

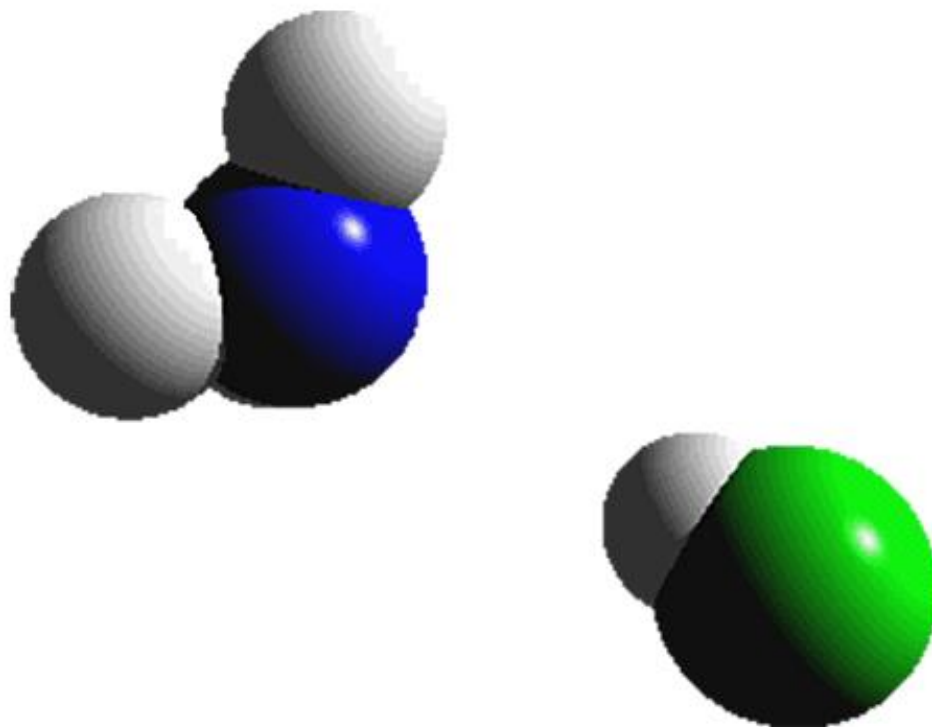
KINETICS OF CHEMICAL REACTIONS

How do reactions occur?

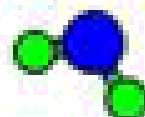
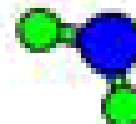
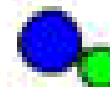
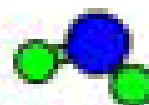
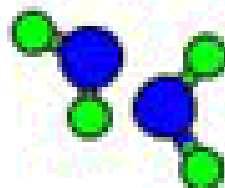
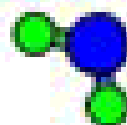
-According to one theory-a **COLLISION** is needed in order to have chemical reaction

- In order to have a chemical reaction, there **MUST BE** a **COLLISION** between the Molecules of **REACTANTS**...
- **Must have** an effective collision between reacting particles for reaction to occur. “**Collision Theory**”
 - **Collision must be energetic** in order the chemical reaction to take place.
 - **Collision must occur at an effective angle.**

Presentation of a collision between two molecules that leads to a chemical reaction



Heat bath



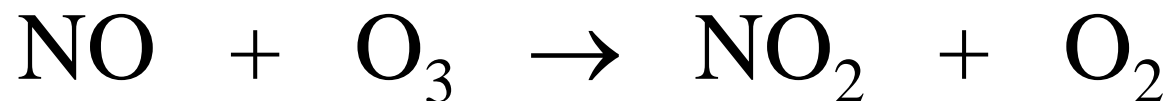
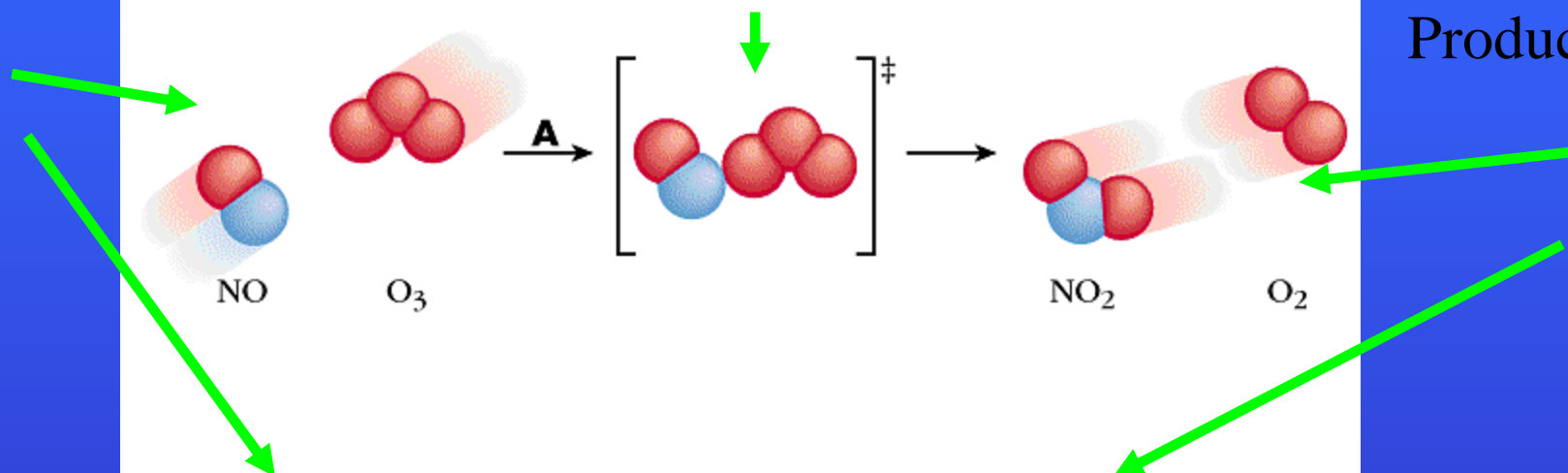
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Particle Diagram of Collision

Reactants

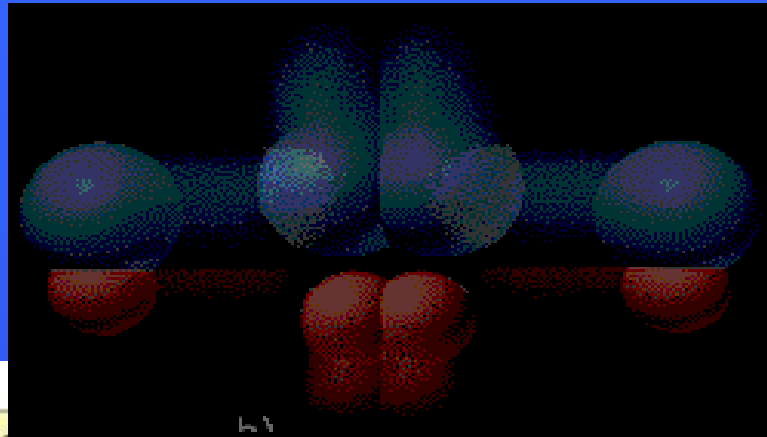
Activated complex or transition state.

Products

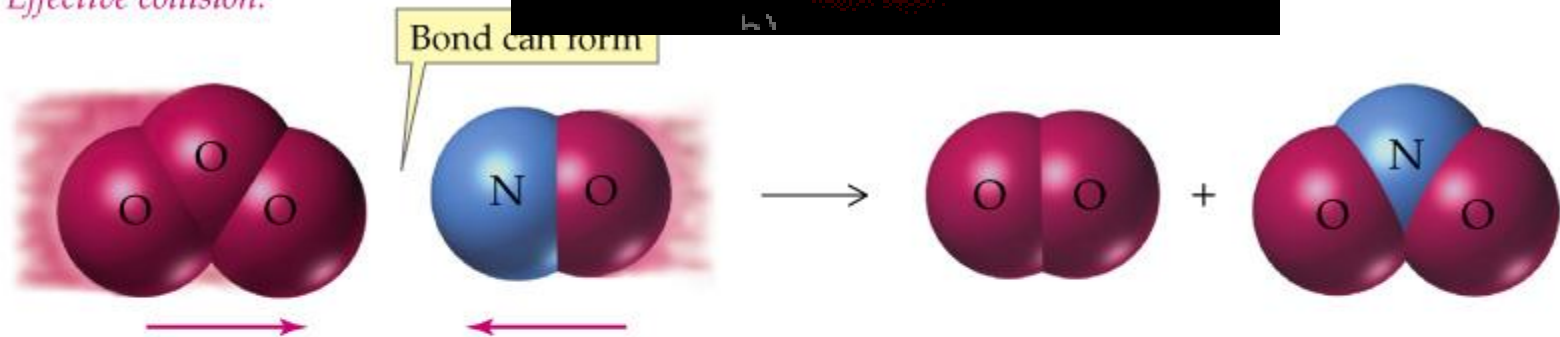


Activated Complex is NOT in equation!

