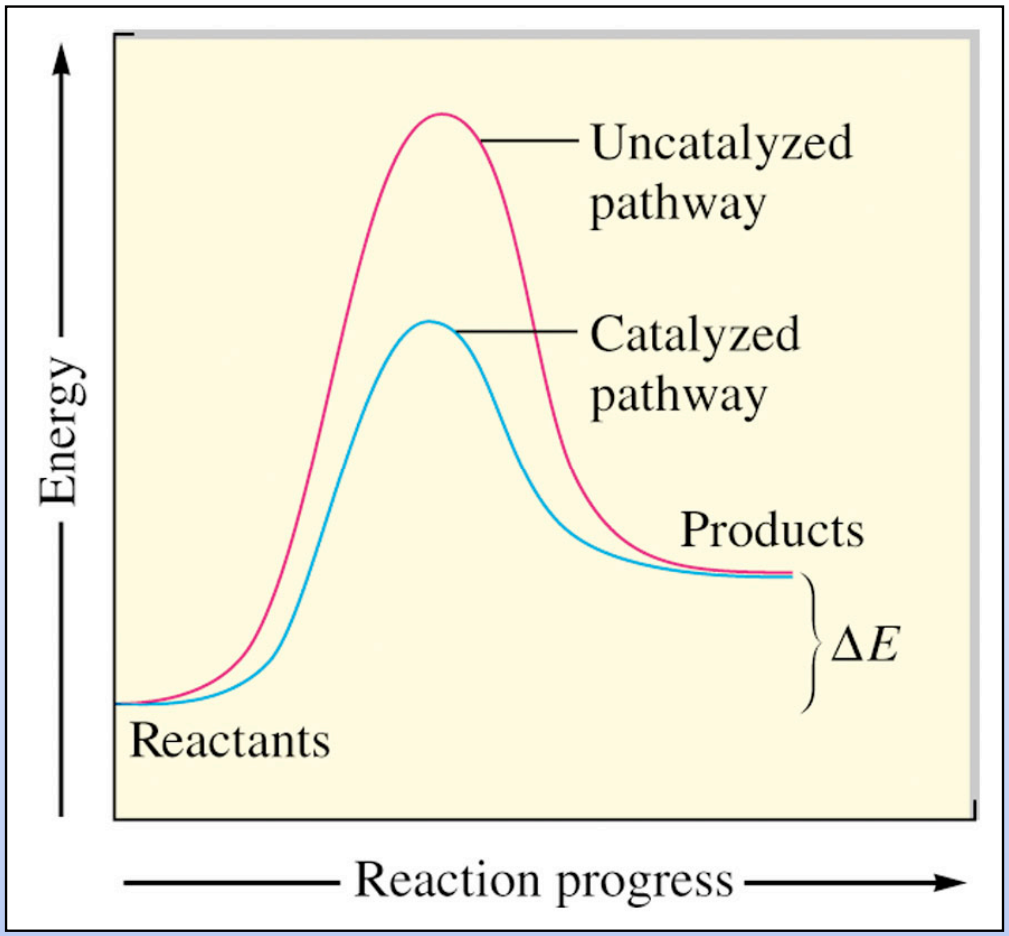
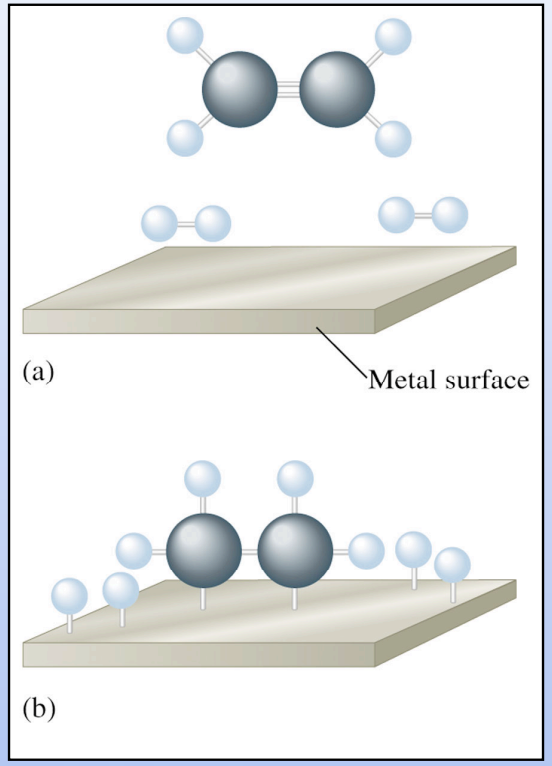
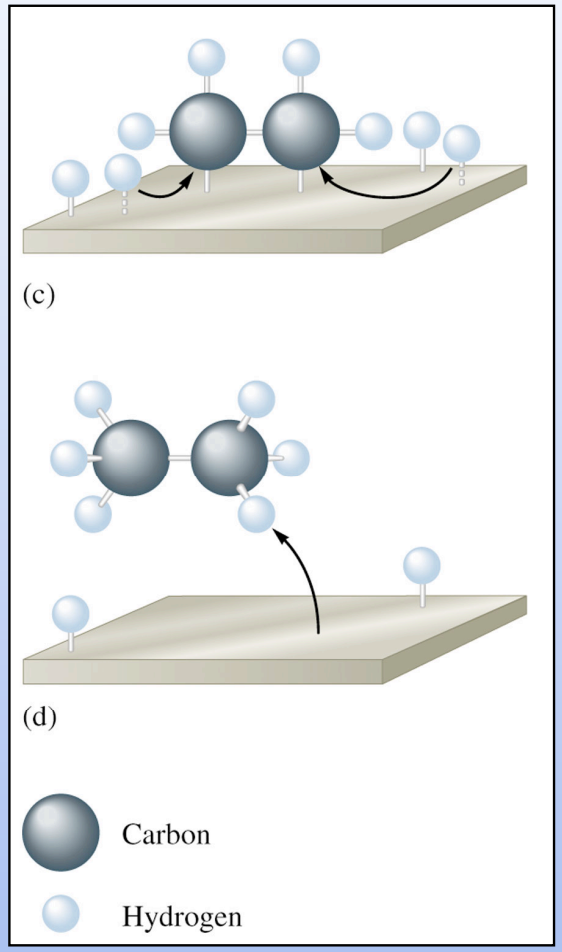
Today

