chemical bonds are related to energy

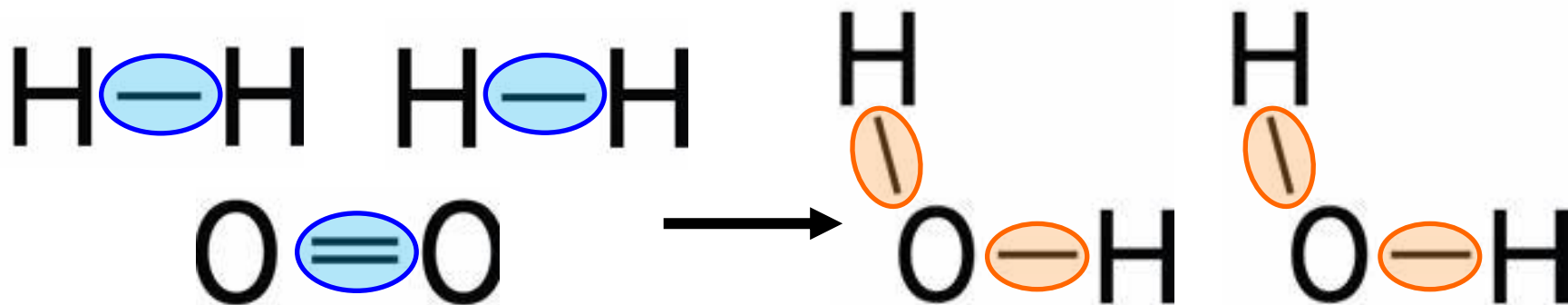
We can use the bond energy in reactants and products to estimate the enthalpy change in a chemical reaction

Bond energy and enthalpy

Let's see a couple of examples: $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$

Broken bonds: $\Delta H > 0$

Created bonds: $\Delta H < 0$



Bond energy $\text{H}_2 = 432 \text{ kJ/mol}$
Bond energy $\text{O}_2 = 495 \text{ kJ/mol}$

Bond energy $\text{H}_2\text{O} = 467 \text{ kJ/mol}$

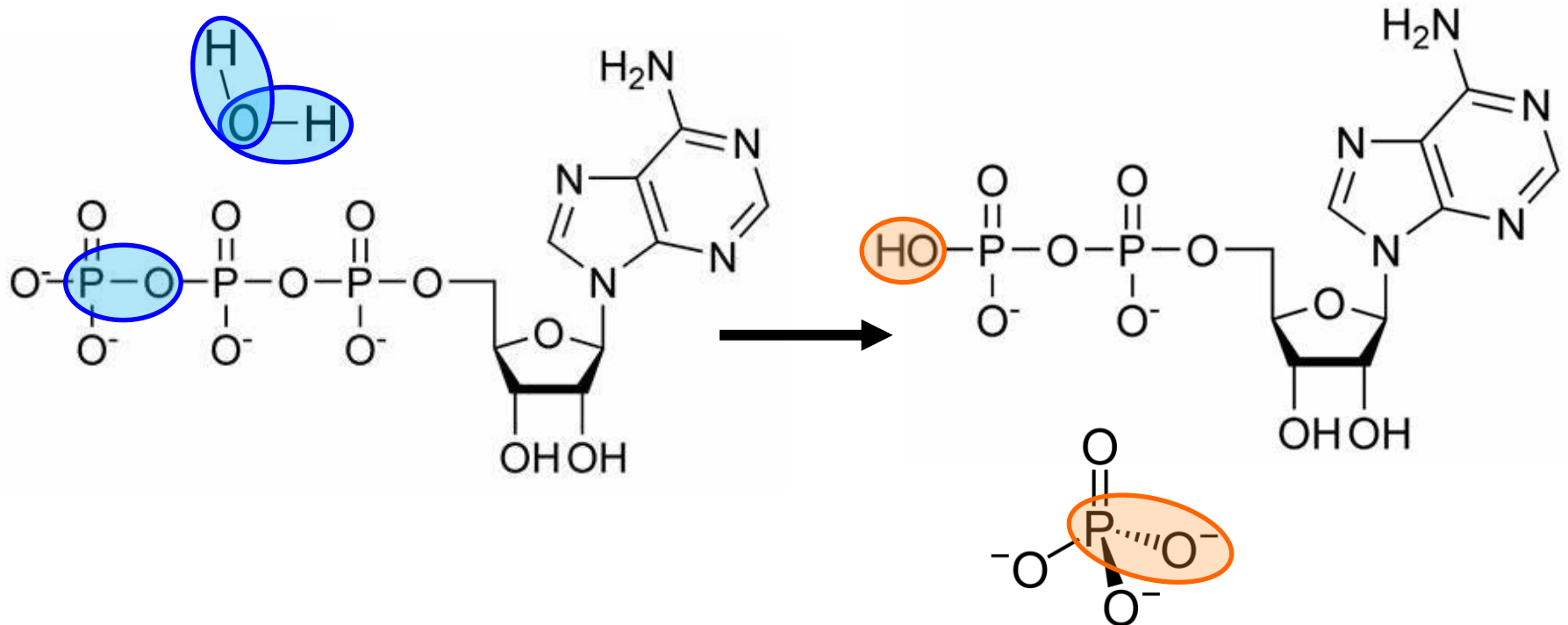
At constant pressure, what is the ΔH of this process?

