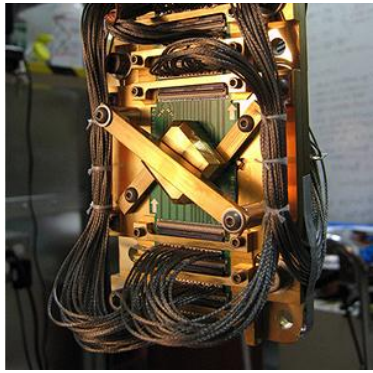
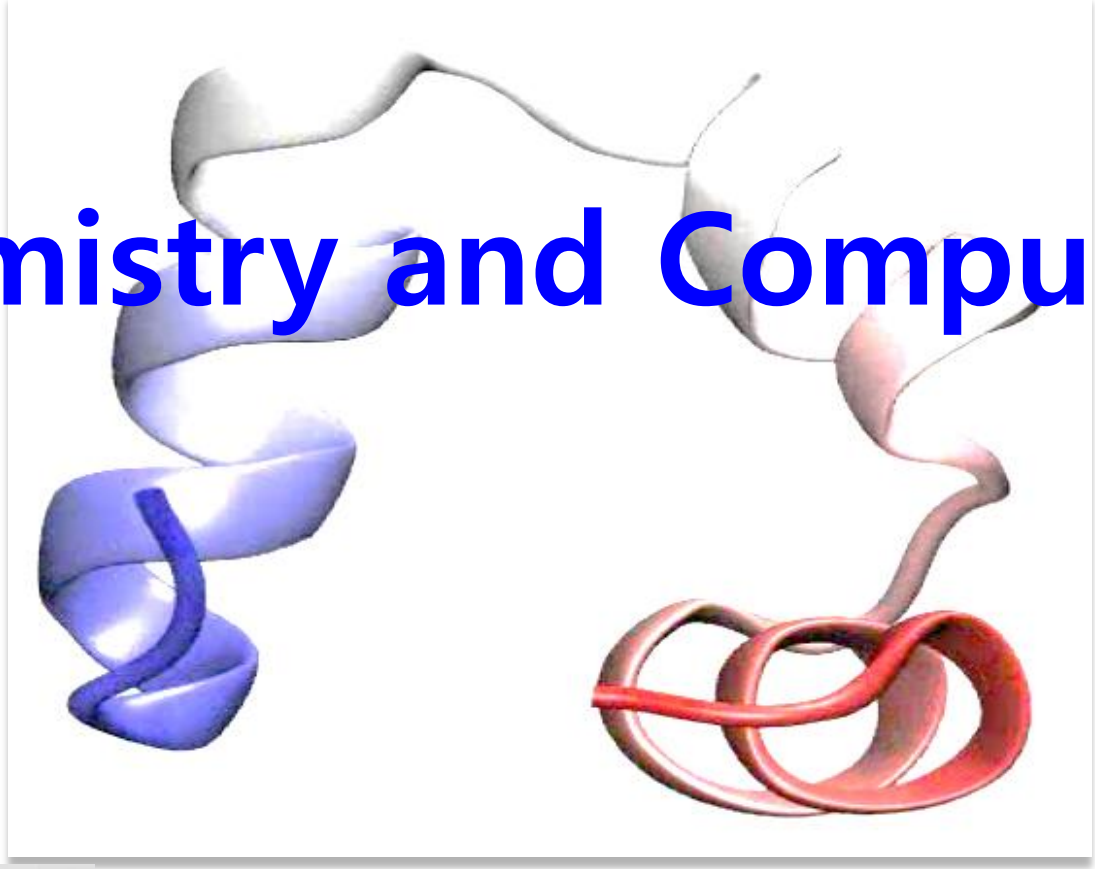


# Chemistry and Computer



화학교육과 양기열

# Modern Computer

## For military purpose (1970 ~

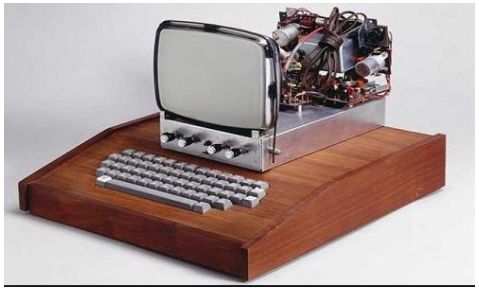
Text (command) oriented monitor/console

| Computer Prices, Computer Speed and Cost/MHz | | | | |
|---|---|---|---|---|
| | **1970** | **1984** | **1997** | **2007** |
| Cost | $4,600,000 | $4,000 | $1,000 | $550 |
| Speed (MHz) | 12.5 | 8.3 | 166 | 1600 |
| Cost per MHz | $368,000 | $482 | $6 | $0.34 |

PC

main frame computer

# Personal computer :8 bit , 16 bit, 32 bit and 64 bit computers



Apple

Apple II (1977)