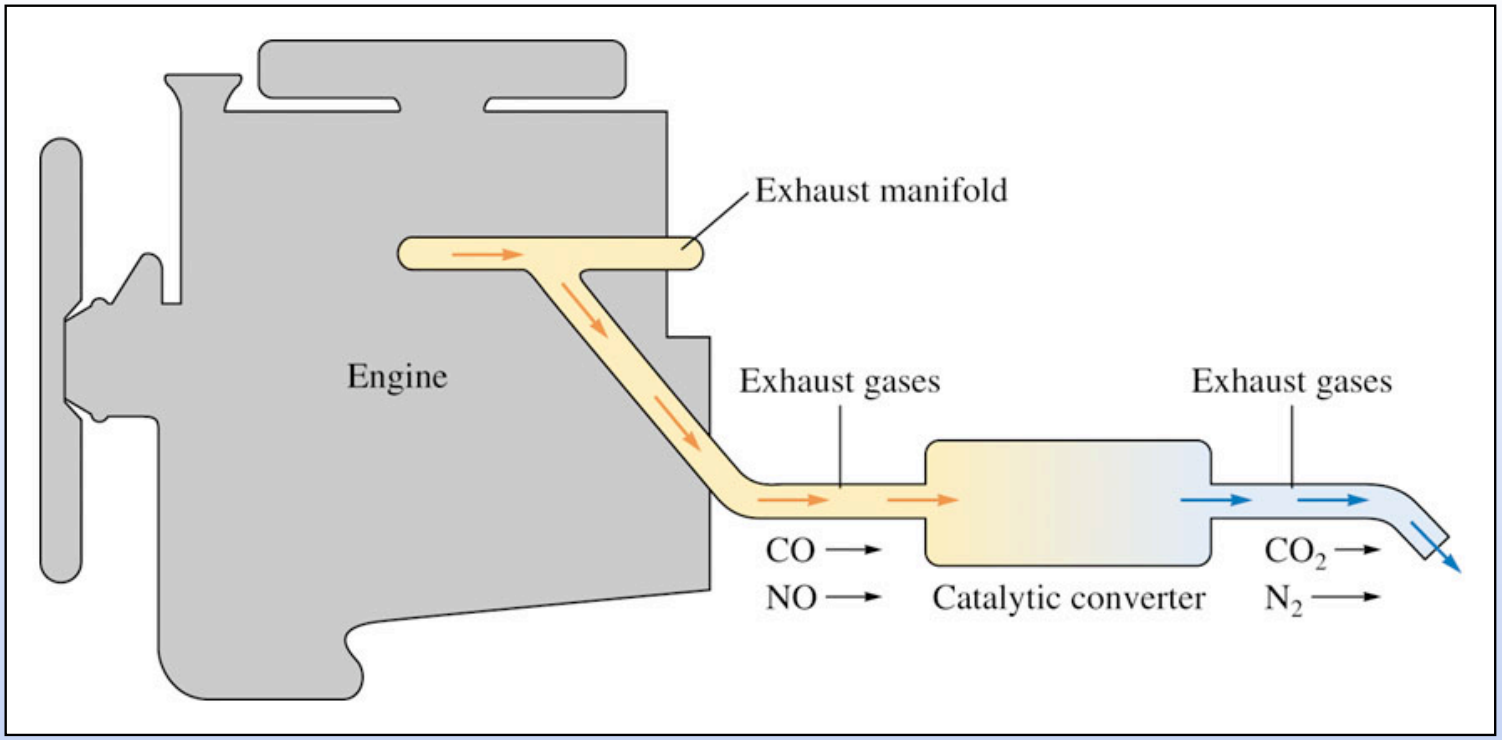
Catalysis




quick note on transition state theory. Once you get to the transition state you are equally likely to go either direction (to reactants or products)






Catalyzes three chemical reactions

$$2NO_x \longrightarrow xO_2 + N_2$$

$$2CO + O_2 \longrightarrow 2CO_2$$

$$2C_xH_y + (2x+y/2)O_2 \longrightarrow 2xCO_2 + yH_2O$$