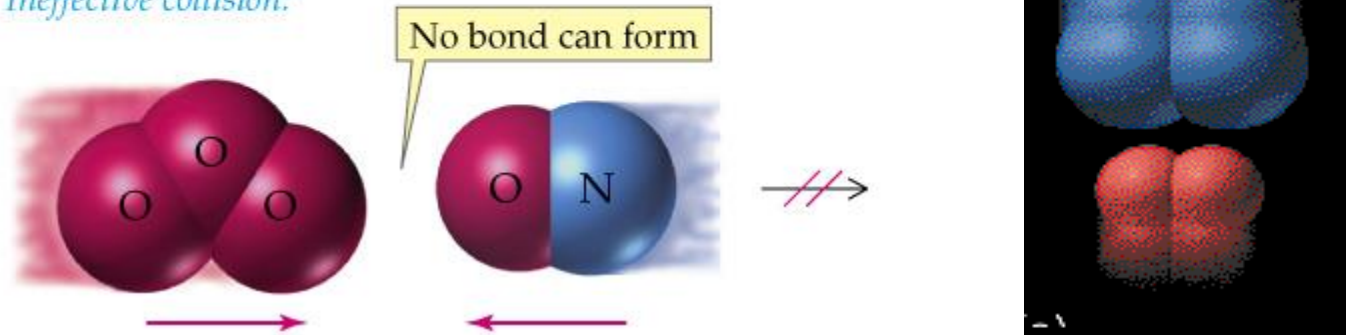
Effective vs. Ineffective Collision



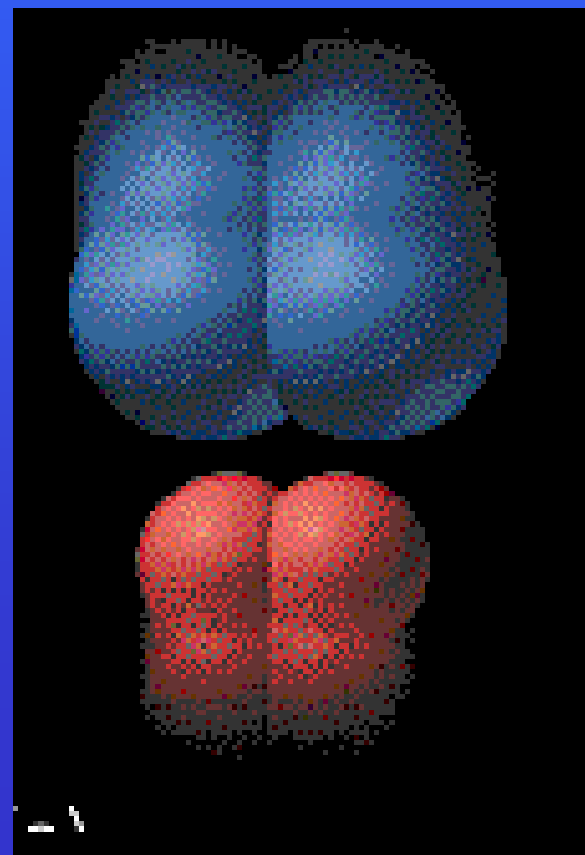
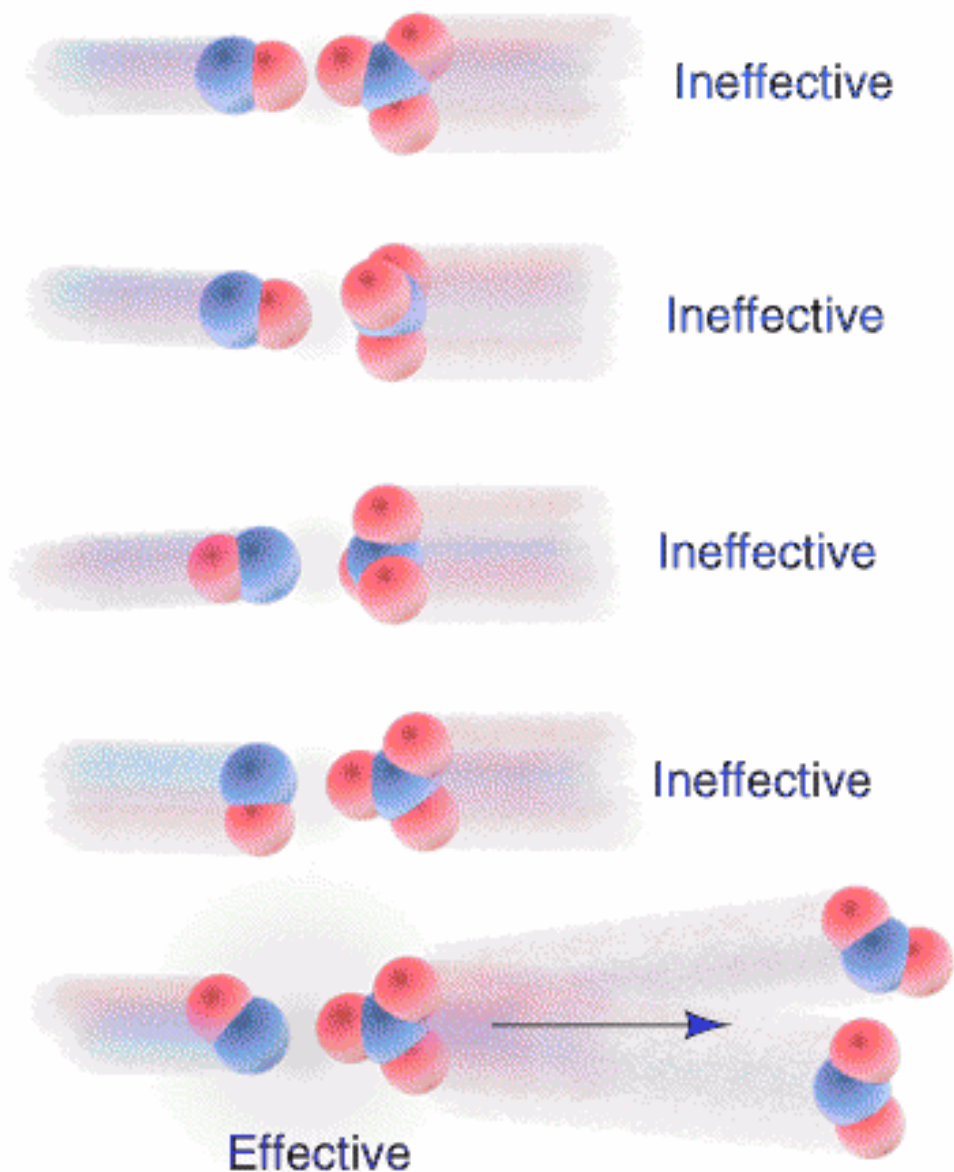
Effective collision:



Ineffective collision:

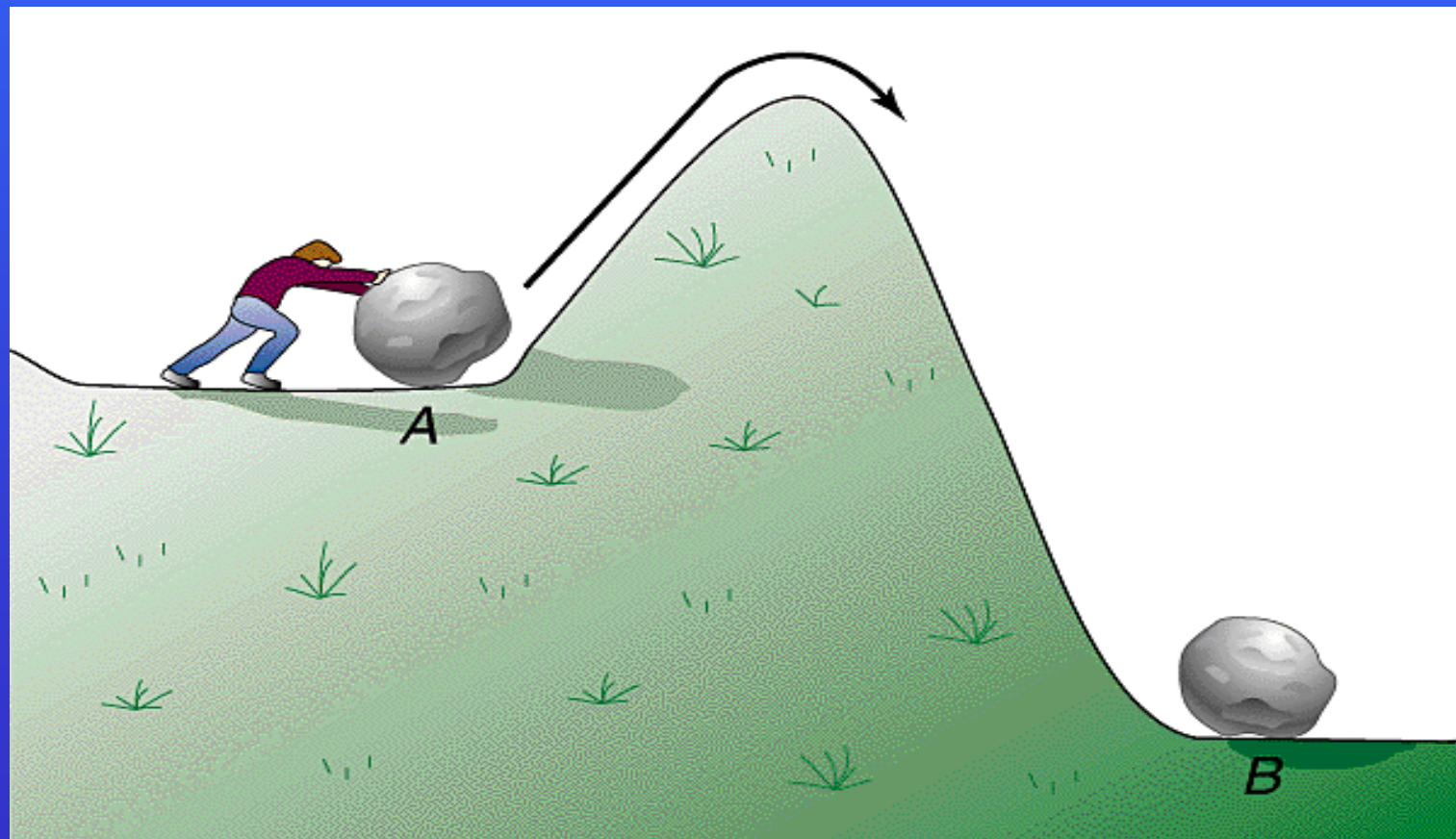


Most
collisions are
NOT
effective!

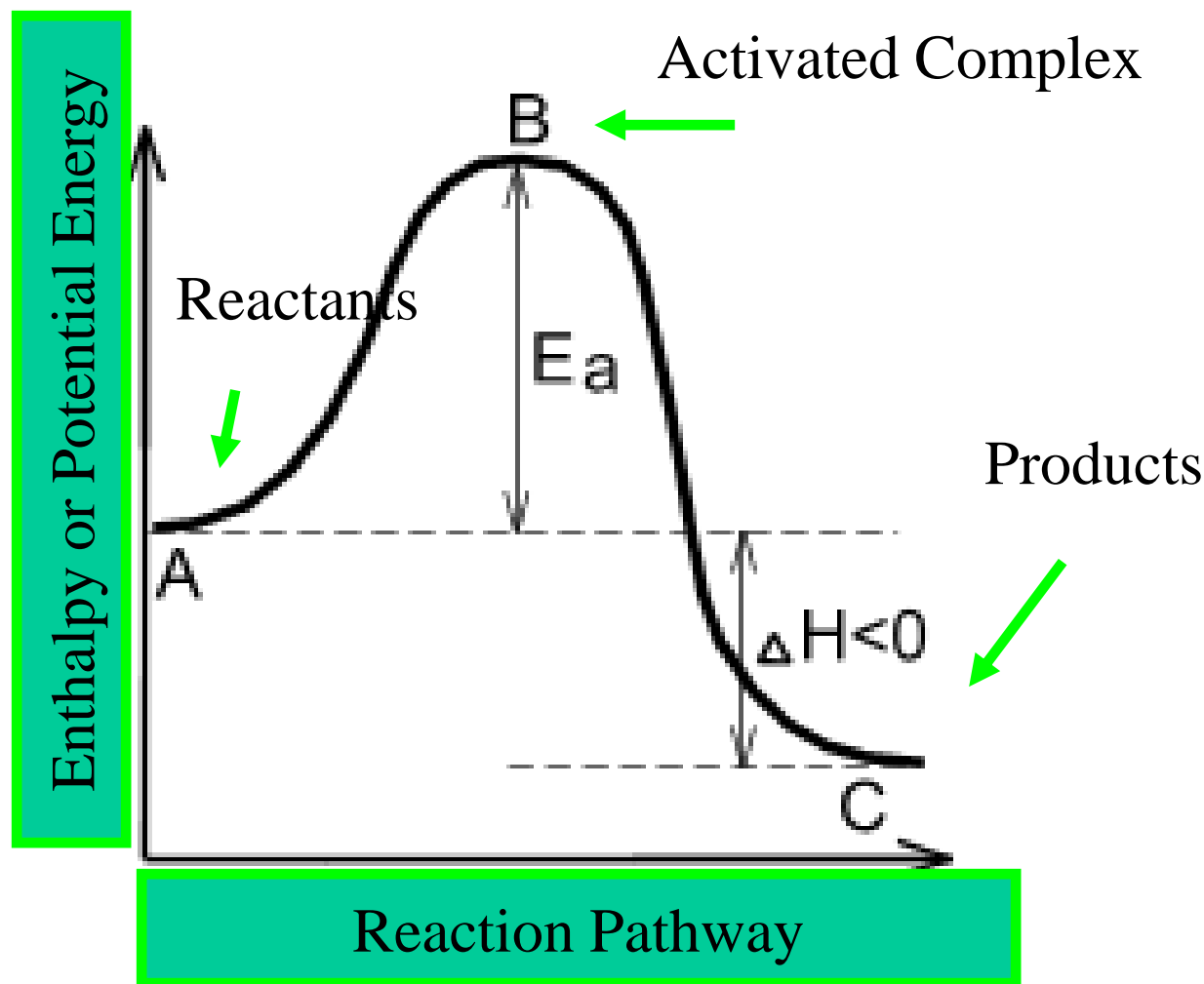


Activation Energy & Reaction

→ what do we understand under the term
“**Activation Energy**” in theory of collision?
-imagine that we have to come from place
“A” to place “B”

