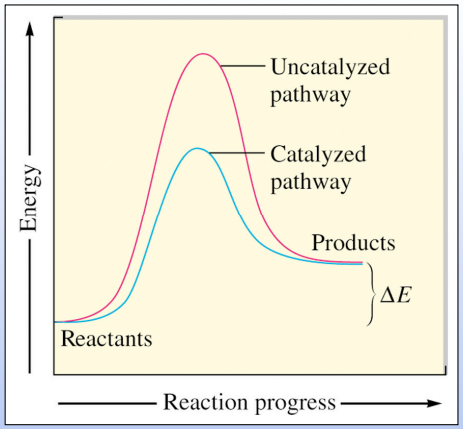
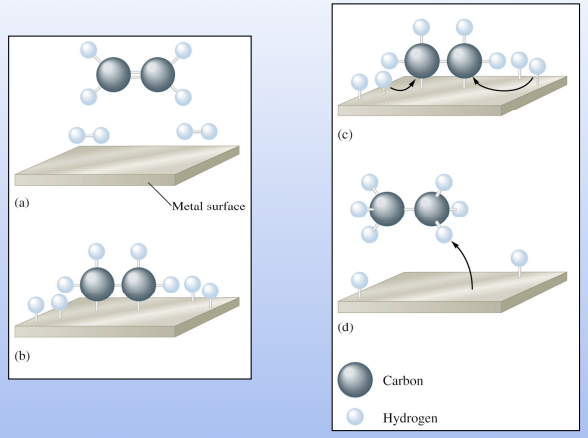
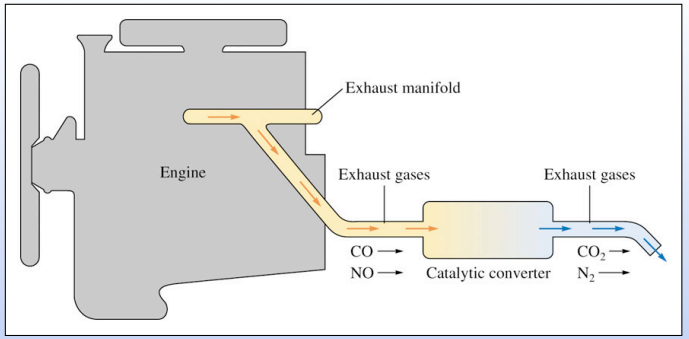
Today

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)