Smog  smoke + $SO_2$ + water

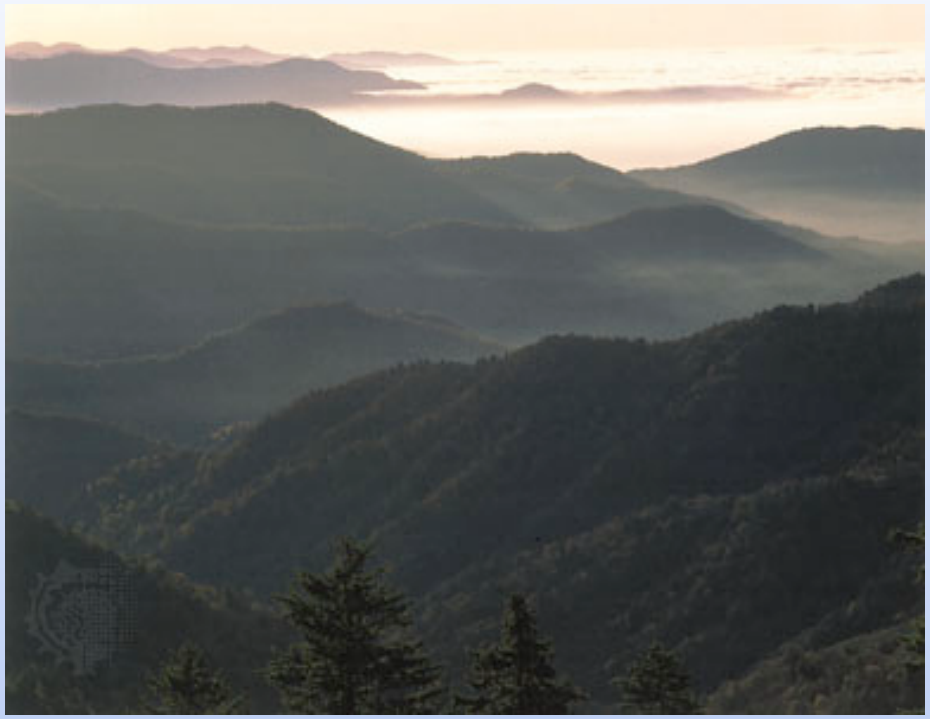
Sun + $NO_x$ + VOC =
photochemical smog

Volatile Organic Compound
(uncombusted fuel for example)

$$OH + CO \rightarrow H + CO_2$$
$$H + O_2 \rightarrow HO_2$$

$$HO_2 + NO \rightarrow OH + NO_2$$
$$NO_2 + hv \rightarrow NO + O$$
$$O + O_2 \rightarrow O_3$$

