Inorganic Molecules, Materials & Medicines

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Lecture: 1

The topics will be covered in the second half

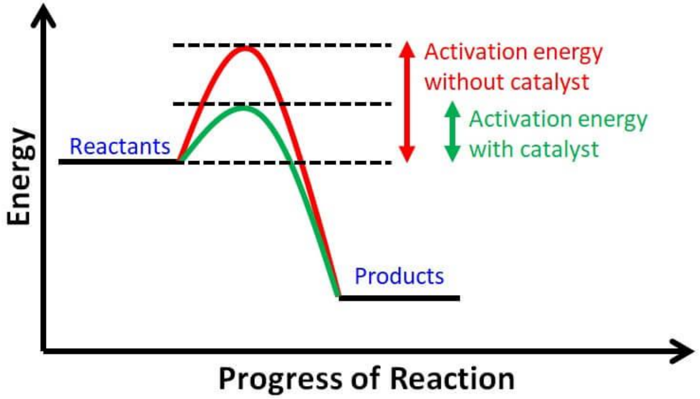
Module IV: Catalysis and sustainability

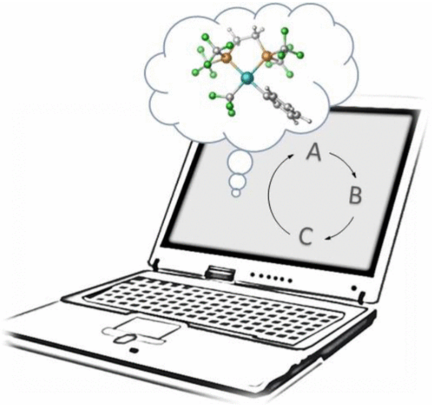
Module V: Electrochemistry and its applications

Module VI: Supramolecular chemistry

Module VII: Graphene and carbon nanotubes

How does a catalyst work?