$OH + CO \rightarrow H + CO_2$

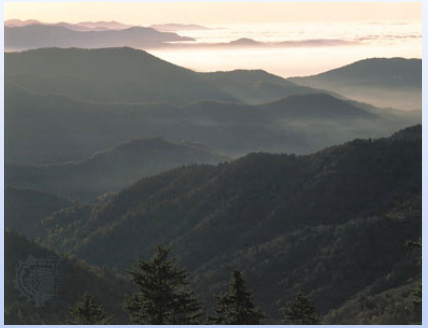
$H + O_2 \rightarrow HO_2$

$HO_2 + NO \rightarrow OH + NO_2$

$NO_2 + hv \rightarrow NO + O$

$O + O_2 \rightarrow O_3$

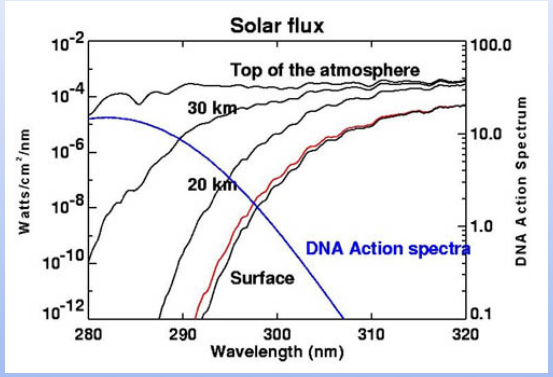
Great Smoky Mountains



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

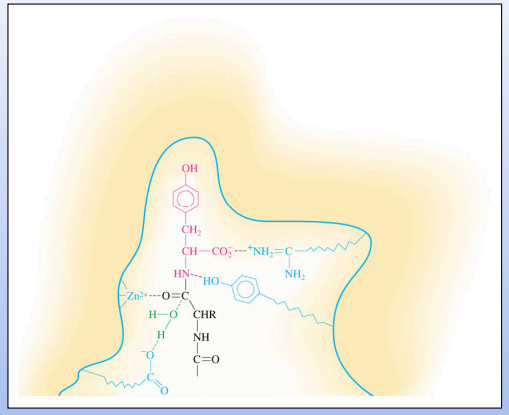
1. $N_2(g) \rightarrow N_2(adsorbed)$
2. **$N_2(adsorbed) \rightarrow 2N(adsorbed)$**
3. $H_2(g) \rightarrow H_2(adsorbed)$
4. $H_2(adsorbed) \rightarrow 2H(adsorbed)$
5. $N(adsorbed) + 3H(adsorbed) \rightarrow NH_3(adsorbed)$
6. $NH_3(adsorbed) \rightarrow NH_3(g)$

originally osmium and uranium

Now iron (keep out the O_2)

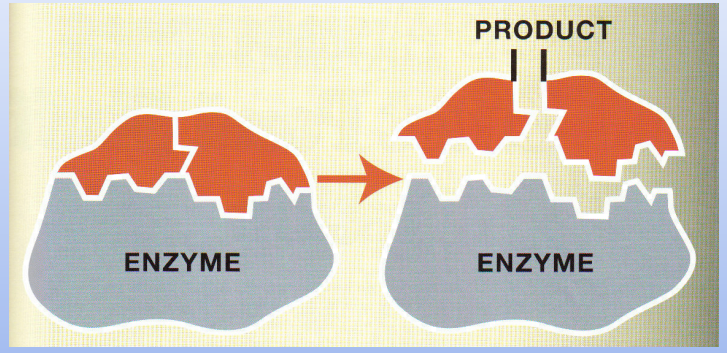
Ertl Nobel Prize 2008

Enzymes
Biological Catalysts



Substrate + Enzyme = Complex = Product + Enzyme

S + E = [SE] = P + E



Enzyme Name = Function

Glucose Oxidase
Oxidizes Glucose

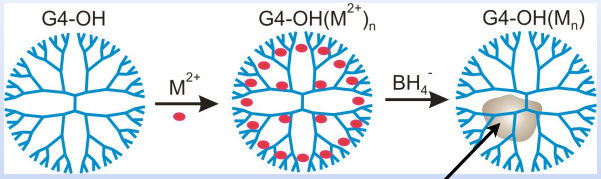
Aromatic Amine Dehydrogenase
removes Hydrogen from an aromatic amine

Hydrolase Hydrolyze reactions

Isomerase Isomerize molecules

Transferase Transfers functional groups

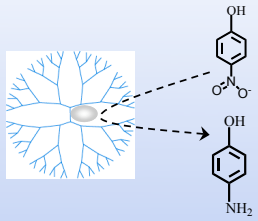
Freshman Research Initiative Project
Nanomaterials

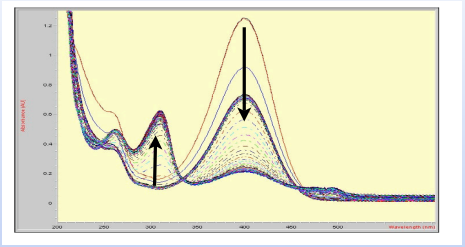


Dendrimer encapsulated nanoparticle

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

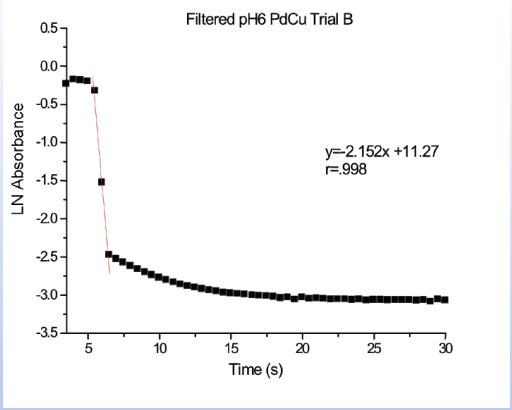
How good is the catalyst? Measure the kinetics





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

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

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

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

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