

# **Computational Chemistry**

*Learning by Prompting*

Pembelajaran 'DEEP LEARNING'  
Terintegrasi AI

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NotebookLM Kimia Komputasi

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# Methods of Doing Science:

Modern science utilizes four basic approaches to the study of how nature works:

- |                           |                           |
|---------------------------|---------------------------|
| 1) observational science, | 2) experimental science,  |
| 3) theoretical science,   | 4) computational science. |

- Computational science is the newest, made possible by the tremendous improvements in both computer hardware and software over the past 30 years.
- Computational science, sometimes known as modeling and simulation or scientific computing, is used extensively in chemistry, and is known as **computational chemistry** or **molecular modeling**.
- Computational scientists deal with a specific application, to which an algorithm is defined, which is then computed using a specific architecture

# Definition of Computational Chemistry

- *Chemistry is the science dealing with construction, transformation and properties of molecules.*
- *Theoretical chemistry is the sub field where mathematical methods are combined with fundamental laws to study processes of chemical relevance.*
- *Computational chemistry is a collection of (computer based) techniques for deriving, representing and manipulating the structures and reactions of molecules, and those properties that are dependent on these three dimensional structures.*

# Computational Chemistry

- A branch of chemistry that uses computer simulation to assist in solving chemical problems.
- It uses methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids.

# Computational Chemistry

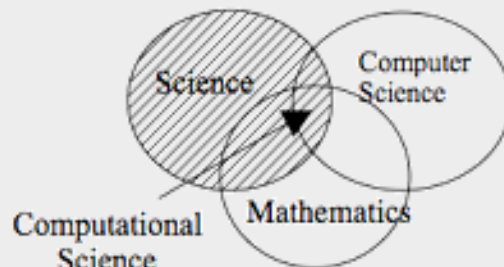
- \* Computational results normally complement the information obtained by chemical experiments, it can in some cases predict unobserved chemical phenomena.
- \* It is widely used in the design of new drugs and materials.

# Computational Chemistry

Examples of such properties are:

1. structure (i.e. the expected positions of the constituent atoms),
2. absolute and relative (interaction) energies,
3. electronic charge distributions,
4. dipoles and higher multipole moments,
5. vibrational frequencies,
6. reactivity
7. or other spectroscopic quantities

# Computational Chemistry



- The branch of chemistry that uses computers to generate information that is complementary to experimental data on the structures, properties, and reactions of substances
- Mostly based on one algorithm :  
**SCHROEDINGER'S EQUATION**
- Historically, computational chemistry has required use of high-performance systems

# Computational Chemistry

“Computational chemistry simulates chemical structures and reactions numerically, based in full or in part on the fundamental laws of physics.”

*Foresman and Frisch*

*In Exploring Chemistry with Electronic Structure Methods*

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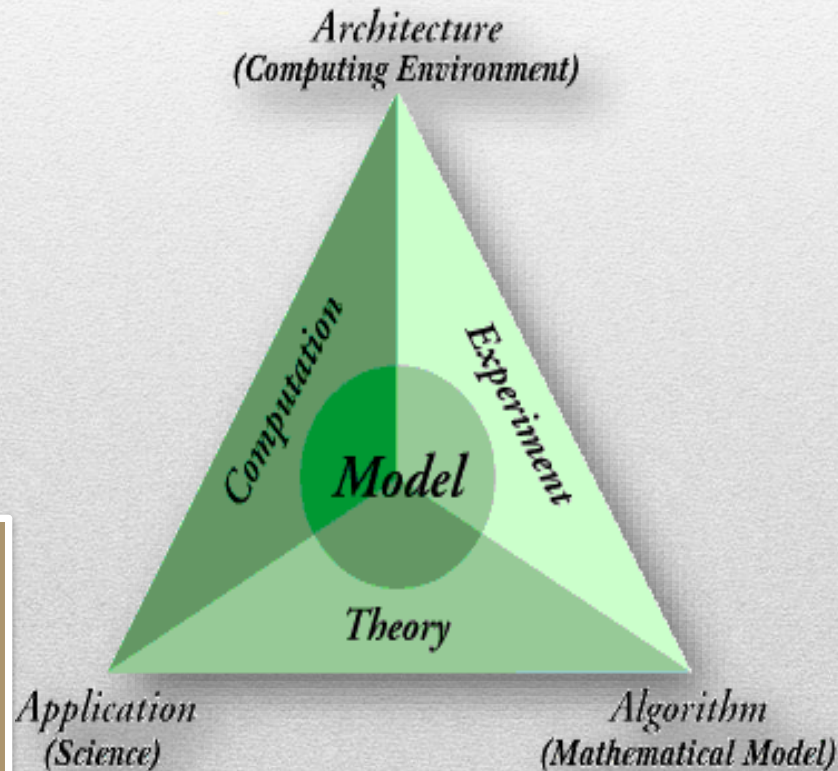
- Computational chemistry is a branch of chemistry concerned with theoretically determining properties of molecules.
  - Because of the difficulty of dealing with nanosized materials, computational modeling has become an important characterization tool in nanotechnology.
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# Why Computational Chemistry ?