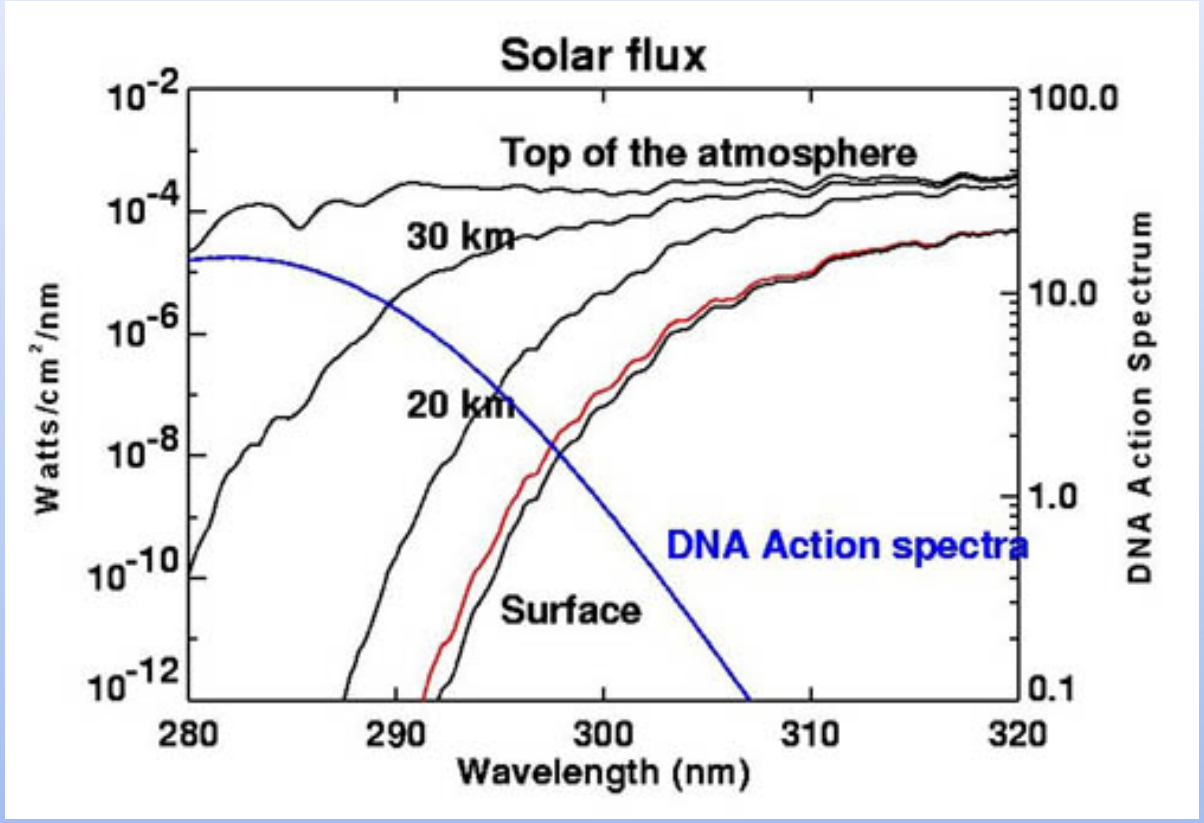
# Great Smoky Mountains



VOC released from the trees lead to a sort of "natural smog"
Greatly enhance by adding $NO_x$

# Ozone $O_3$

Great in the upper atmosphere



Ozone $O_3$

Bad down here

$O_3$ is a great oxidizing agent

$O_3$ + lungs = reacted lung tissue

| AQI | Air Quality | Color |
|---|---|---|
| 0 - 50 | Good | |
| 51 - 100 | Moderate | |
| 101 - 150 | Unhealthy for sensitive groups | |
| 151 - 200 | Unhealthy | |
| 201 - 300 | Very Unhealthy | |
| 301 + | Hazardous | |

April | 10 | 2008 | Select a Different Date

| Metropolitan Area | Ozone Forecast* for April 10, 2008 | April 10, 2008 as of 8:10 am CDT | | |
|---|---|---|---|---|
| | | Peak Ozone Concentrations | | Ozone AQI Rating |
| | | One-Hour | Eight-Hour | |
| Houston-Galveston-Brazoria [1] | No | 22 ppb | †† | ** |
| Beaumont-Port Arthur | Season Begins 05/01/2008 | 23 ppb | †† | ** |
| Dallas-Fort Worth | Season Begins 05/01/2008 | 51 ppb | †† | ** |
| Tyler-Longview-Marshall | Season Begins 05/01/2008 | 40 ppb | †† | ** |
| Austin | No | 47 ppb | †† | ** |
| San Antonio | No | 37 ppb | †† | ** |
| Corpus Christi | No | 30 ppb | †† | ** |
| Victoria | Season Begins 05/01/2008 | 21 ppb | †† | ** |
| El Paso-Juarez [1] | Season Begins 05/01/2008 | 59 ppb | †† | ** |