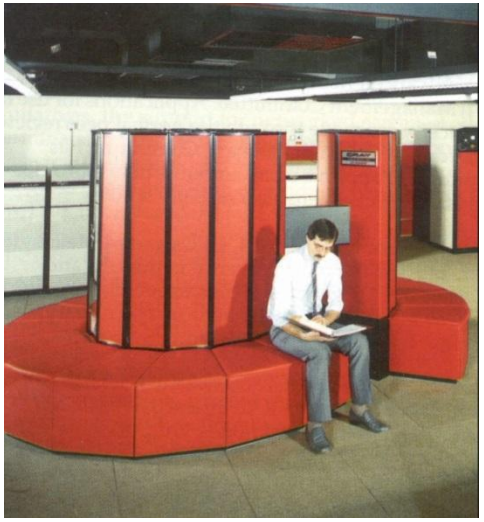

국내 제조 (1981)

**16 bit 컴퓨터 시초 : IBM-XT**
8086(1978, 4.77MHz~10MHz) 80186, 80286 (1982, 6MHz~20MHz, 90년도 초반까지 사용)

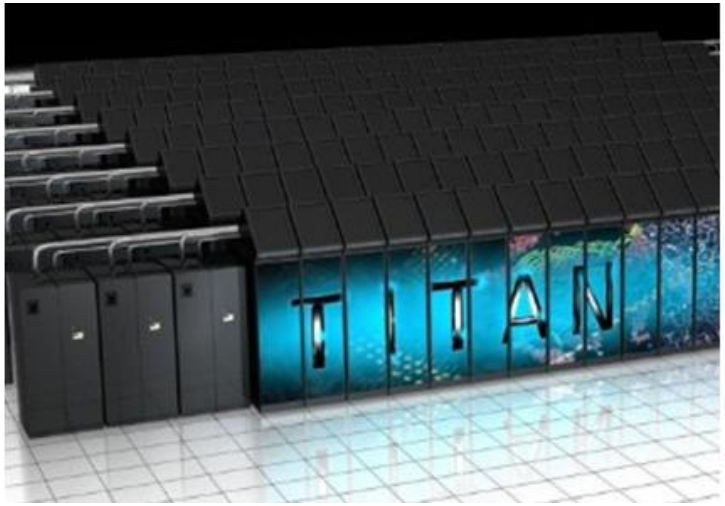
애플 매킨토시(1984): 마우스 및 윈도우
**(최초로 화학구조식 작성 가능)**

**32 bit computer** : Intel 80386(1985), 80486 etc **: 화학계산에 이용 가능**
**64 bit computer : 최근 pc**

# Supercomputer and cluster computer



80~90년대 수퍼컴퓨터(cray)

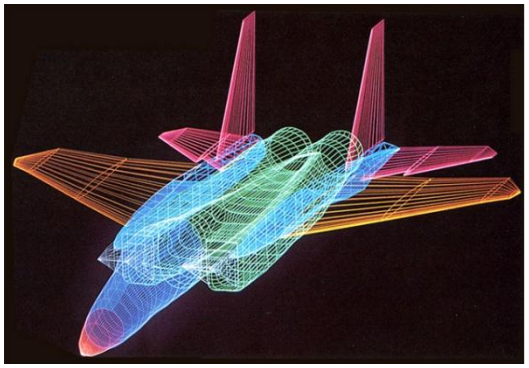
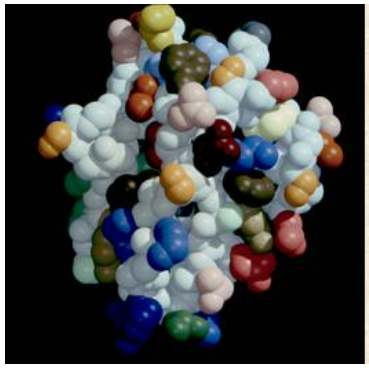


현재(2013.06) 가장  빠른 수퍼 컴퓨터: 병렬처리 컴퓨터(pc cluster)
중국 National University of Defense Technology (NUDT)
 PC(server) cpu(core) 260,000 cpus x 12 core=3,120,000 개 core 연결

# Workstation

**Main frame computer 와 personal computer의 장점 포함)**

-크기는 개인용 컴퓨터 정도이나 연산성능은 대형 컴퓨터(main frame computer) 수준이며, 탁월한 그래픽 기능을 보유한 컴퓨터로 CAD(computer aided design) 가능


Evans & Sutherland, Sun, HP, Compaq etc.

