CHM222A: Basic Physical Chemistry

The Basics:

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Office SL302, Tel: X6037
Lectures: MWF 10-10:50 L9

Advanced Information:

Quiz 1 : 10 % (on Tuesday, January 19 – 40 mins)
Quiz 2 : 10% (on Tuesday, March 15 – 40 mins)
Mid Sem: 30 % (2 hours)
Final : 50 % (3 hours)
2 sided A4 page of hand written notes allowed for each exam

Most Advanced Information:

A Grade above 70%, Passing grade above 30%

Course Topics

- Equilibrium Thermodynamics – Nonreactive (physical) and reactive (chemical)
- Gases, liquids, solutions
- Kinetic Theory of Gases
- Physical transport processes in Gases
- Chemical Reaction Kinetics

.....but they will not be followed sequentially

Texts and References

Text Book:

Physical Chemistry: A Molecular Approach, by D.A. McQuarrie, Viva Student Edition.

Other References:

- *Physical Chemistry* by P.W.Atkins and J. De Paula
- *Physical Chemistry* by Ira N. Levine
- *Physical Chemistry* by R.J. Silbey, R.A. Alberty, M.G. Bawendi
- Use many online and offline resources but

DO NOT TRUST, VERIFY !!!

(Barack Obama after lifting Iran sanctions)

Many Worlds of Physical Chemistry

- Microscopic World: Atomic and Molecular structure, interatomic and intermolecular interactions, molecular understanding of reactions

  Quantum Chemistry, Molecular Reaction dynamics

- Macroscopic World: Thermodynamic equilibrium and thermodynamic laws, constitutive laws of matter (ideal and nonideal gases, solutions, electrolytes, interfaces), Reaction kinetics, rate laws

  Thermodynamics, Phenomenological Kinetics, Transport phenomena, Gas and Solution laws

- Statistical Mechanics: Link between the two worlds

Many Worlds of Physical Chemistry

- Experimental – how to probe phenomena at different scales
- Theoretical and Mathematical – develop new models/methods
- Computational – apply models/methods to more things than you can do manually

Modern Physical Chemistry offers exciting challenges in all levels

Example: Spectroscopic probes of molecular processes

- Ruby Laser (microwave) 1960 – Theodore Maiman – continuous wave
- 1961 – Pulsed semiconducting lasers
- Nanosecond laser (10^{-9}) – Electronic relaxations
- Picos econd Laser (10^{-12}) – Electronic/vibrational relaxations
- Femtosecond laser (10^{-15}) – Vibrational processes
- Attosecond laser (10^{-18}) – Electronic motion in molecules

http://www.osa.org/en-us/history/exhibits/laser_history_timeline/

Challenges in making better laser technology, materials, pulses, electronics, etc.

3 breakthroughs

- Haber-Bosch Ammonia synthesis – illustrates thermodynamics, kinetics, gas transport processes, reaction dynamics, catalysis, surface processes
- Water phase diagram– illustrates phase equilibrium, molecular motions, solvation, electrolytic effects
- Kinesin molecular motors – illustrates irreversible processes, thermodynamics, kinetics.

Lets get going

Consider the reaction

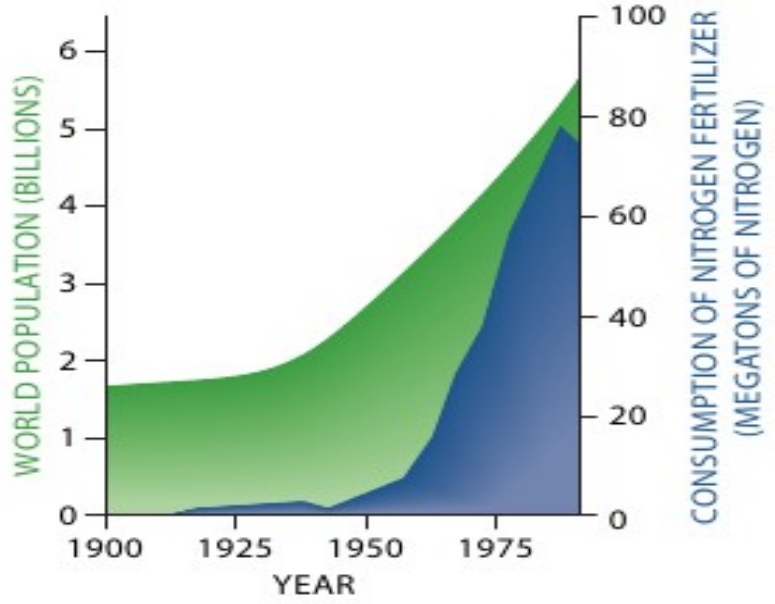
$$N_2 + 3\ H_2 \Longrightarrow 2NH_3$$

- Simple looking reaction, Exothermic reaction
- Requires 700 K, 200 Bar pressure
- Negligible rate without a catalyst – Fe
- Fritz Haber: Nobel Prize 1918 (Discovery)
- Carl Bosch : Nobel Prize 1931 (Commercialized the Haber process)
- Elucidation of the mechanism : Gerhard Ertl (Nobel Prize 2007)

Why is it such a big deal ?

Greatest discovery of the last century ??