# Haber Process (Fritz Haber Nobel 1918)
# Formation of Ammonia

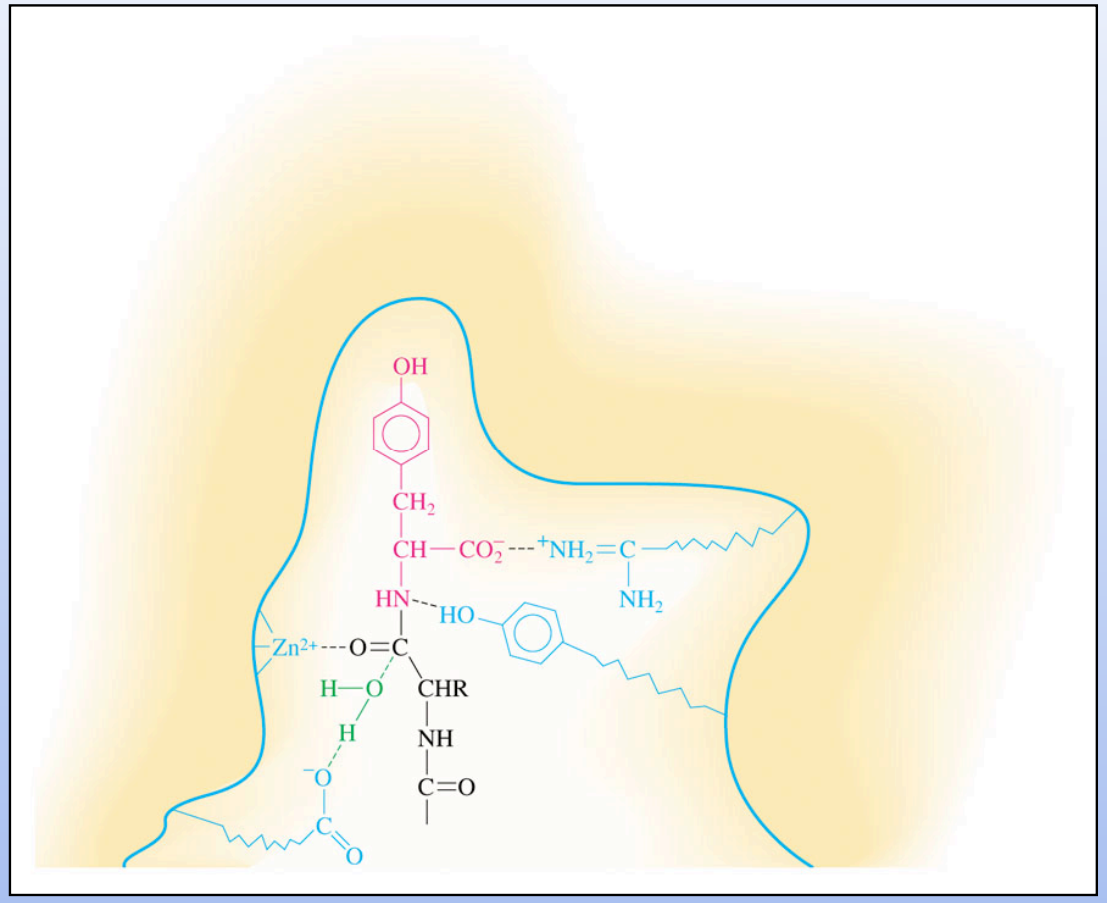
1. $N_2(g) \rightarrow N_2(adsorbed)$
2. **$N_2(adsorbed) \rightarrow 2N(adsorbed)$**
3. $H_2(g) \rightarrow H_2(adsorbed)$
4. $H_2(adsorbed) \rightarrow 2H(adsorbed)$
5. $N(adsorbed) + 3H(adsorbed) \rightarrow NH_3(adsorbed)$
6. $NH_3(adsorbed) \rightarrow NH_3(g)$

originally osmium and uranium

Now iron (keep out the $O_2$)