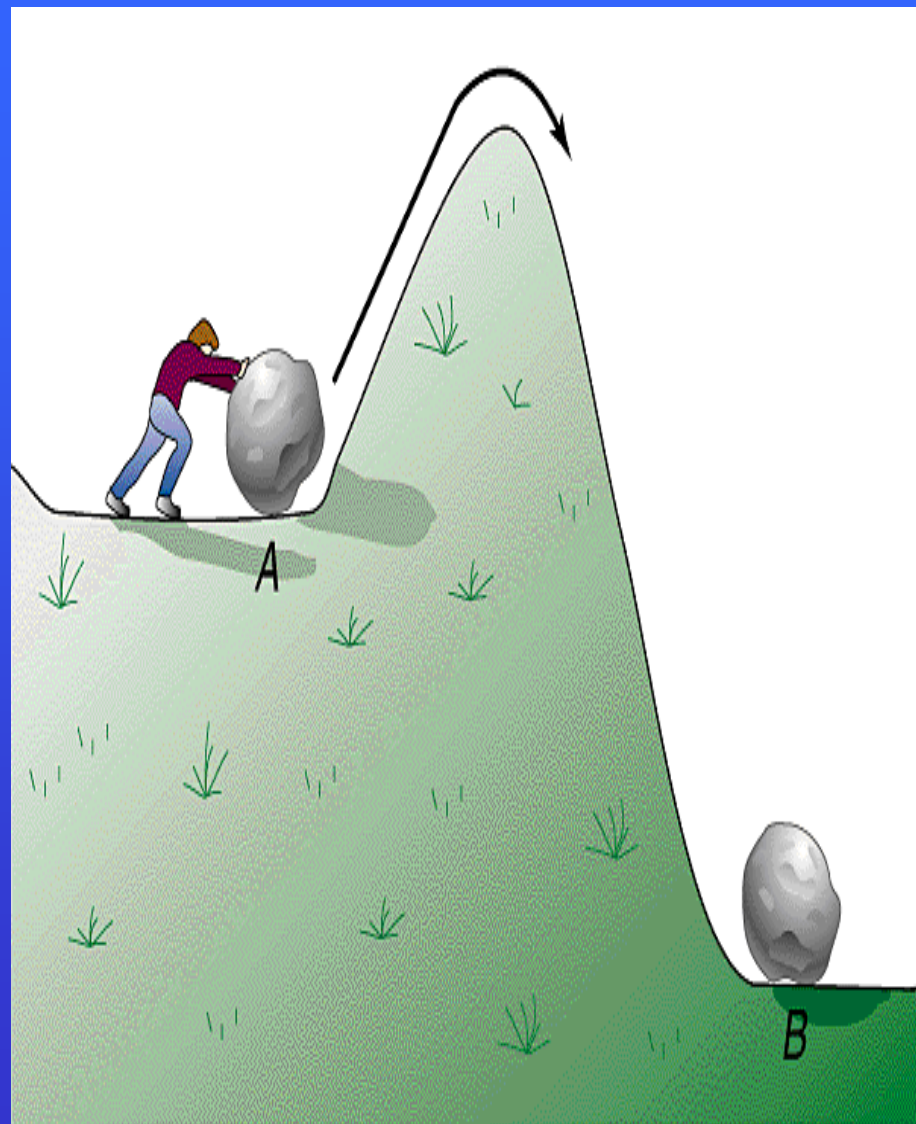


Energy Diagram of a Reaction



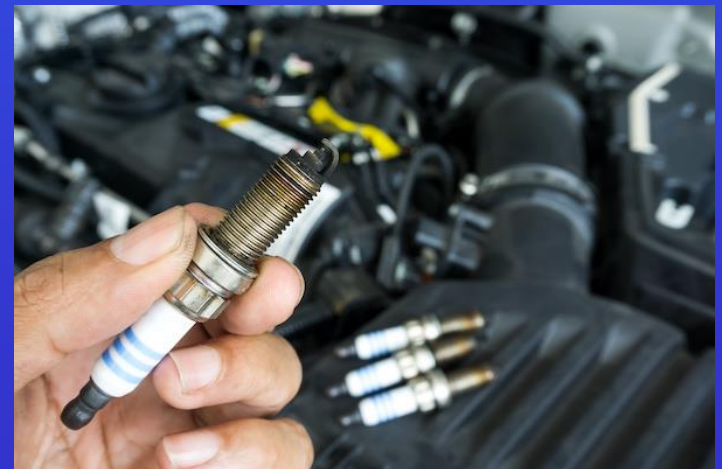
What is Activation Energy

- Energy needed to initiate the reaction.
- Energy needed to overcome the reaction barrier.
- The difference between the top of the hill & where you start.
- Difference between activated complex & reactants.



Activation Energy in everyday life

- Using a match to start a fire.
-
- The spark plug in a car engine.

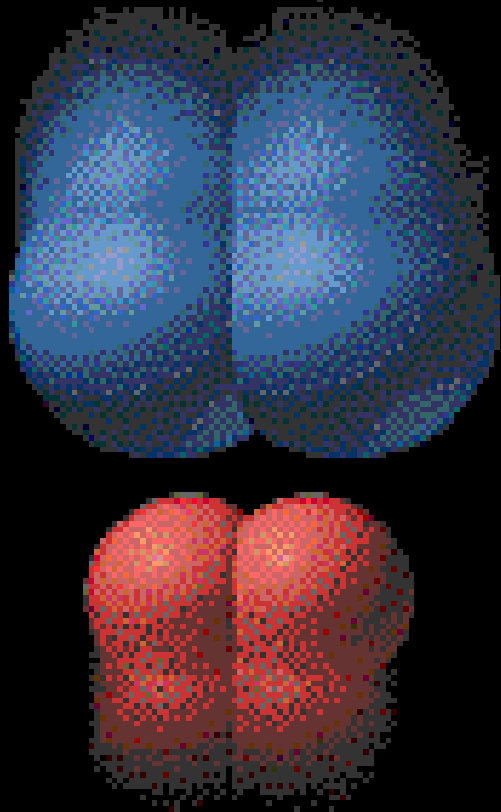


Why does the collision have to be energetic?

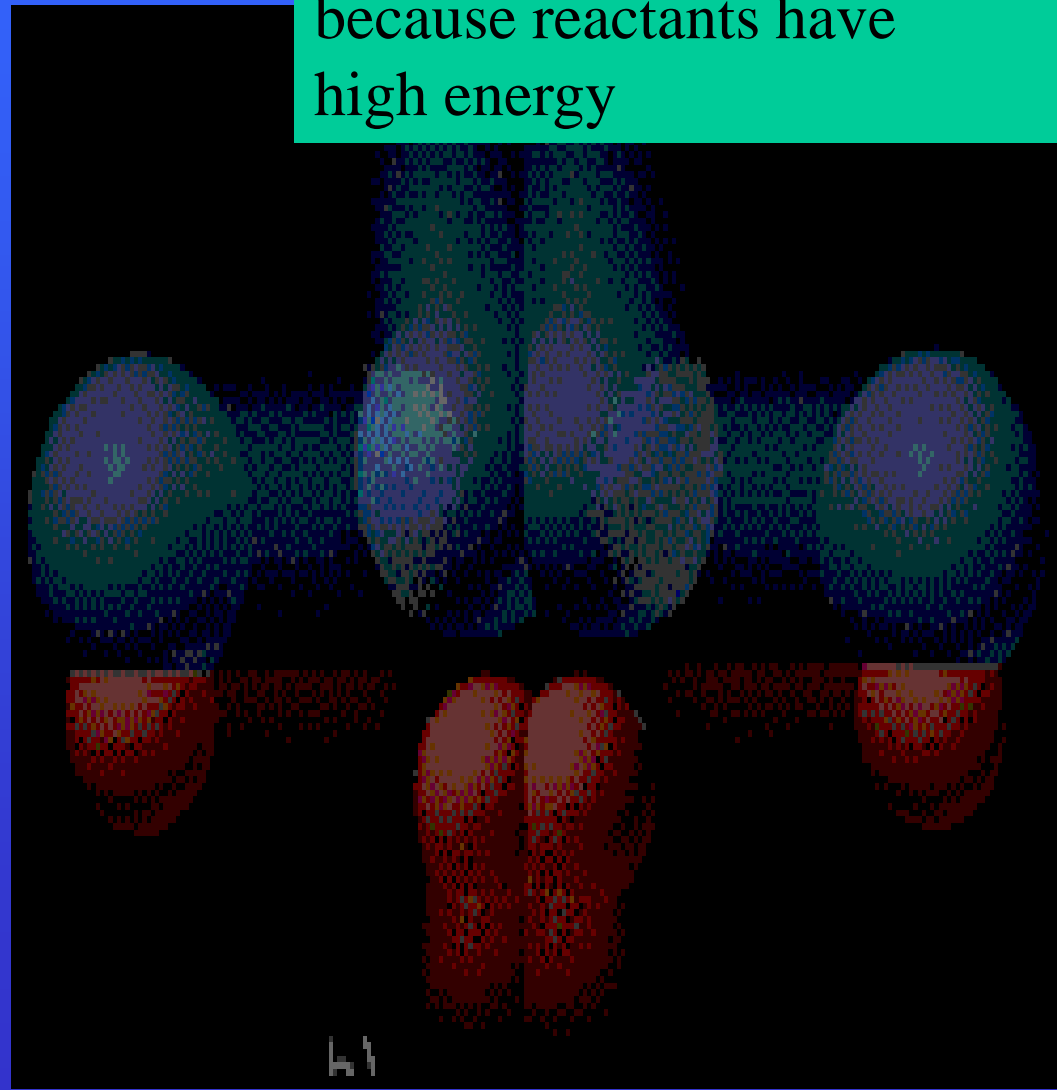
- The kinetic energy of the reactants is used to overcome the reaction barrier.
- The kinetic energy is transformed into potential energy.

Why Do Collisions Have to be “Highly Energetic” in order to have a chemical reaction?