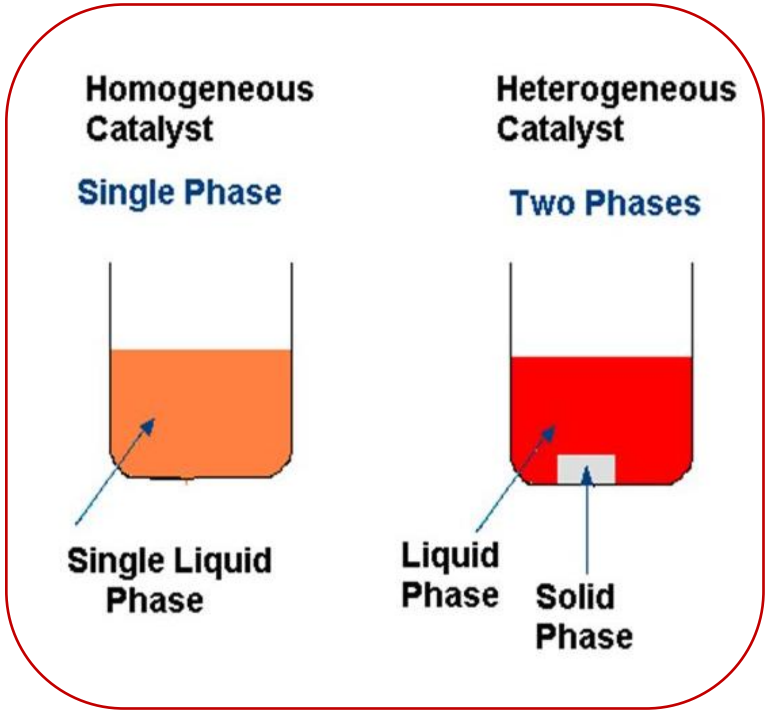


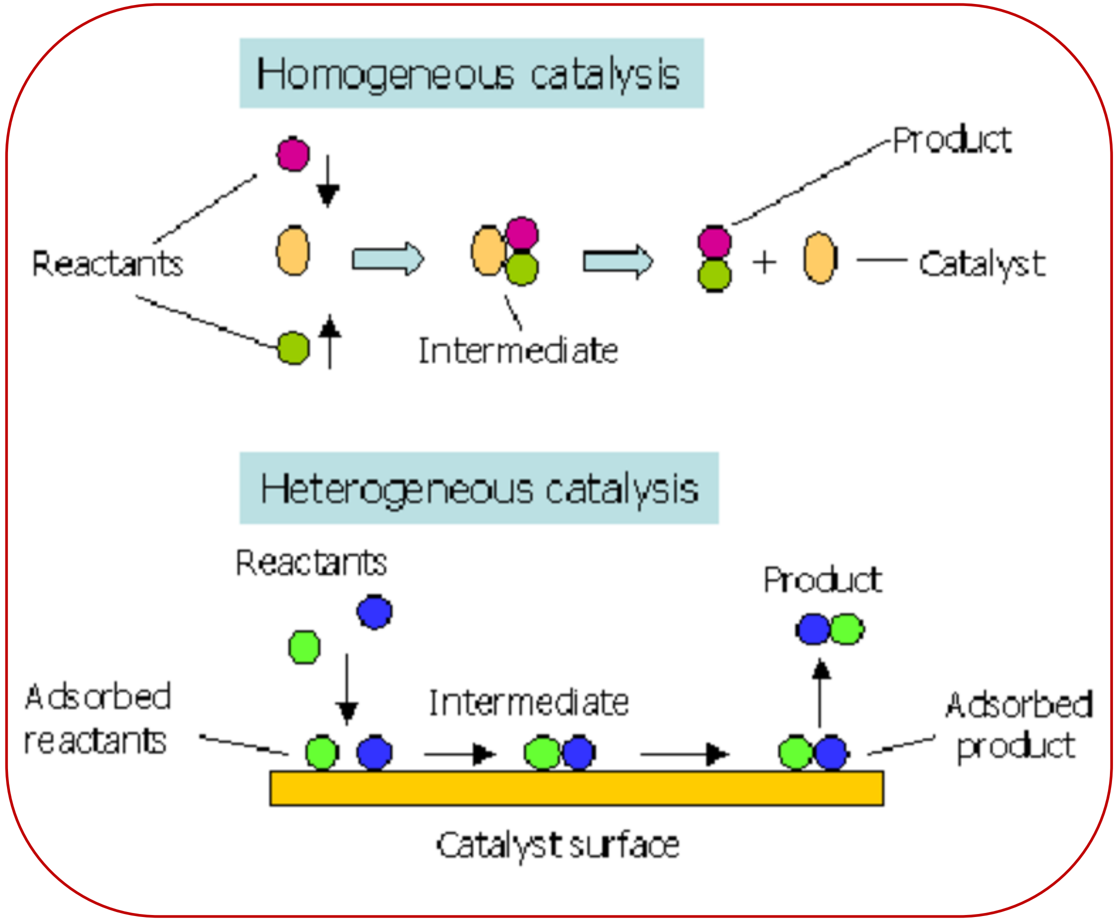
A catalyst lowers the activation energy, Ea, thus enhancing the rate of a chemical reaction.

A catalyst does not get consumed in the chemical reaction. Its chemical composition and mass remain unchanged.

A catalyst provides an alternative reaction pathway with a lower activation energy (Ea).
Ea: It is the minimum energy required for a chemical reaction to occur. At the cost of Ea, the reactant molecules are converted into products.