-현재는 개인용 컴퓨터와 Workstation의 구분이 없음

동일한 하드웨어(PC)에 운영체제(OS)로서 Windows 설치하면 "일반 PC"

Mac OS 설치하면 "애플 맥 컴퓨터"

**리눅스(linux)를 설치하면 "서버, 워크스테이션,클러스터(수퍼컴퓨터)"**

# Operation System (OS) : 운영체제

▣ **Main frame computer (대형컴퓨터)**
제조사마다 다른 자체 cpu를 사용하므로 모두 다른 OS로 출발하였으나 후에 거의 Unix로 통일

▣ **Workstation: Unix**

▣ **개인용 컴퓨터**
애플컴퓨터 ; Mac OS(초기부터 윈도우, 마우스 사용), Mac OS X
일반 PC (IBM PC) : MS-DOS, Windows

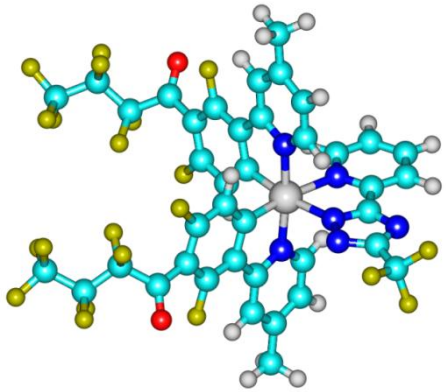
▣ **리눅스(linux)의 등장 : Linus B. Torbalds가 26세 때인 1991년 386 PC에 적용하여 개발이 시작된 open source 기반의 OS (linus Unix -> Linux)**

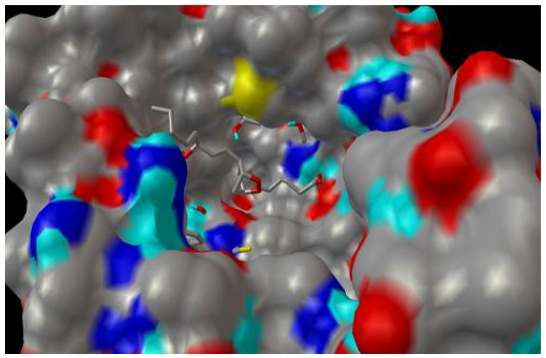
"전문적인 컴퓨터 사용자들에겐 가장 큰 영향을 준 운영체제"

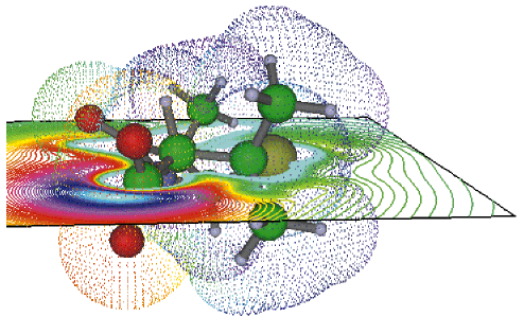
*스마트폰 OS : ios(apple), android(google), MS windows mobile, Samsung bada 등

# 컴퓨터 시뮬레이션 : 분자 설계 및 특성 시험

~ 1960년대 양자역학 및 양자화학의 수식 체계 및 문제해결 개념 정립
1970년대 : 일부 **계산화학**의 시작(컴퓨터 사용의 제한으로 극히 일부 연구팀에 국한)
~ 1981년 최초의 계산화학 저널 등장(J. Computational Chemistry)
1990~ 중형컴퓨터, Workstation 등장 및 보급에 따른 계산화학의 관심 증대확산 : 실험-이론 병행 연구의 활성화
1990 중반 : PC 성능 증가 및 Linux OS 등장으로 개인 연구실 수준의 연구 기반 가능



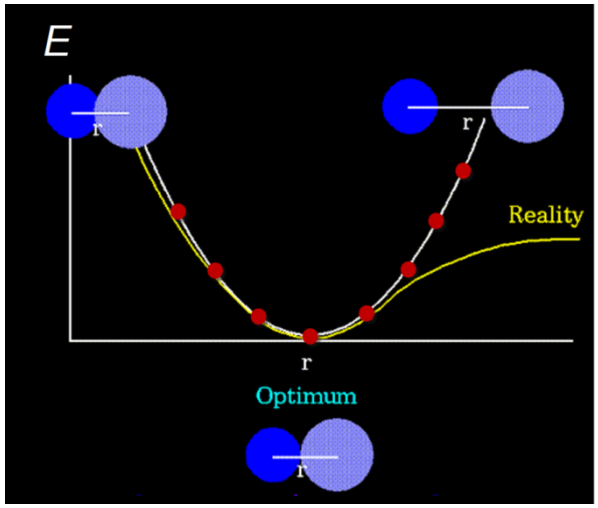




# Structure-reactivity relationship : determination of electronic structure of molecules

- Experimental methods
  X-ray crystallography for solid state
  other spectroscopic methods for gas phase and liquid state

- Theoretical method
  Energy minimization for geometry optimization




양자역학적(Quantum Mechanics)

고전역학적(뉴튼역학, Classical Mechanics)