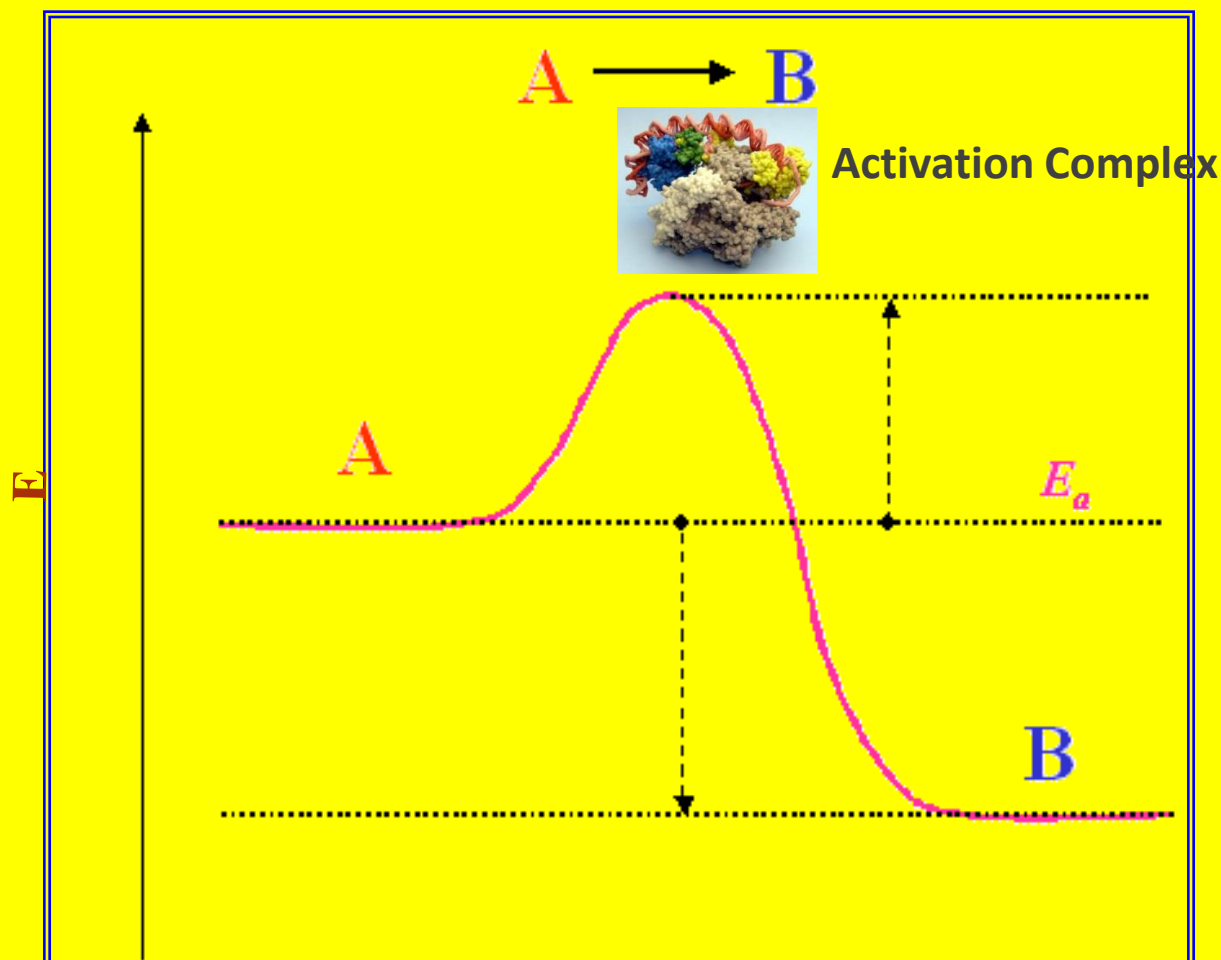
No chemical reaction
Because reactants have
Low energy



Chemical reaction takes place
because reactants have
high energy



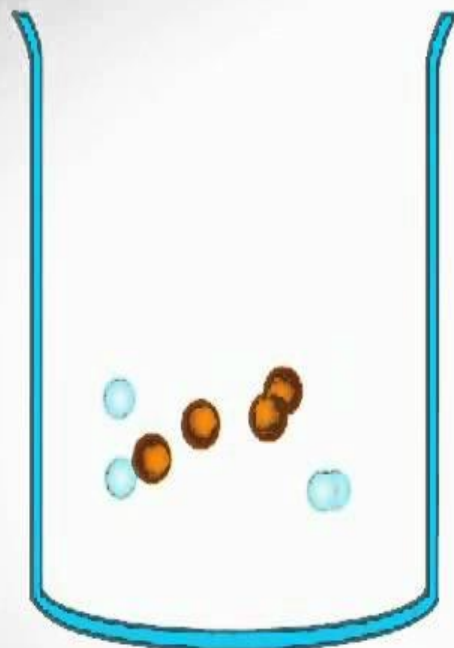
Activation Energy is an **ENERGETIC BARRIER** that **MUST BE OVERCOMED** via collisions between the reactants molecules in order to obtain **PRODUCTS** created via chemical reactions of the reactants



Factors that affect the rate of chemical reactions

- Nature of the reactants (ions vs. molecules)
- Temperature
- Concentration
- Pressure (for gases)
- Surface Area
- The presence of a catalyst

The Effect Of Concentration

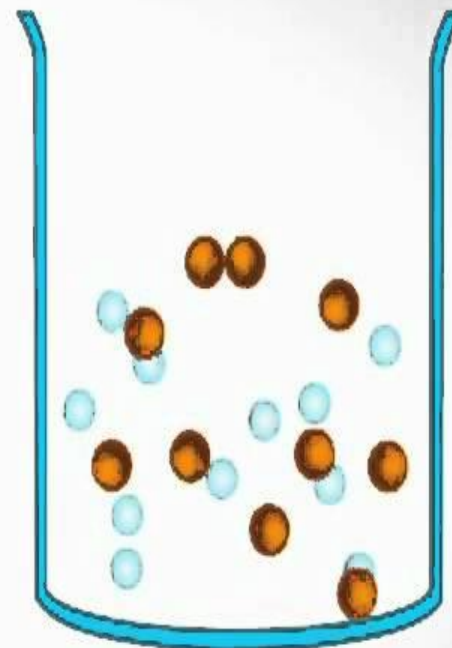


Condition A

Condition A has less :

- Concentration
- Frequency of Collision
- Frequency of Effective Collision
- Rate of Reaction

than Condition B



Condition B

● = Acid molecule ● = Water molecule

Nature of the reactants: Ions or Molecules?

- Ions in solution react quickly.
- Covalently bonded molecules react slowly.
It takes time to break all those bonds!
- 2 gas phase reactants tend to react more quickly than 2 liquids or 2 solids.