Bond energy and enthalpy

Let's see a couple of examples: ATP hydrolysis

Broken bonds: $\Delta H > 0$

Created bonds: $\Delta H < 0$



Enthalpy

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

When bonds are created, energy is released as heat

$$\Delta H < 0$$

Processes with $\Delta H < 0$
favor spontaneity
($\Delta G < 0$)

When bonds are broken, energy is taken as heat

$$\Delta H > 0$$

Processes with $\Delta H > 0$
oppose to spontaneity
($\Delta G > 0$)

Enthalpy

Try to solve the following exercises without doing calculations, just thinking:

1. Consider two complementary molecules of single stranded DNA inside the cell nucleus. If they hybridize, will this process increase or decrease the enthalpy of the DNA molecules?
2. Imagine a protein with a lot of alpha helices:
 - Does it has hydrogen bonds?
 - What happens if we increase the temperature of the protein?
 - What is the ΔH of this process?

The Gibbs free energy equation

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

Try to solve the following exercises without doing calculations, just thinking:

1. Consider a block of ice and a glass of liquid water:
 - What is the ΔH for going from solid ice to liquid water?
 - What is the ΔS for going from solid ice to liquid water?
 - Under what conditions becomes spontaneous going from solid ice to liquid water?
2. Consider two water molecules floating in vacuum, if they create a hydrogen bond between themselves:
 - What is the ΔH of the process?
 - What is the ΔS of the process?
 - What value is larger in absolute values? $|\Delta H|$ or $|T \cdot \Delta S|$?

The Gibbs free energy equation

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

When creating bonds:

ΔS opposes to it

ΔH favors it

When breaking bonds:

ΔS favors it

ΔH opposes to it

Some videos for you to study

A better description of entropy – YouTube

<https://www.youtube.com/watch?v=w2iTCm0xpDc>

What is entropy? - Jeff Phillips – YouTube

https://www.youtube.com/watch?v=YM-uykVfq_E

Enthalpy: Crash Course Chemistry #18 – YouTube

<https://www.youtube.com/watch?v=SV7U4yAXL5I&t=385s>

Lecture 03, concept 12: Phase transitions from entropy-enthalpy balance – YouTube

<https://www.youtube.com/watch?v=NITMgwZgohI&list=PLuIpgNT2hMwTyjpKVevMHUofykrXFtNVW&index=12>

Lecture 03, concept 15: Hydrogen bond formation in water interpreted with entropy/enthalpy – YouTube

<https://www.youtube.com/watch?v=CR7rfTyNpdo&list=PLuIpgNT2hMwTyjpKVevMHUofykrXFtNVW&index=15>