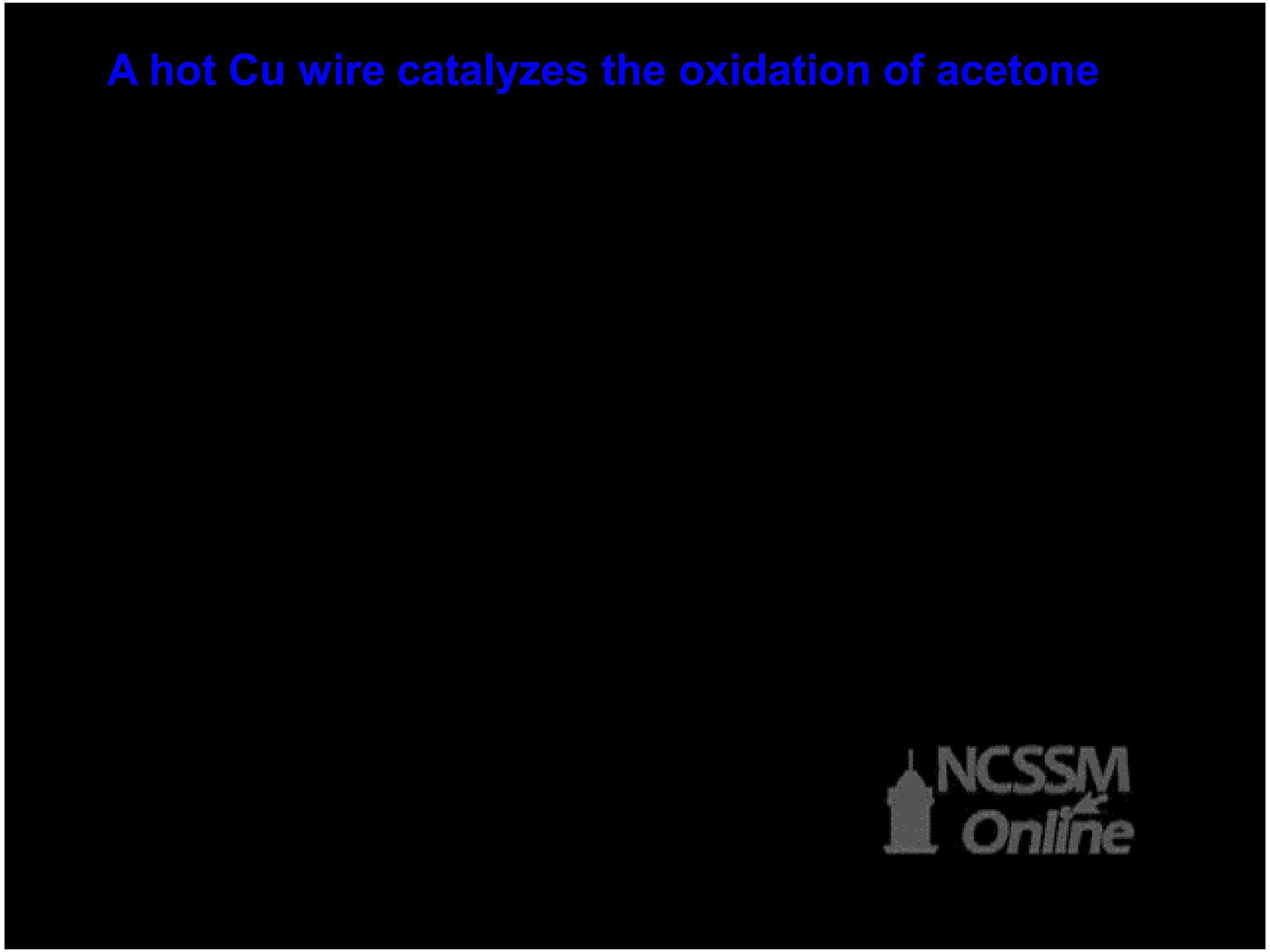
Homogeneous Vs. Heterogeneous Catalysis





- **Homogeneous catalysis: Catalyst and reactants are in the same phase.**
- **Heterogeneous catalysis: Catalyst and reactants are in the different phase (the catalyst is usually insoluble; reaction occurs on its surface).**

Heterogeneous Catalysis



Heterogeneous Catalysis

Examples of industrial catalysts (metals, metal oxides, zeolites)

Terminologies in Catalysis : TON and TOF

- **Each time the complete catalytic cycle occurs, we consider one catalytic turnover (one mole of product formed per mole of catalyst) to have been completed.**

- **TON: The lifetime of the catalyst before its deactivation is measured in terms of turnover number (TON).**

- **TOF: The catalytic rate can be conveniently given in terms of the Turnover Frequency (TOF) measured in turnovers per unit time.**

- **How many cycles can a catalyst perform → TON**

Example: If **0.1 mole** of catalyst converts **100 moles** of substrates in **5 minutes** (**100% yield**) then

TON = 100/0.1 = 1,000 (unitless)

TOF = TON/time = 1000/5 min = 200 min^{-1}

Why are the catalysts so important?

- Apart from speeding up a chemical reaction, they are more energy-efficient.
- They can also reduce unwanted byproducts through a process called 'selectivity'.
- This allows us to produce new compounds/materials with fewer negative side effects or no harmful effects on the environment.
- We can produce environmentally friendly fuel sources, fertilizers, and even biodegradable plastics.
- Catalysts have profoundly changed modern life and driven evolutionary advances in industrial applications.