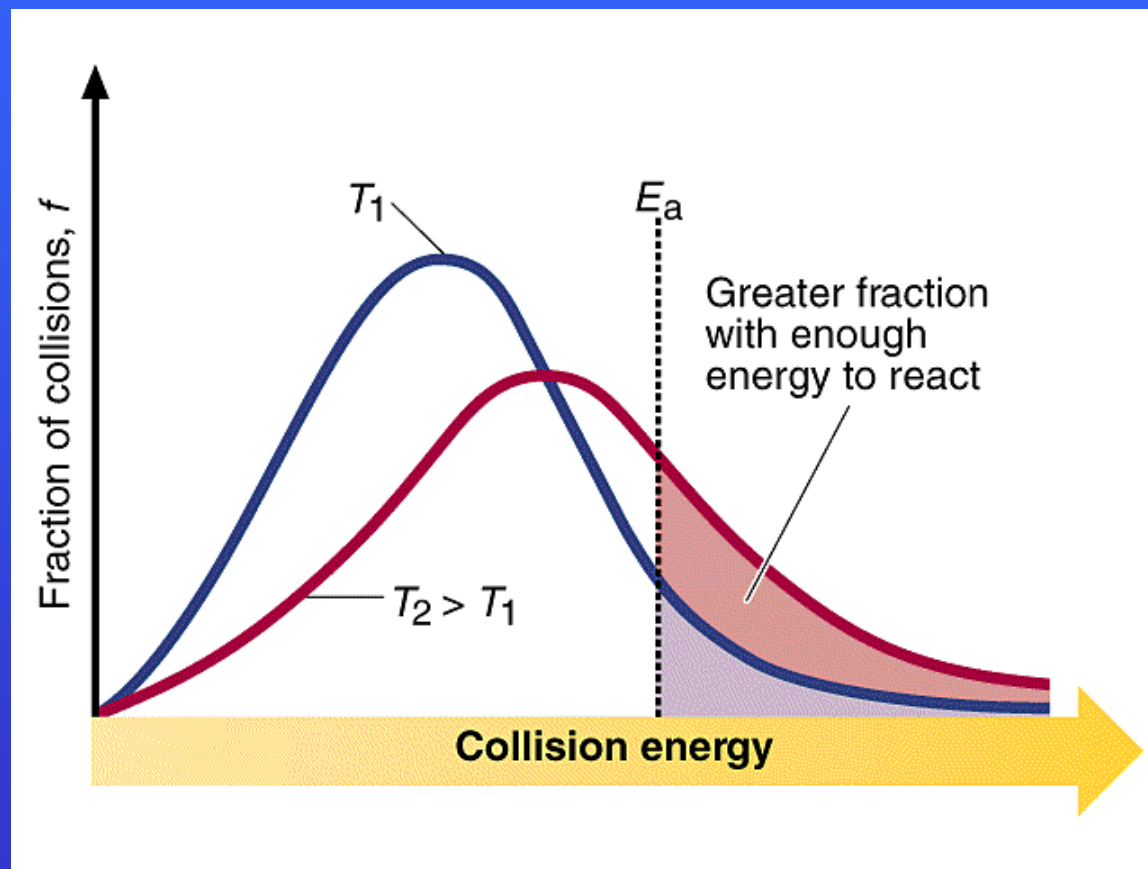
Temperature

- Rule of thumb:
- Increasing the temperature 10°C doubles the reaction rate.

Temperature

- A measure of the average kinetic energy of the molecules in a system.
- The faster they are moving, **the more often** they will collide.
- The faster they are moving, **the more energetic** the collisions.

Maxwell-Boltzmann Distribution



Increase in Temperature

- Increases the frequency of collisions between the reactants molecules
- Increases the percentage of collisions that lead to reaction.

Concentration

- **Increase in concentration** means more particles per unit volume – so **more collisions in a given amount of time.**

Pressure

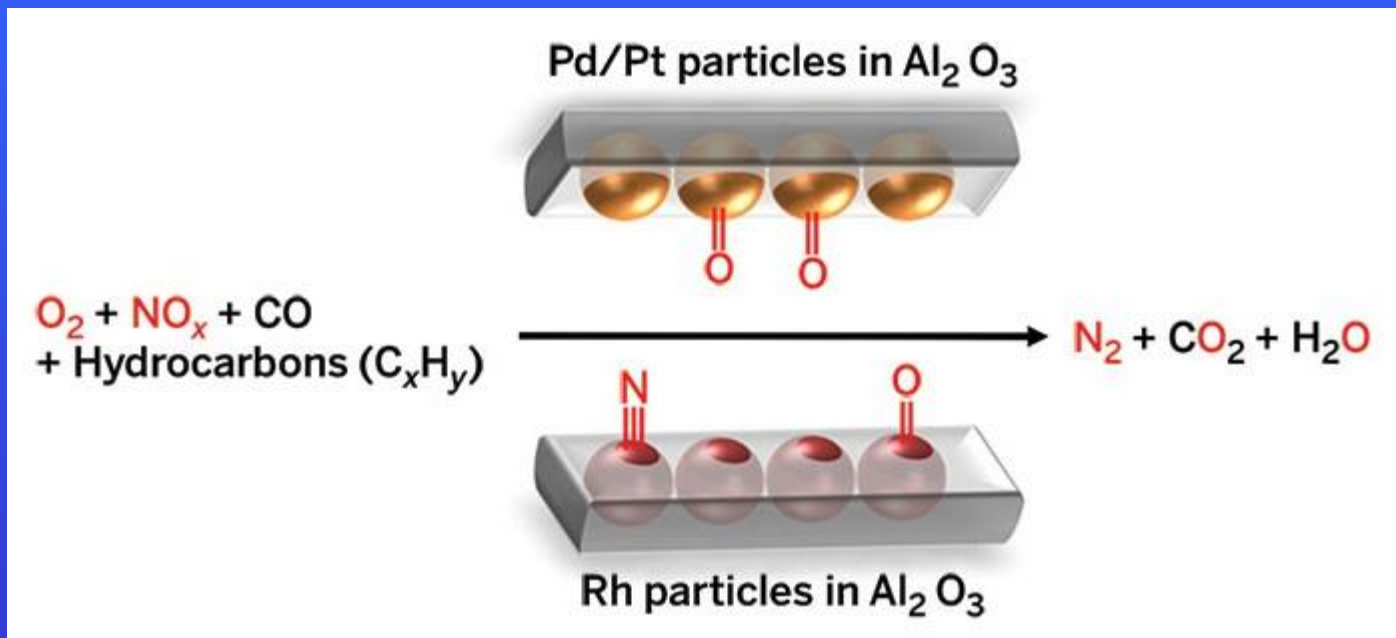
- For systems involving gases.
- Analogous to increasing concentration.
- \uparrow Pressure, \uparrow number of particles per unit volume.

Surface Area

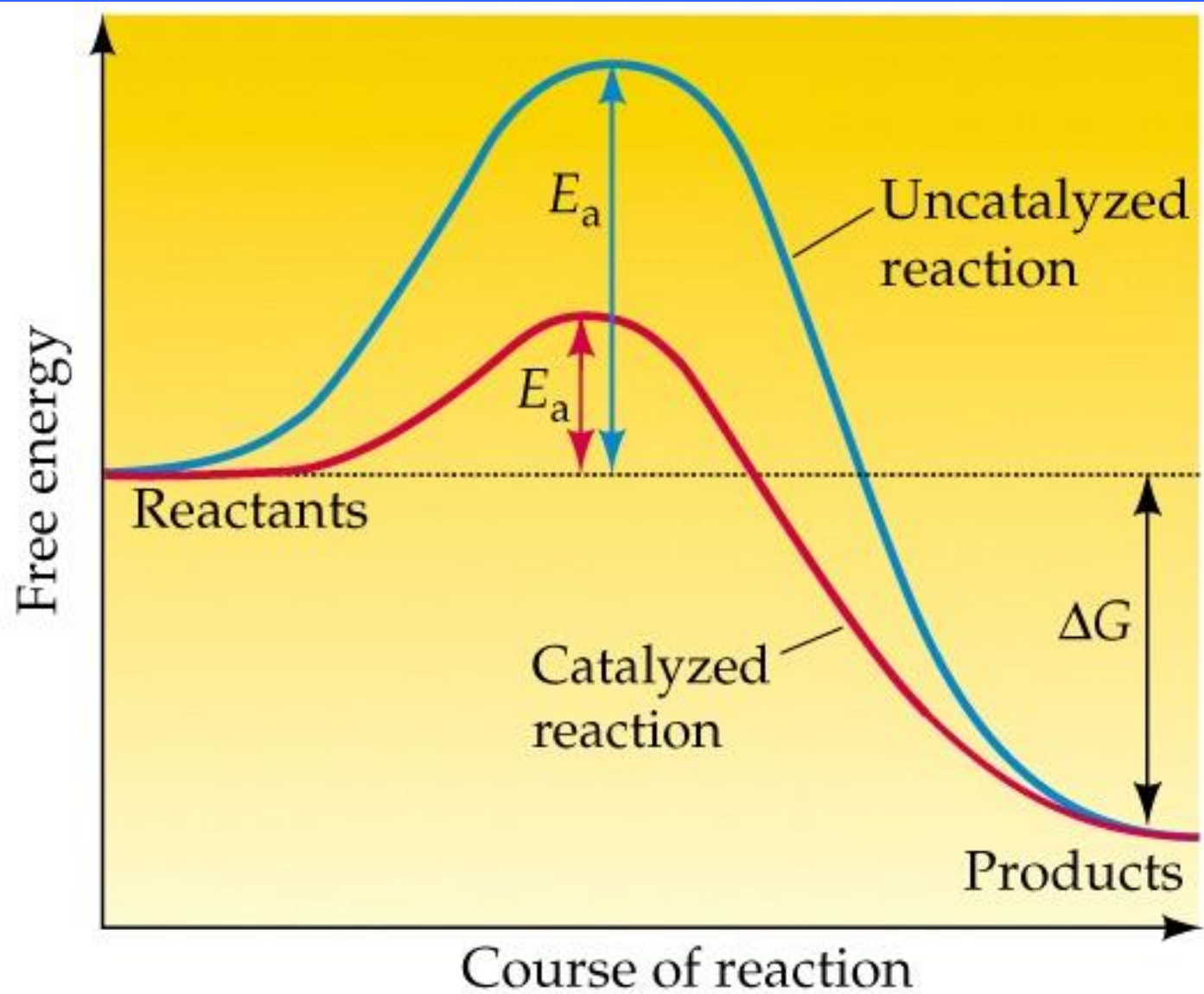
- Higher surface area – more particles exposed for reaction.
- Higher surface area means smaller particle size.
- (For heterogeneous reactions.)