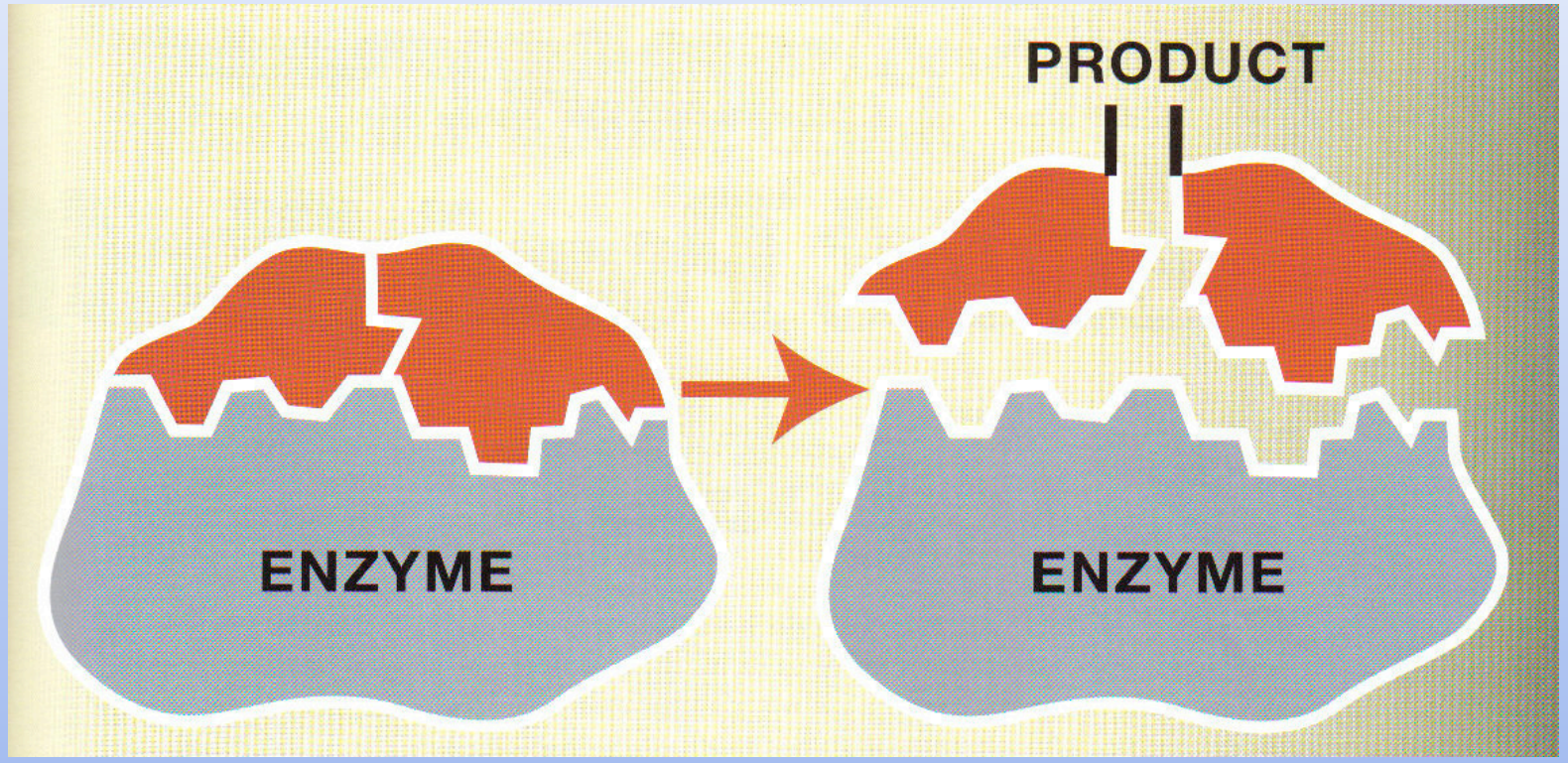
Ertl Nobel Prize 2008

# Enzymes
# Biological Catalysts



Substrate + Enzyme = Complex = Product + Enzyme

S + E = [SE] = P + E



Enzyme  Name = Function

Glucose Oxidase
Oxidizes Glucose

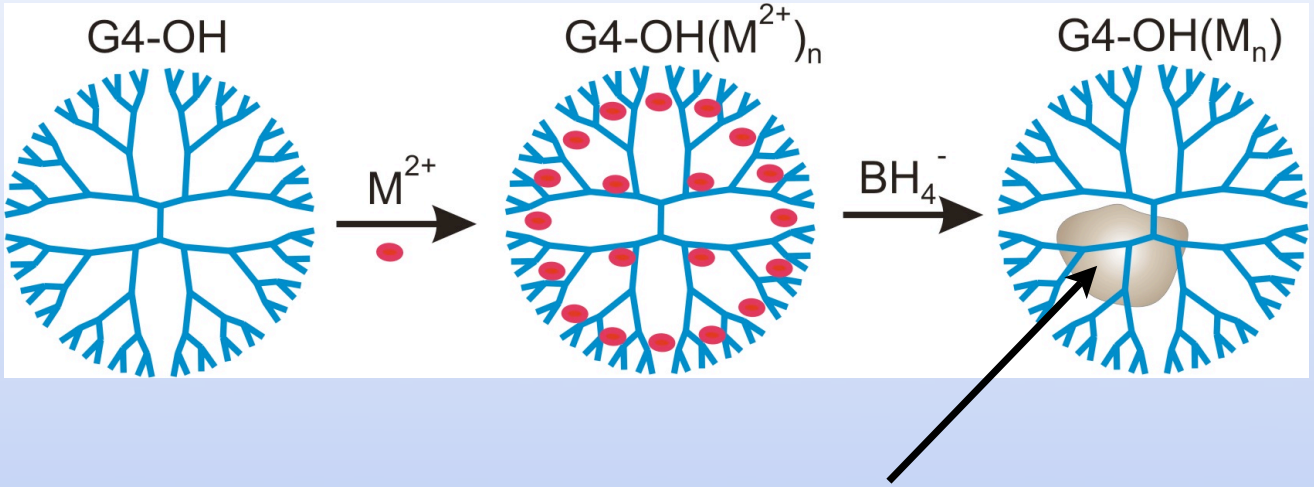
Aromatic Amine Dehydrogenase
removes Hydrogen from an aromatic amine

Hydrolase  Hydrolyze reactions