# Quantum mechanical treatment

1. Calculation of Energy of Molecule/Electronic Structure
   - ▣ Quantum Mechanics (QM): small molecules
   - ▣ Molecular Mechanics (MM): large molecules (classical treatment)

   - ▣ **Differences between QM and MM**

     **Energy quantization and uncertainty principle**

Schrodinger Wave Equation (QM)

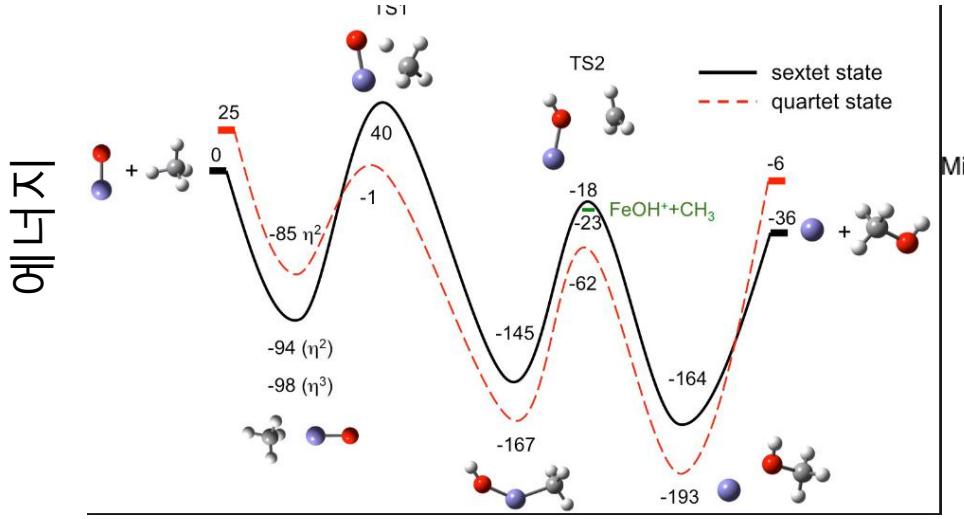
$$\hat{H}\psi = E\psi$$

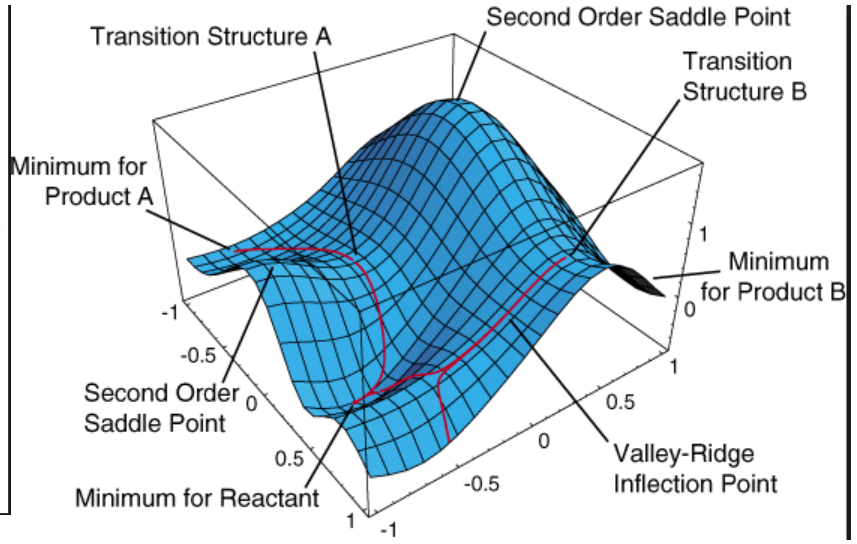
$E$ : energy of system(molecule)

$\psi$ : wave function, $\psi^2$ : probability density

- **계의 에너지와 파동함수만 알면 그 계에 대한 거의 모든 정보를 알 수 있다**

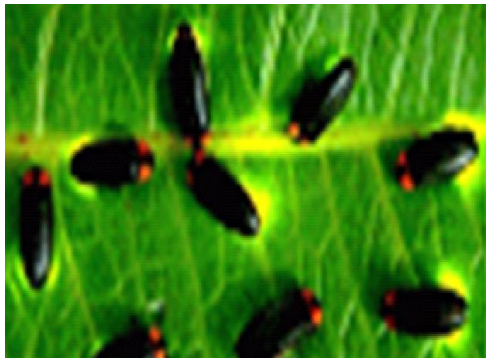
# 화학 반응 경로에 대한 Potential Energy Surface (PES) 추적