Catalysts-are accelerators of the chemical reactions

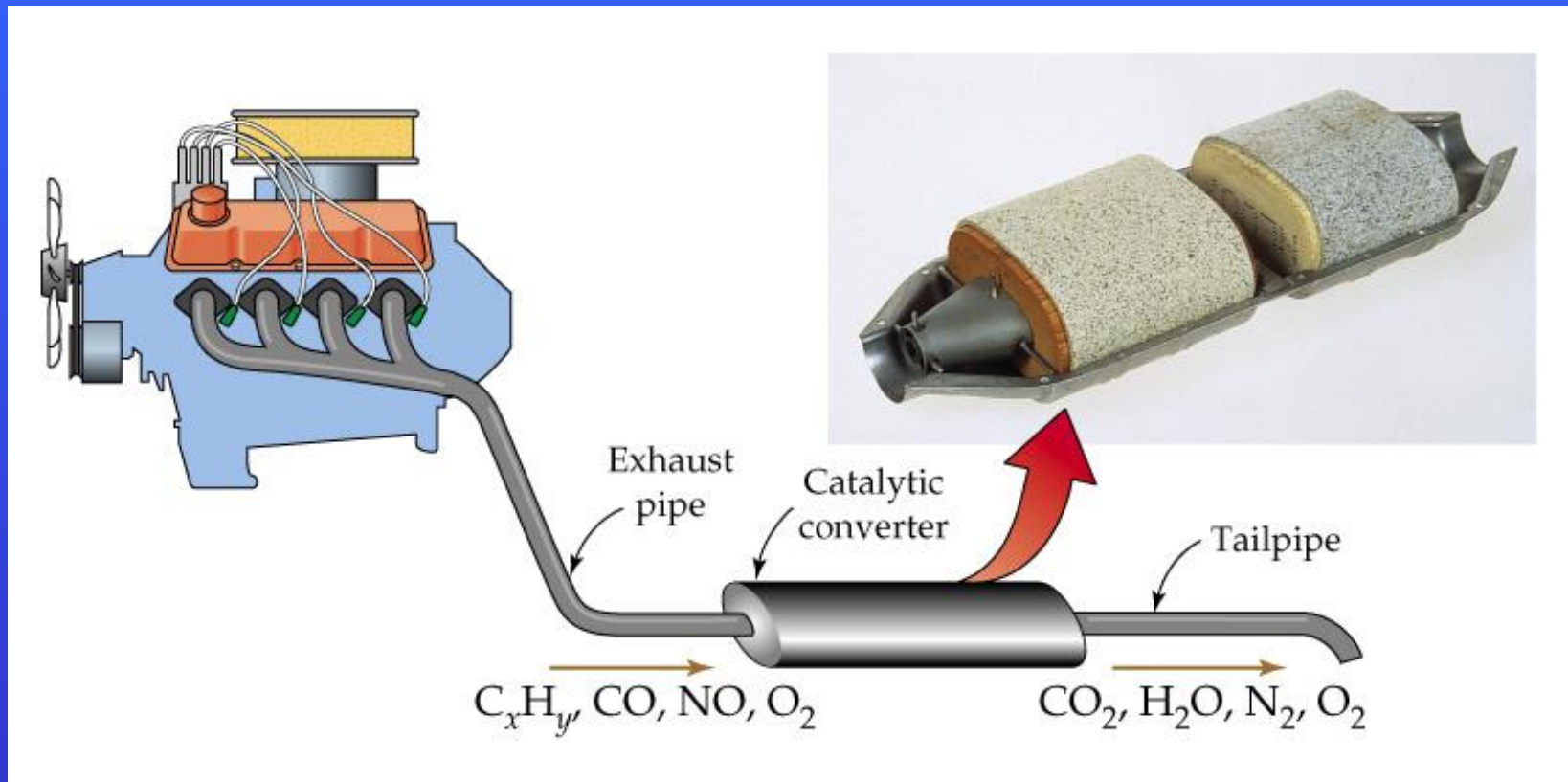
- Substance that increases the rate of reaction without itself being consumed.



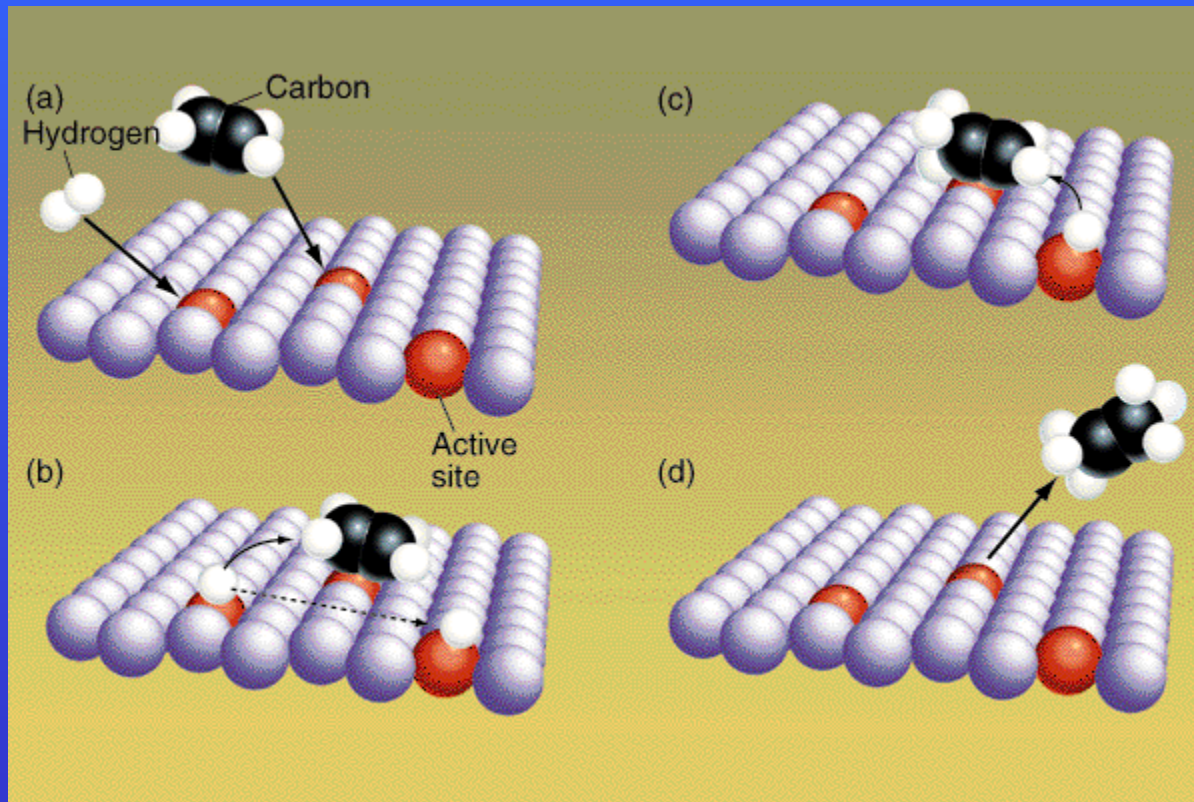
- Provides an alternate reaction pathway with a lower energy barrier.