- Ammonia production is the first stage of fertilizer preparation and the most difficult



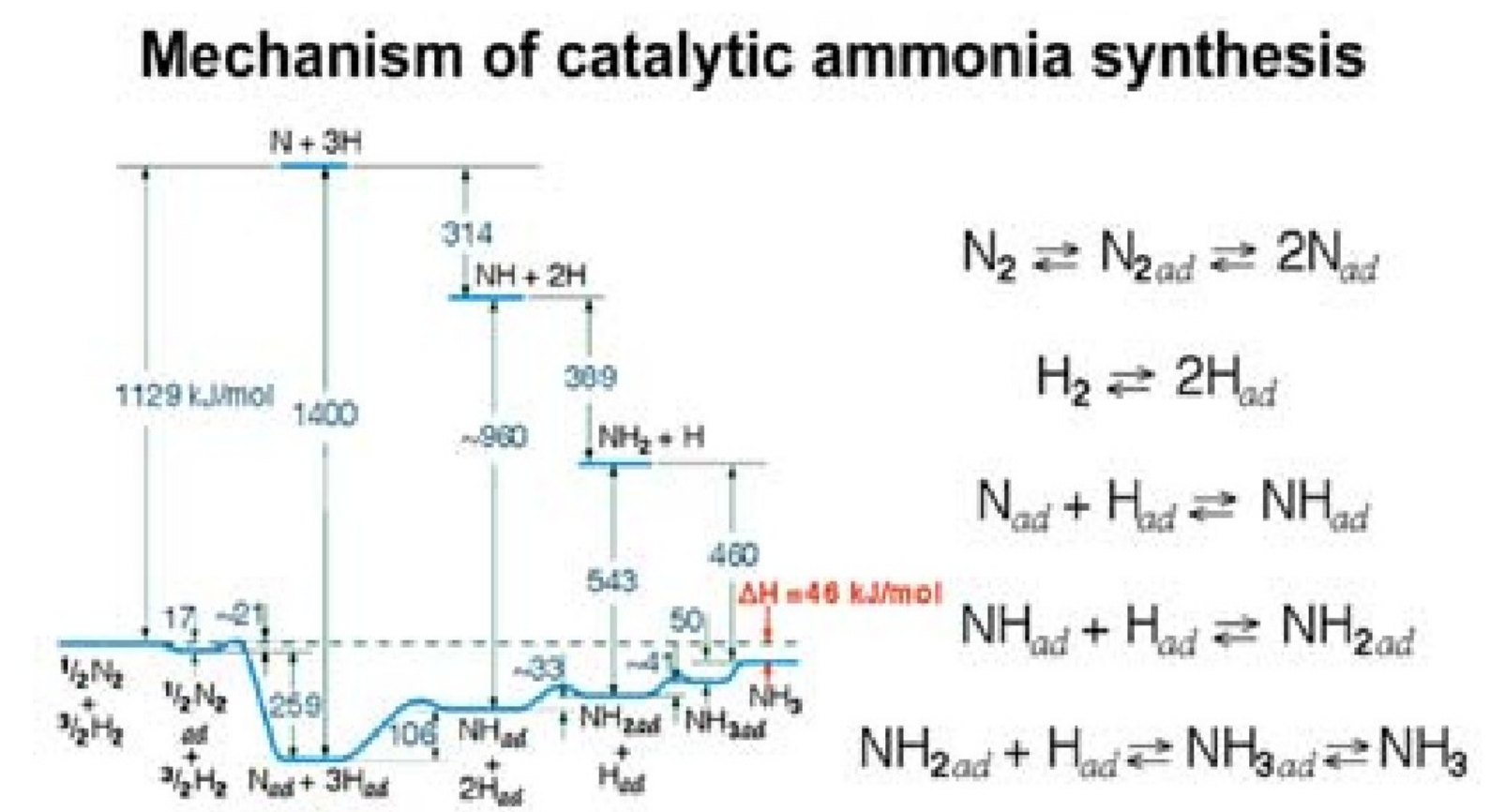
Global population and the nitrogen cycle, Vaclav Smil, Scientific American, July 1997

Fritz-Haber process replicated that of N-fixing bacteria and transformed the N-cycle

Nitrogen compounds are also used in explosives – World War II

The Physical Chemistry elements involved - Gas laws and transport processes, reaction thermodynamics, kinetics, catalysis, surface chemistry, experiments, Ultra-High vaccuum

Gerhard Ertl's Mechanism



Why is this reaction so difficult ?

- N – N triple bond
- One of the strongest known bonds
- The inertness of N_2 is well known
- Liquid Nitrogen is frequently used to cool
- Nitrogen is easily available in the atmosphere but fixing it artificially is very hard

Reading Assignment

- Gerhard Ertl's Nobel lecture:

  http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2007/ertl-lecture.html

- PDF of lecture: Reactions at Surfaces: From Atoms to Complexity

  https://www.nobelprize.org/nobel_prizes/chemistry/laureates/2007/ertl_lecture.pdf

- 42 minute video of presentation.

  http://www.nobelprize.org/mediaplayer/index.php?id=784

- Read the part dealing with Haber-Bosch process

- Nobel Prize page also has several other links on the left such as Popular information, Advanced information, which are also useful.