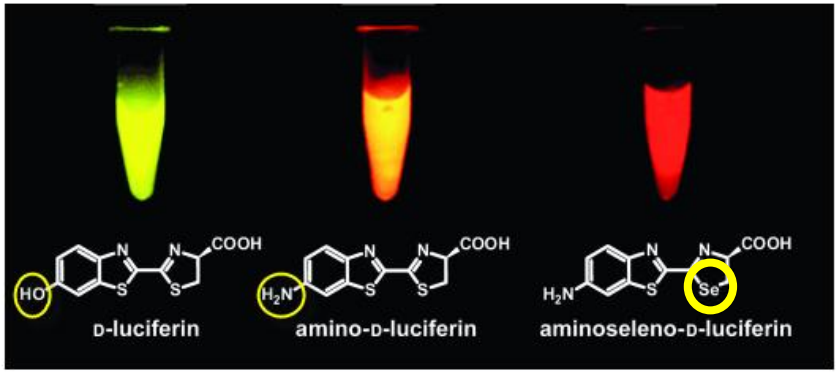


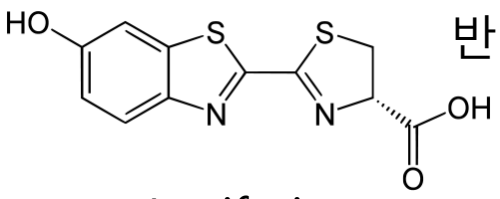

**(수명이 짧아 실험적으로는검출이 어려운 화학종에 대한 에너지 계산 가능)**

# 유기반도체, OLED 물질의 설계 및 특성 예측



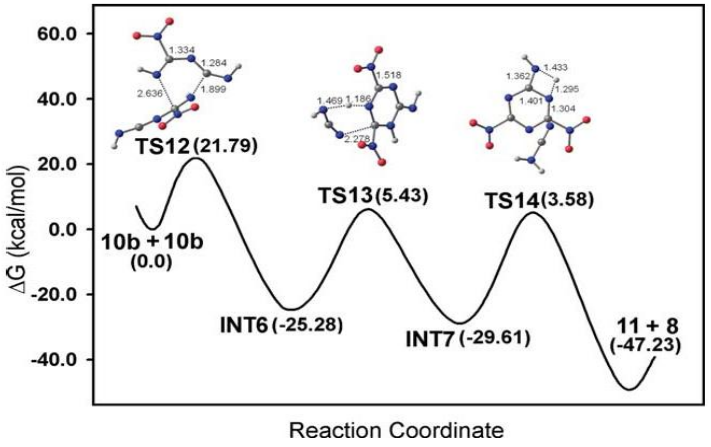

무기 금속화합물

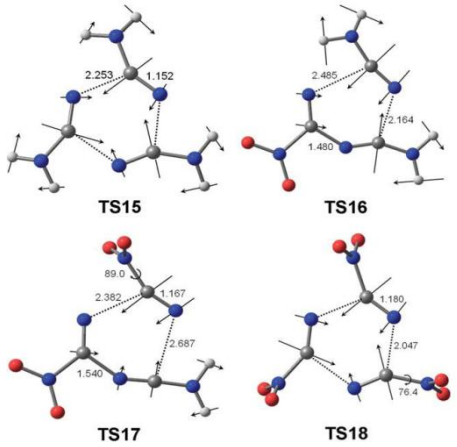



Luciferin

반딧불이의 발광 및 치환기에 따른 색 변화

# 화학, 추진체 설계 및 특성 연구




설계된 물질의 화약특성 계산

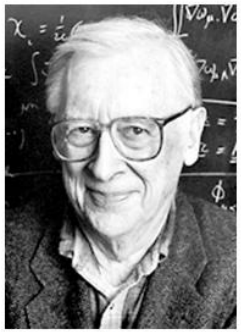
| | DANTA | | ADNTA | | TNTA | | | |
|---|---|---|---|---|---|---|---|---|
| | L[a] | U[a] | L | U | L | U | RDX | HMX |
| $\Delta H_f$ (s) (kcal/mol) | −8.52[b] | −8.52 | 21.14[b] | 21.14 | 47.00[c] | 63.73[c] | 18.9[d] | 18.0[d] |
| Density ($g/cm^3$) | 1.620[e] | 1.796[f] | 1.755[e] | 1.932[f] | 1.904[e] | 2.010[f] | 1.82 | 1.91 |
| $I_{sp}$ (s) | 175.7 | 175.7 | 231.7 | 231.7 | 257.0 | 261.4 | 265 | 265 |
| $v_{det}$ (km/s) | 6.601 | 7.280 | 8.059 | 8.694 | 9.044 | 9.618 | 8.754 | 9.1 |
| $P_{CJ}$ (GPa) | 14.94 | 20.13 | 26.01 | 32.96 | 33.80 | 39.83 | 34.7 | 39.5 |
| IS (cm) | 297.9 | | 201.9 | | 17.4 | | 28 | 32 |