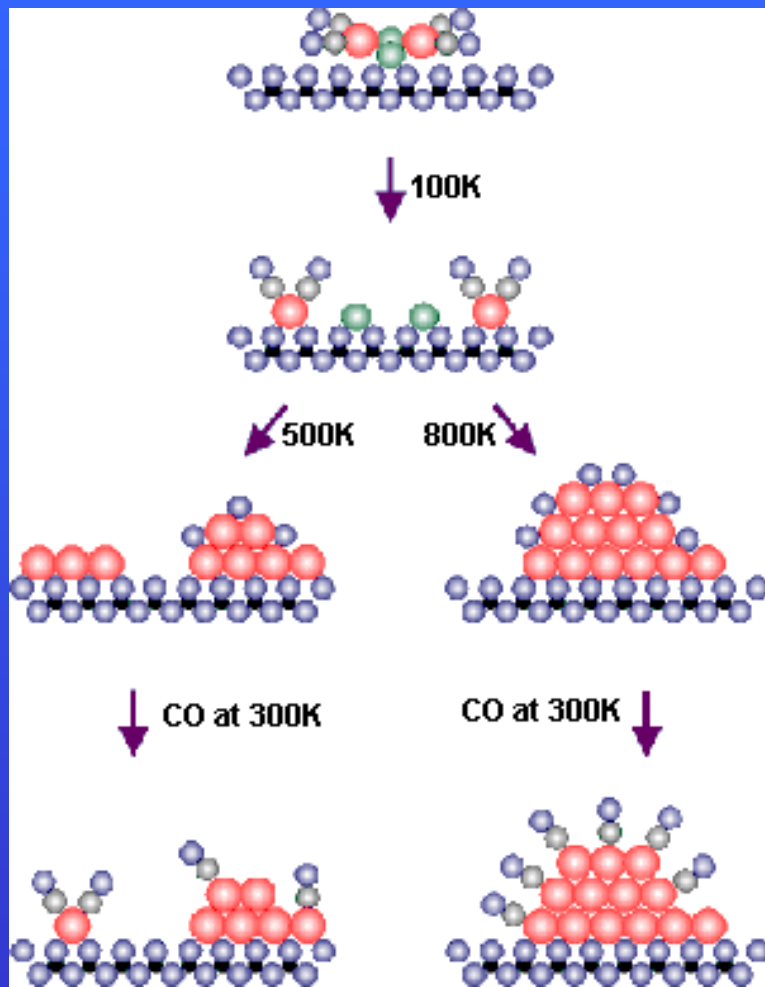
Catalytic Converter in Engines



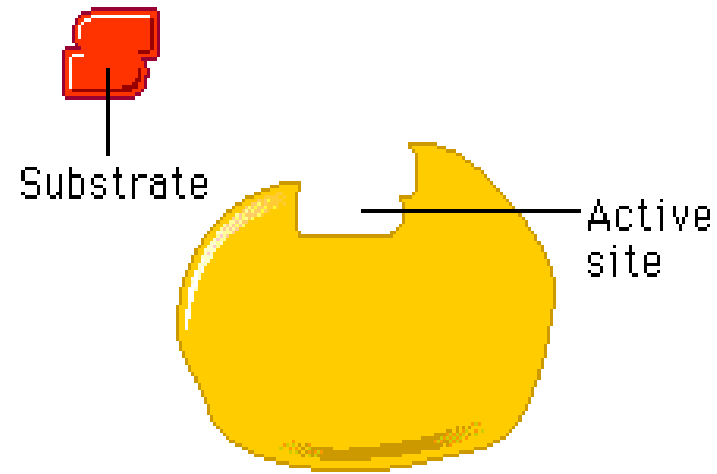
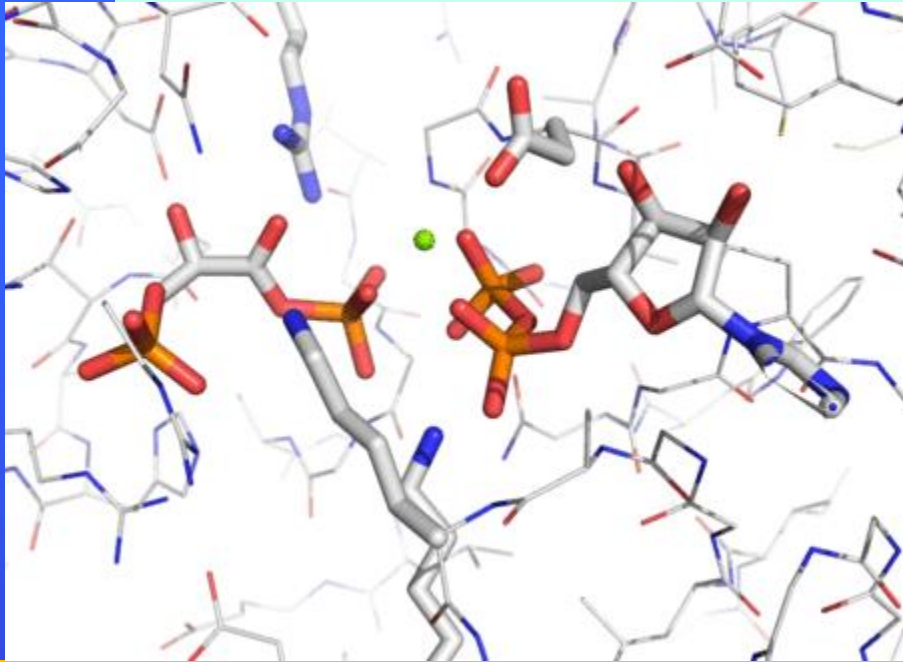
Hydrogenation & Surface Catalysis



Surface Science

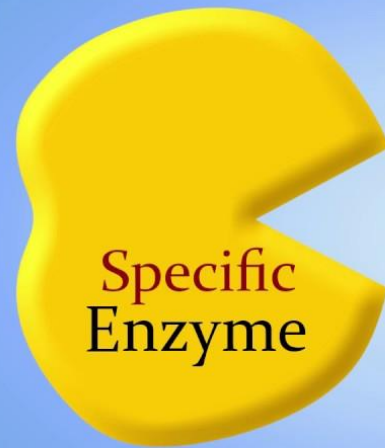


Enzymes are bio-catalysts!



Enzymes are **PROTEINS** that have so-called **ACTIVE SITE** in their Structure. In this active site, **ONLY** a given molecule named **SUBSTRATE** can be accommodated, and it can be transformed to final **PRODUCT**.

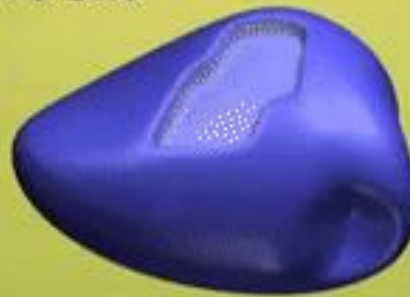
ENZYMES are SPECIFIC systems---it means in given enzyme **ONLY** Defined **MOLECULE** (substrate) can undergo chemical reaction
Example: Glucose-oxidase is specific enzyme for Glucose only!



Substrate



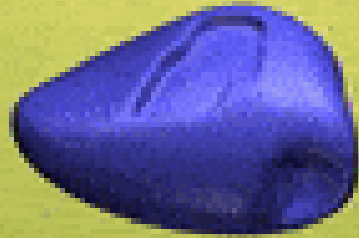
Active Site



Enzyme

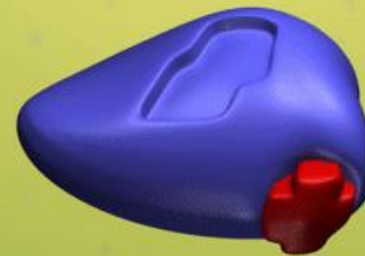


Competitive Blocker



Enzyme

Inhibition of the Enzymes
is a way in which
given enzyme
gets inactivated



Enzyme

Non-Competitive Blocker

Which conditions affect the activity of the enzymes?



All parameters that can affect the Active site of the enzyme will Affect its activity...these are

- pH
- Heavy metals
- Temperature

...



Optimal pH

REFERENCES

1. R Gulaboski, F Borges, CM Pereira, M Cordeiro, J Garrido, AF Silva, *Combinatorial Chemistry & High Throughput Screening* 10 (2007) 514-526
2. R Gulaboski, ES Ferreira, CM Pereira, MNDS Cordeiro, A Garau, Vito Lippolis, A Fernando Silva, *Journal of Physical Chemistry C* 112 (2008) 153-161
3. V. Mirceski, R. Gulaboski, *The Journal of Physical Chemistry B* 110 (2006) 2812-2820
4. M Janeva, P. Kokoskarova, V. Maksimova, R. Gulaboski, *Electroanalysis* 31 (2019) 2488-2506
5. R Gulaboski, V Mirčeski, S Mitrev, *Food Chemistry* 138 (2013) 116-121
6. P. Kokoskarova, R. Gulaboski, *Electroanalysis* 32 (2020) 333-344