

# A Brief Introduction to Physical Chemistry

CHM 320

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Dr. Lee

# What is Physical Chemistry?

- Physical chemistry is the study of the underlying *physical principles* that govern the properties and behavior of chemical systems.  
In principle, we can answer any chemistry question “*exactly*” using quantum mechanics.
- Quantum Mechanics and Chemistry

*“The underlying physical laws necessary for the mathematical theory of a large part of physics and **the whole of chemistry are thus completely known**, and the difficulty is only that the exact solution of these laws leads to equations much too complicated to be soluble.”*

By Paul Dirac (Nobel Prize in Physics, 1933)



# Physical Chemistry according to textbooks

*Quantum chemistry: CHM320* “Exact” descriptions of molecular structures, chemical bondings and reactions at the molecular level (*microscopic*) via *quantum mechanics*.

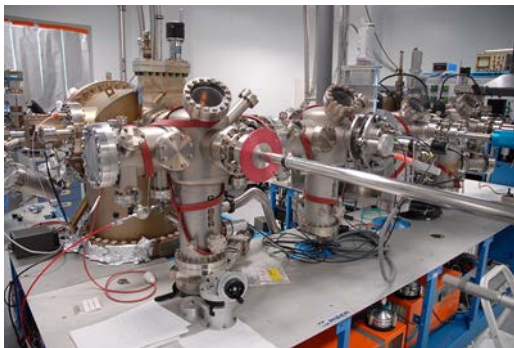
*Thermodynamics: CHM321* A study of *macroscopic* properties of matter, especially the energy and its transformation to various forms. As applied to chemical problems, it is primarily concerned with the position of chemical equilibrium and the direction of chemical change.

*Chemical kinetics: CHM321* A study of reaction rates and mechanisms as a chemical equilibrium is approached.

*Statistical thermodynamics: CHM521* Links the three areas mentioned above: thermodynamics, quantum chemistry, and kinetics. It provides a basic relationship between the microscopic and macroscopic worlds.

# Physical Chemistry in Research Lab

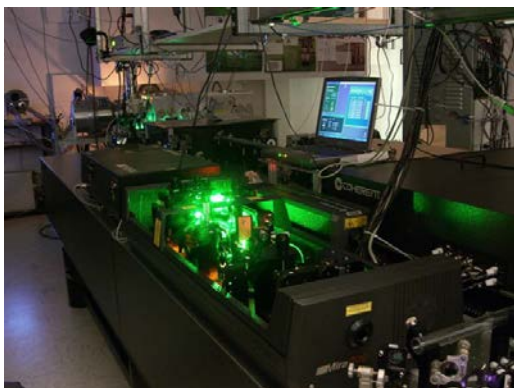
## *Kinetics and dynamics of gas phase reactions*



**Nobel prize in 1986** : Herschbach, Lee and Polany  
*“for their contributions concerning the dynamics of chemical elementary processes”*

developed crossed-molecular beam technique

## *Chemistry with Laser (spectroscopy and dynamics)*

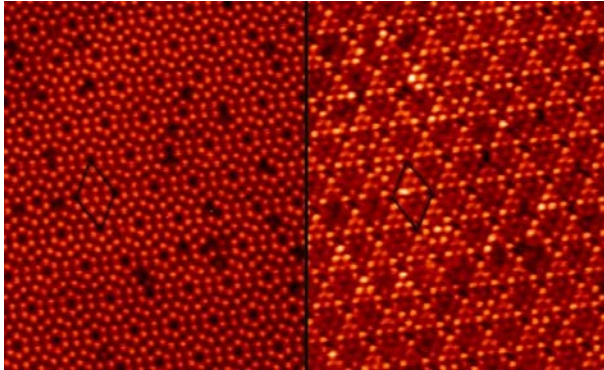


**Nobel prize in 1998** : A. H. Zewail  
*“for his studies of the transition states of chemical reactions using femtosecond spectroscopy”*

opened a new area called femtochemistry ( $10^{-15}$  sec.)

# Physical Chemistry in research lab

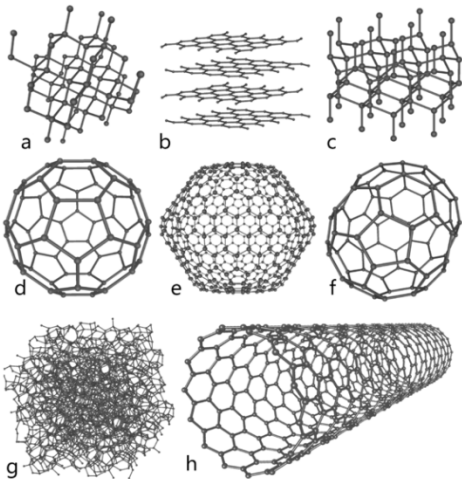
## Surface chemistry



**Nobel prize in 2007:** Gerhard Ertl  
*“for his studies of chemical processes on solid surfaces”*

**Nobel prize in 1986:** G. Binnig and H. Rohrer  
*“for their design of the scanning tunneling microscope”*

## Nano chemistry (material science in general)

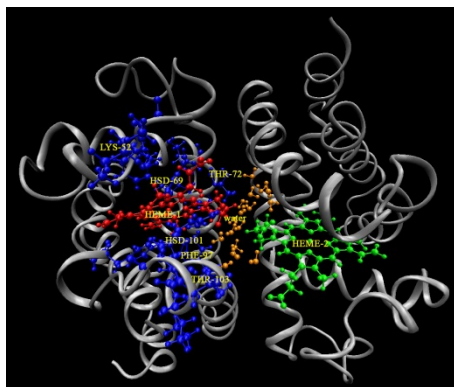


**Nobel prize in 1996:** R. Curl Jr., H. W. Kroto, R. E. Smalley  
*“for their discovery of fullerene”*

opened a new area studying nano material

# Physical Chemistry in research lab

## *Biophysical chemistry*



**Nobel prize in 1982:** Aaron Klug

*“for his development of crystallographic electron microscopy and his structural elucidation of biologically important nucleic acid-protein complexes”*

## *Theoretical and computational chemistry*



Schrodinger



Cray XT-3

**Nobel prize in 1998:** Walter Kohn and John Pople

*“for their development in computational methods in quantum chemistry”*

**Nobel prize in 2013:** Martin Karplus

*“for the development of multiscale models for complex chemical systems”*

# What do we learn in CHM320

- I. Classical mechanics Review & Failure of classical mechanics
- II. Dual nature (matter and wave) of light
- III. The Schrodinger equation (1-dimensional version)
- IV. Postulates in quantum mechanics & mathematical machinery
- V. Quantum mechanics in multi-dimension (2- and 3-dimensional)
- VI. Hydrogen Atom
- VII. Multi-electron atoms
- VIII. Quantum mechanics for molecule: chemical bonding