Isomerase  Isomerize molecules

Transferase  Transfers functional groups

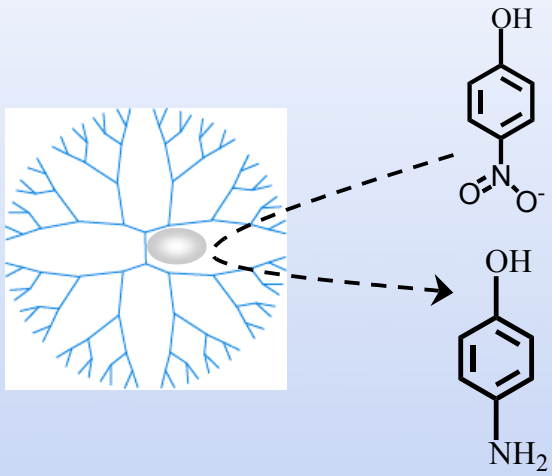
# Freshman Research Initiative Project
# Nanomaterials

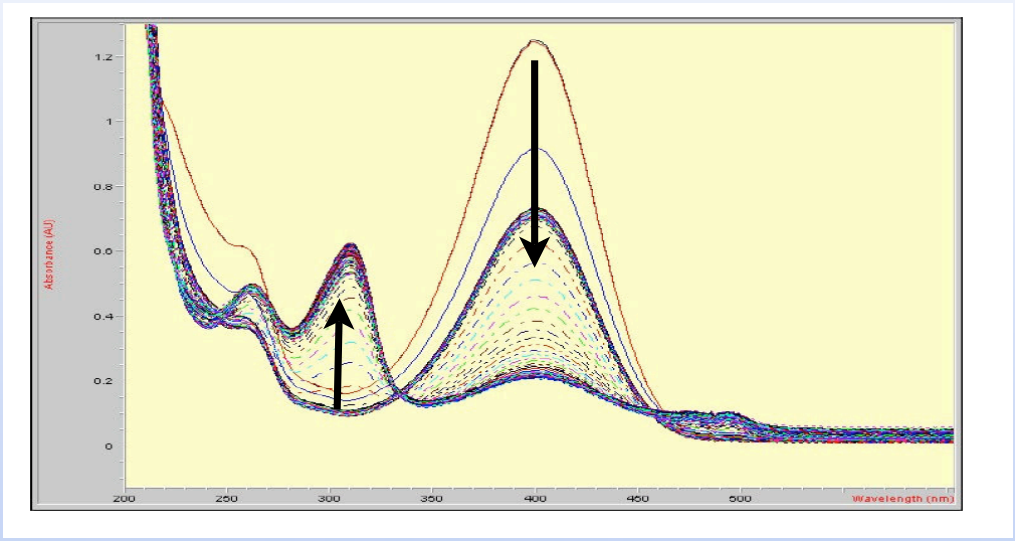



Dendrimer encapsulated nanoparticle

small metal particle
can be made of a variety of materials
(Au,Ag, Pd, Pt, Cu, Pt/Cu, Pd/Cu,....)