설계된 물질의 반응경로 및 전이상태 구조

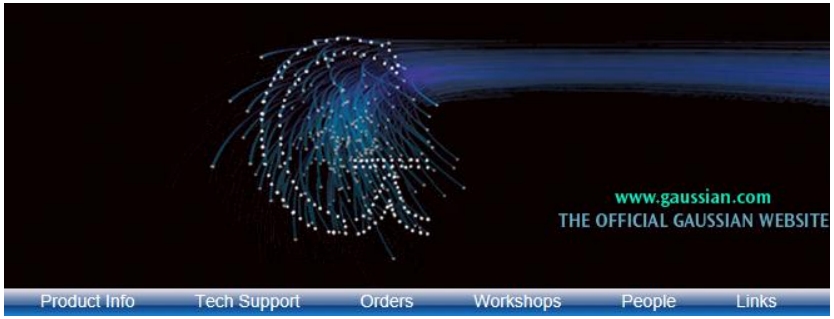
# Nobel Prize in 1998

## The Nobel Prize in Chemistry 1998

Walter Kohn



John A. Pople




The Nobel Prize in Chemistry 1998 was divided equally between Walter Kohn *"for his development of the density-functional theory"* and John A. Pople *"for his development of computational methods in quantum chemistry"*.

**Computational Chemist**

밀도범함수/양자역학계산 컴퓨터 프로그램 작성 및 연구

Gaussian70 – Gaussian09 (starting 1970): *ab initio* 계산

# Classical Mechanical Computation (Molecular Mechanics)

Using Newton Mechanics : suitable for large molecules like protein and DNA etc.

$$E^{Total} = \sum_{i}^{b} E_i^{str.} + \sum_{i}^{a} E_i^{bend} + \sum_{i}^{d} E_i^{tors.} + \sum_{ij}^{p} E^{vdw} + \sum_{ij}^{p} E^{electro.}$$

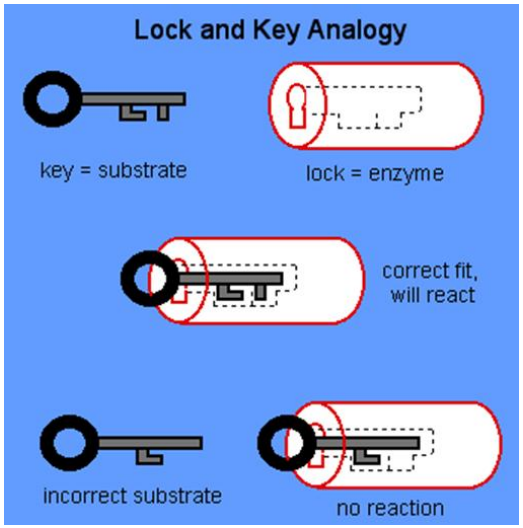
Covalent Non-covalent

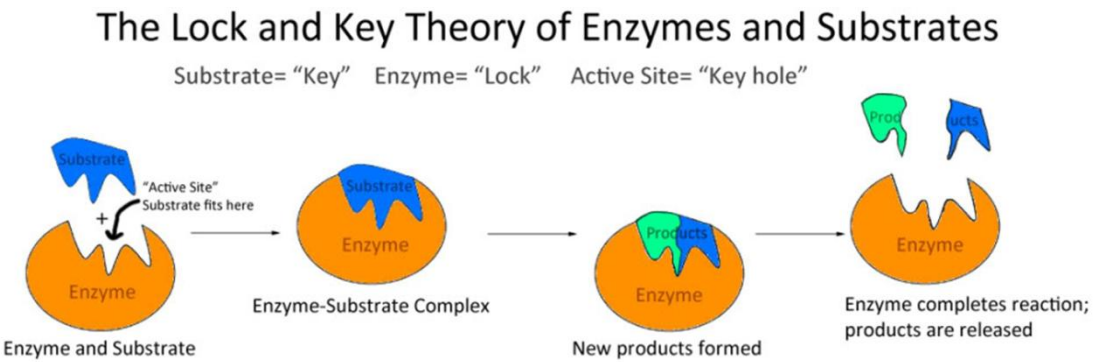
## Molecular Dynamics (MD)

