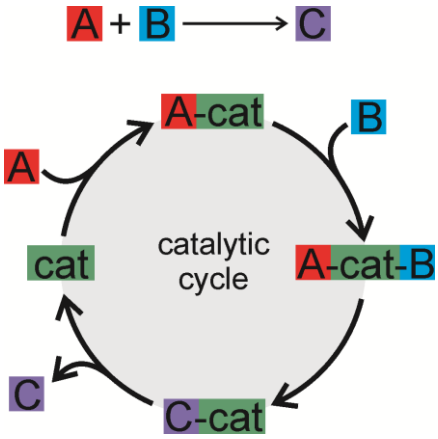
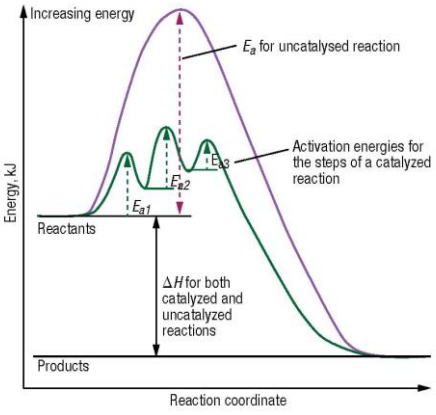
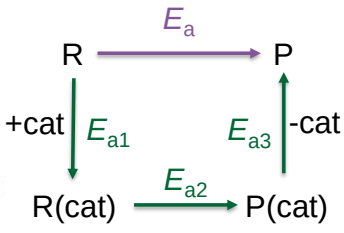
Catalysis



- What is catalysis?

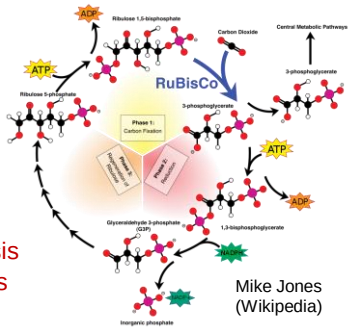




Catalysts
- speed up the rxn
- lower the rxn T
- do not get consumed

Catalysis in nature

- catalysts (enzymes) in most parts of the life cycle (forming, growing, decaying)
- catalysis contributes to the processes of converting sun energy to other forms of energy (e.g., photosynthesis)



Mike Jones (Wikipedia)

Chemical industry

- Catalysts - USD 34 billion in 2019
- 90% chemical industry involves catalysis (everything from fuels to drugs to paints to cosmetics)
- Catalysis reduces emissions of cars, secures fresh food, provides new farmaceuticals.

The Grand Challenge for the 21st century

→ to understand how to design catalyst structure to control catalytic activity and selectivity

Aims:

- to selectively activate a single bond in a multifunctional reactant to produce a desired product
- to achieve predictive capability do design catalyst that will provide ~100% selectivity for a desired product with minimal use of energy

Opportunities for Catalysis in the 21st Century (Basic energy sciences advisory committee subpanel workshop report 2002)

Research in catalysis

- Reaction kinetics and mechanism
  - reaction paths, intermediate formation and action, generalizing reaction types, predict catalyst performance..
- Catalyst development
  - catalyst design, material synthesis, structure properties, catalyst stability, compatibility
- Analysis techniques
  - detection methods, detection limits, extreme conditions (T, P, H^+), new spectroscopy, imaging, … techniques
- Reaction modelling
  - elementary reactions and rates, computational chemistry, physical chemistry
- Reactor modelling
  - mathematical representation and interpretation, reactor design, structure and efficiency of heat and mass transfer
- Catalytic process
  - heat and mass transfer, energy balance, efficiency of process

Opportunities for catalysis

- Efficient H_2 production
- Efficient CO_2 reduction
- Efficient ammonia production
- Decomposition of NO_x
- Depolymerization of plastic materials
- Production of new fuels and chemicals by selective oxidation of alkanes, methane in particular
- Synthesis of enantiomerically pure drugs
- Etc.

Learning objectives

- Understand principles of catalysis
- Understand basic approaches and mechanisms in homogeneous catalysis
- Understand principles of heterogeneous catalysis and basic reaction mechanisms
- Basic knowledge of photocatalysis and electrocatalysis
- Applications of catalysis in green chemistry

Do the quiz and see you in the class!