# How good is the catalyst? Measure the kinetics

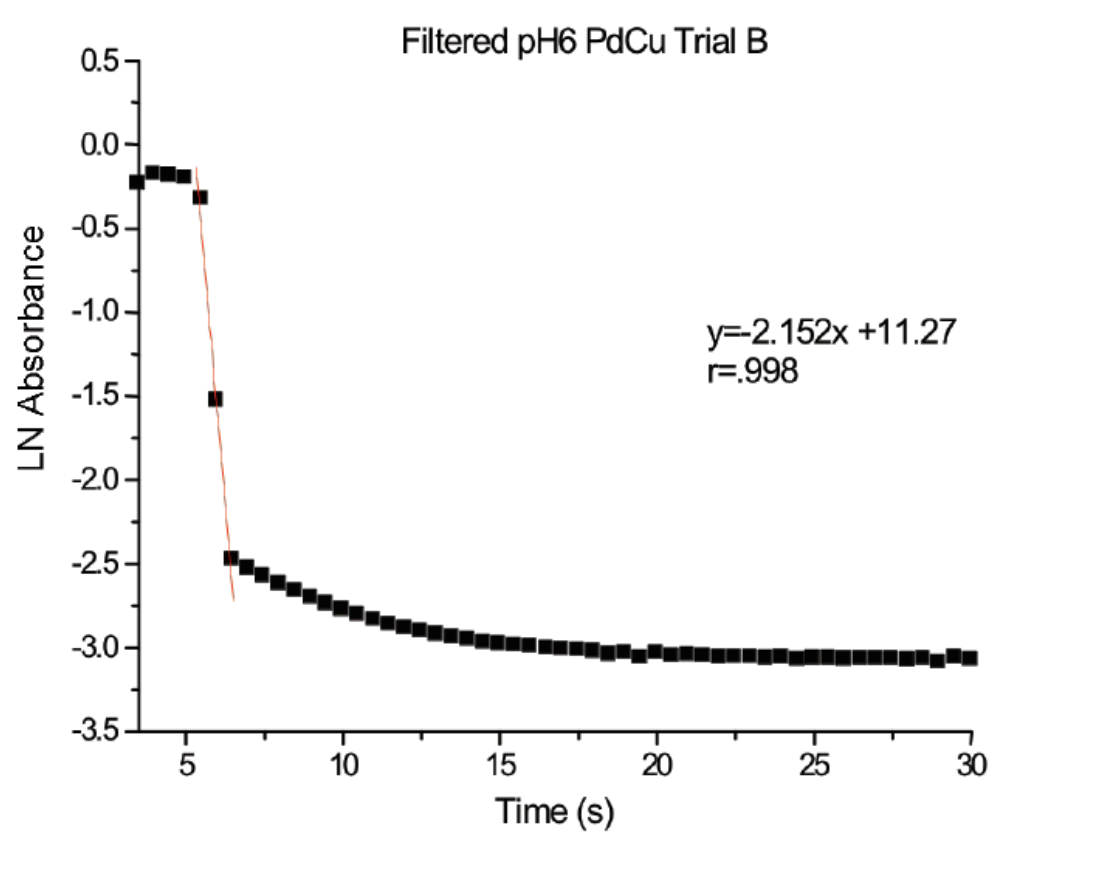



Measure the concentration as a function of time.

Kinetics are first order in reactant

plot ln[concentration] vs time slope = -k




Kinetics Wenly Ruan, Alex Guevaraal 2007

$$[A] = [A]_0 - akt \qquad t_{1/2} = [A]_0/2k$$

$$\ln[A] = \ln[A]_0 - akt \qquad t_{1/2} = 0.693/k$$

$$1/[A] = 1/[A]_0 + akt \qquad t_{1/2} = 1/k[A]_0$$

$$k = A\, e^{-Ea/RT} \qquad \ln(k_2/k_1) = \frac{-E_a}{R}\left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$