Why are the catalysts important for living organisms?

- Do you know that the human body also runs on catalysts?
- Yes, these are proteins, known as ‘enzymes’ (biocatalysts, considered as a third category), which are responsible for helping you move, digest your food, and produce energy. To say that catalysts are the ‘holy grail’.

- Using catalysts for many chemical reactions can help make things greener – they’re also better for living organisms.

- The main reasons for using a catalyst: (i) it makes a faster chemical reaction by lowering Ea, (ii) it reduces the harmful and potentially toxic by-products produced by the uncatalyzed reaction, (iii) it improves yield, (iv) it enhances efficiency (for industrial processes), (v) it is cost effective, (vi) less time-consuming.

Haber-Bosch process for NH3 preparation

Nobel Prize in Catalysis

Fritz Haber (1918) & Carl Bosch (1931, Chemistry)


Fritz Jakob Haber, a German chemist

For the Haber–Bosch process, which uses an Fe-based heterogeneous catalyst to synthesize ammonia from N_2 and H_2.


Carl Bosch was a German chemist and engineer

Carl Bosch: His work enabled the mass production of ammonia

The process converts atmospheric dinitrogen (N_2) to ammonia (NH_3) by a reaction with dihydrogen (H_2) from natural gas (methane) using finely divided iron metal as a catalyst

Haber-Bosch process for NH3 preparation

The Haber-Bosch Heritage:
The Ammonia Production Technology

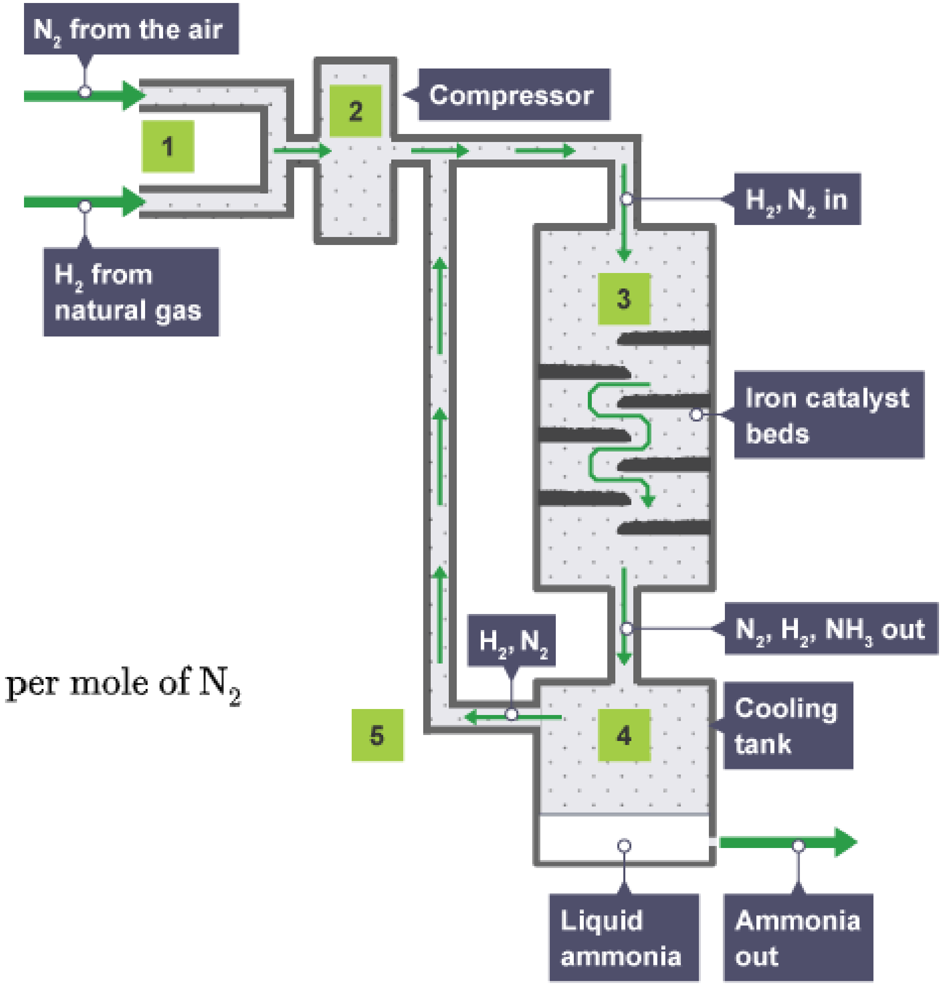

Haber


Bosch


Mittasch

Based on the fundamental research work of Fritz Haber, Carl Bosch and his engineering team developed industrial-scale ammonia (NH_3) synthesis using an iron-based catalyst found by Alwin Mittasch and his co-worker.