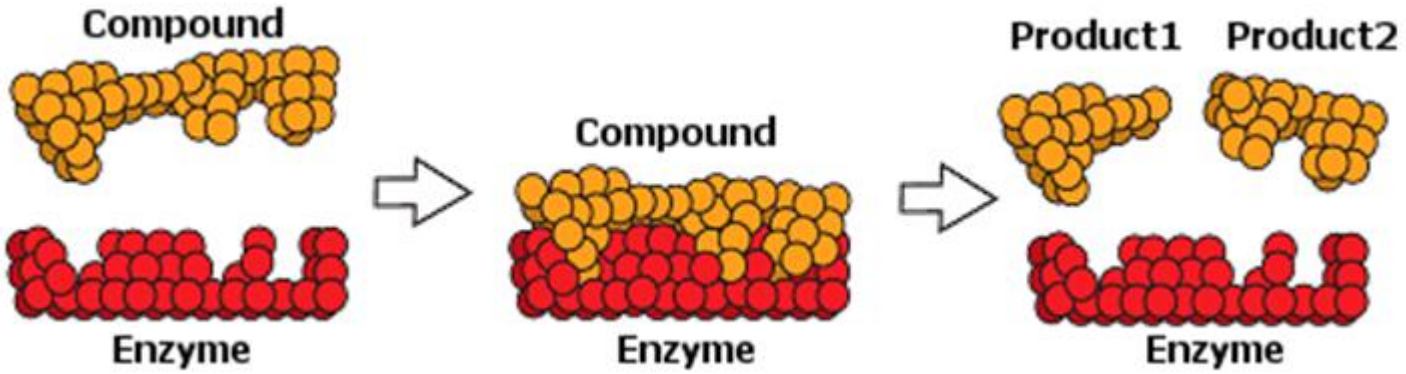
$$F = ma = m\frac{d^2\overline{x}_i}{dt^2} = -\frac{\partial E}{\partial x_i}, \qquad x_i = f(t)$$

양자역학 계산에 비해서 기본 원리는 매우 단순하나 매우 큰 분자를 다루고 시간에 따라 분자의 움직임 1펨토초 단위로 추적하기 때문에 역시 계산 시간이 많이 소요됨

# Mechanism of Enzymatic Action

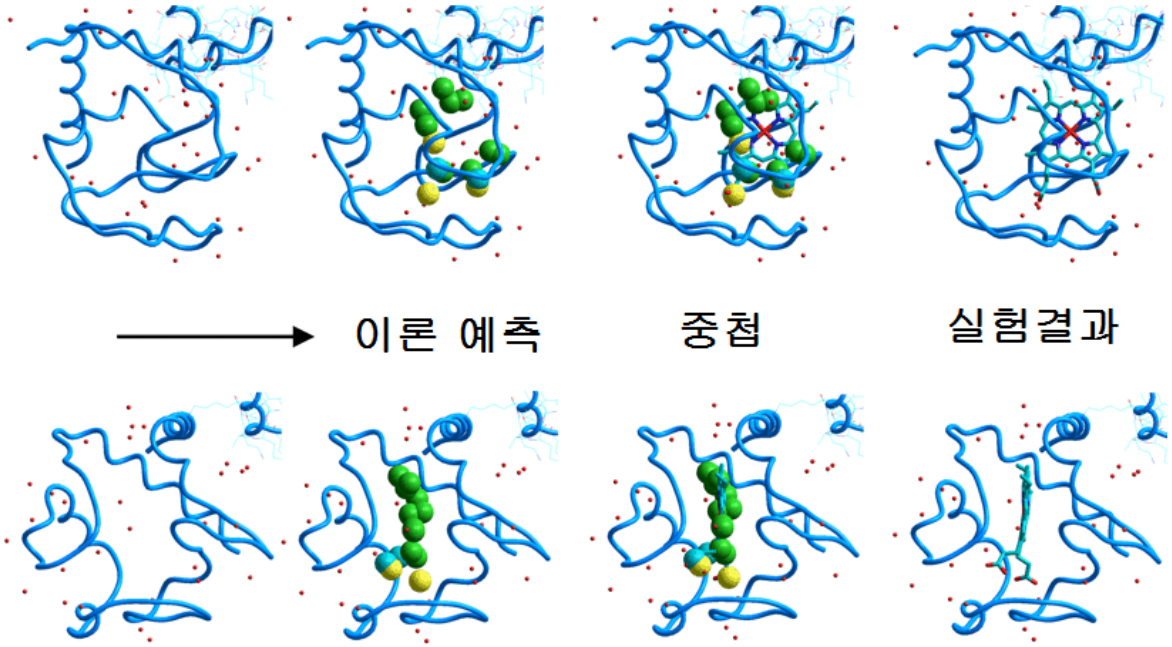


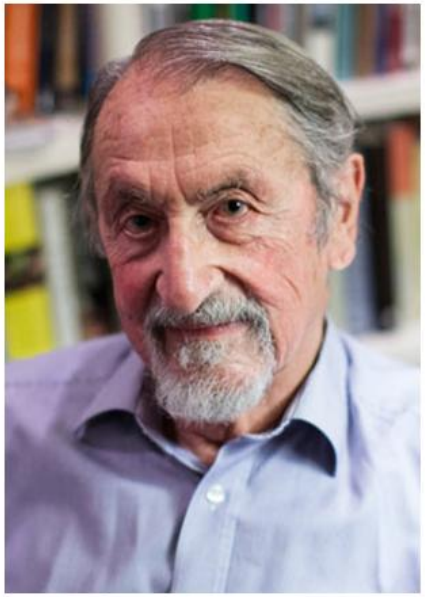
# Drug Design

Fitting drug into receptor (protein)