Haber-Bosch process for NH3 preparation

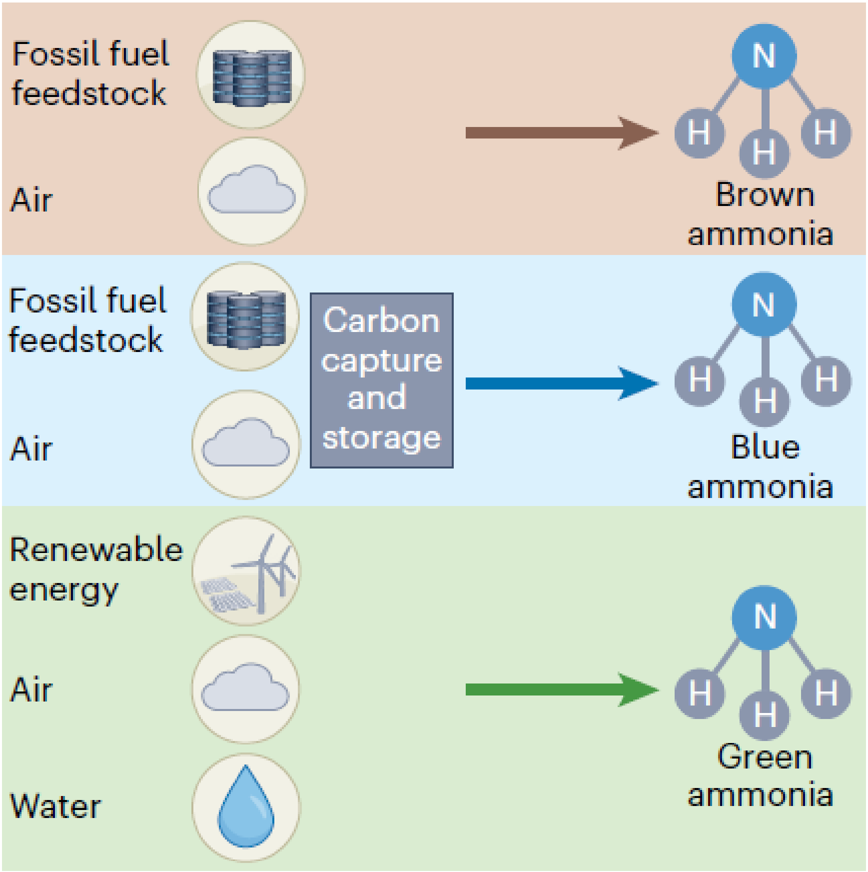


$$N_2 + 3\,H_2 \rightleftharpoons 2\,NH_3 \qquad \Delta H^\circ_{298\ \mathrm{K}} = -92.28\ \mathrm{kJ\ per\ mole\ of\ } N_2$$

Each year, around 170 million metric tons of ammonia are produced globally, with approximately 80% used in fertilizers.

Green ammonia synthesis

The Haber–Bosch process for synthesizing ammonia has enabled a significant increase in food production over the past century. Haber–Bosch process consumes 1–2% of the total global energy production, 3–5% of the world's natural gas production, and produces 1–3% of our CO_2 emissions.



In 1908, Fritz Haber combined nitrogen from the air with hydrogen from natural gas, over a metal catalyst at high pressure and temperature, to produce (brown) ammonia

The Haber–Bosch process has been modified to make ammonia synthesis cleaner. The inclusion of a carbon capture unit negates emissions from the conventional Haber–Bosch process, producing blue rather than brown ammonia

The use of hydrogen from water electrolysis rather than methane, in combination with the use of renewable energy, produces green ammonia.