# Nobel Prize in 2013

## Martin Karplus - Facts



© Harvard University

**Martin Karplus**

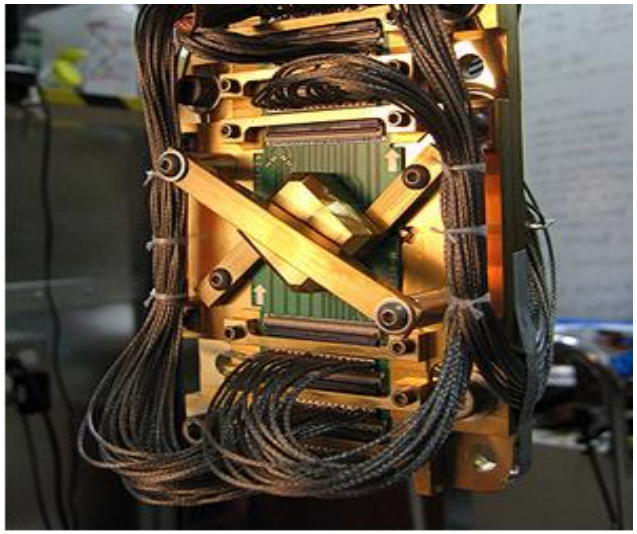
**Born:** 15 March 1930, Vienna, Austria

**Affiliation at the time of the award:** Université de Strasbourg, Strasbourg, France, Harvard University, Cambridge, MA, USA

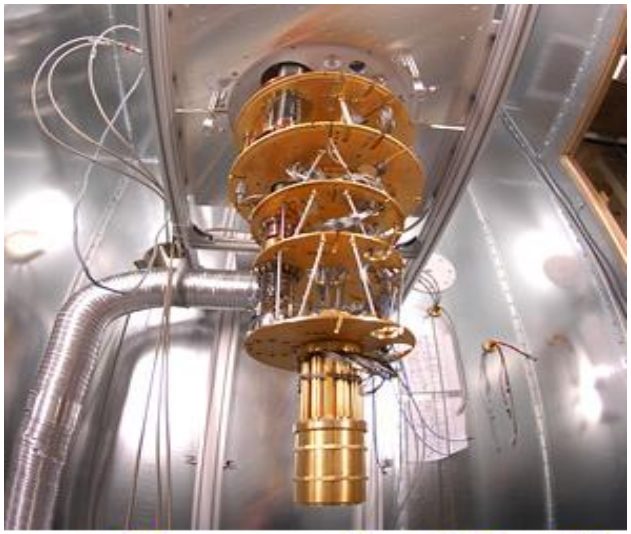
**Prize motivation:** "for the development of multiscale models for complex chemical systems"

**Computational Chemist**
분자역학/분자동력학 컴퓨터 프로그램 작성 및 연구
**CHARMM** (**Chemistry at HARvard Marcromolecular Mechanics**) 1984

# Computer in the future?
# Quantum Computer

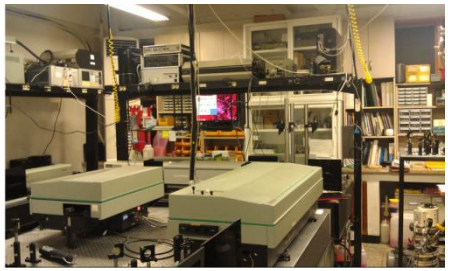
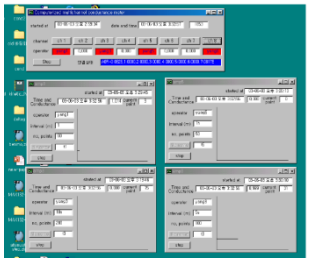
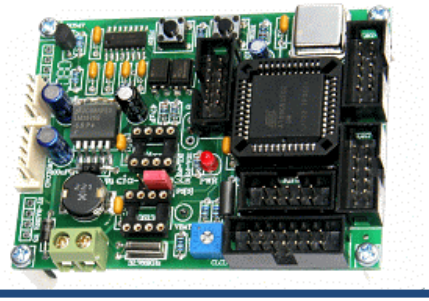
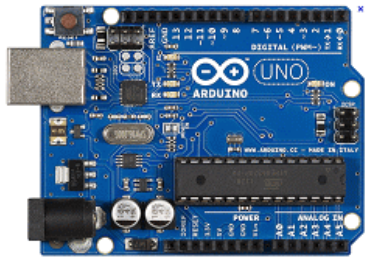


quantum leap



cooling part ~20mK

# Computer in Chemistry Lab.
# (computer interfacing to experimental equipment)


교과목 운영 : Computer Chemistry (1989~2003)
CAI, CAL etc
Microcomputer-based laboratory (MBL) 실험


**Just black box ?**

# Remarks

**How to use computing resources efficiently in science research and learning**

**Basic knowledge of the computer language (high level ) is essential**

**Other keywords in computer resources are 3D printing, Smart equipment including tablet and wearable computer**