- There are many interesting problems that can be solved using this technology that can not easily be solved using traditional methods
    - Too tedious to solve problems using calculator
    - Too dangerous and/or expensive to try to solve problems in the laboratory
    - Problems are only solvable using mathematical techniques or model
  - Establish a true marriage between mathematics, computing and science
-

# Tripartite Approach

**Architecture :**  
Choosing the right platform (hardware)  
to solve the problem



**Application :**  
understanding the  
science of the  
problem

**Algorithm:** creating  
a mathematical  
representation of  
problem, the  
“mathematical  
model”

# Application:

In computational science, the application refers to the type of science being studied, and/or the specific problem being addressed.

For example, this Guide specifically addresses one application: molecular modeling, also known as computational chemistry or computational quantum chemistry.

Specifically, this Guide focuses on electronic structure determination, which involves trying to solve a specific algorithm, known as the Schrödinger equation.

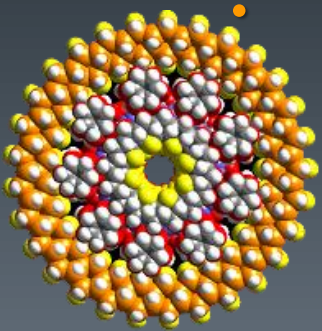
In electronic structure determinations, chemists calculate the structure, properties, and behavior of atoms and molecules, with an emphasis on the electrons.

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# Molecular modelling

Molecular modelling studies involve three stages:

- **Selection of a model;** A model is selected to describe the intra- and inter-molecular interactions in the system. The two most common models that are used in molecular modelling are quantum mechanics and molecular mechanics.
- **The calculation;** such as energy minimization, a molecular dynamics or Monte Carlo simulation, or a conformation search.
- **Analyzing;** The calculation must be analyzed, not only to calculate properties but also to check that it has been performed properly



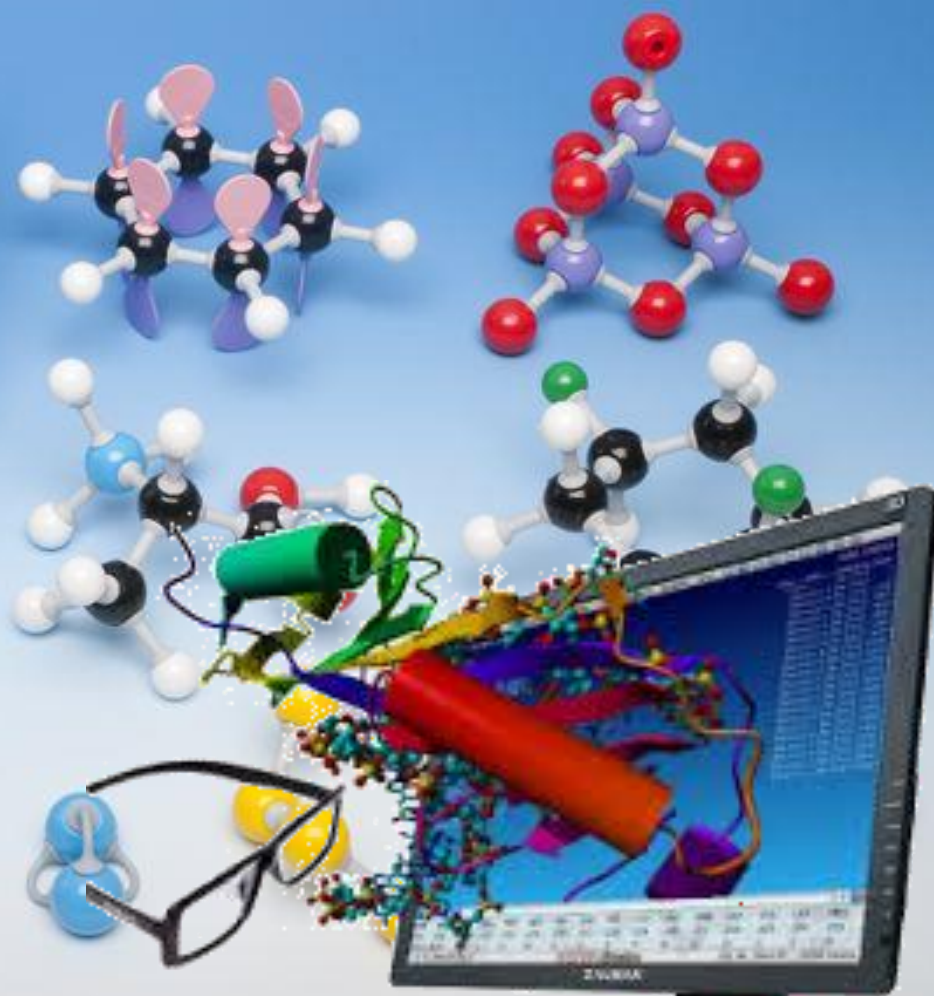
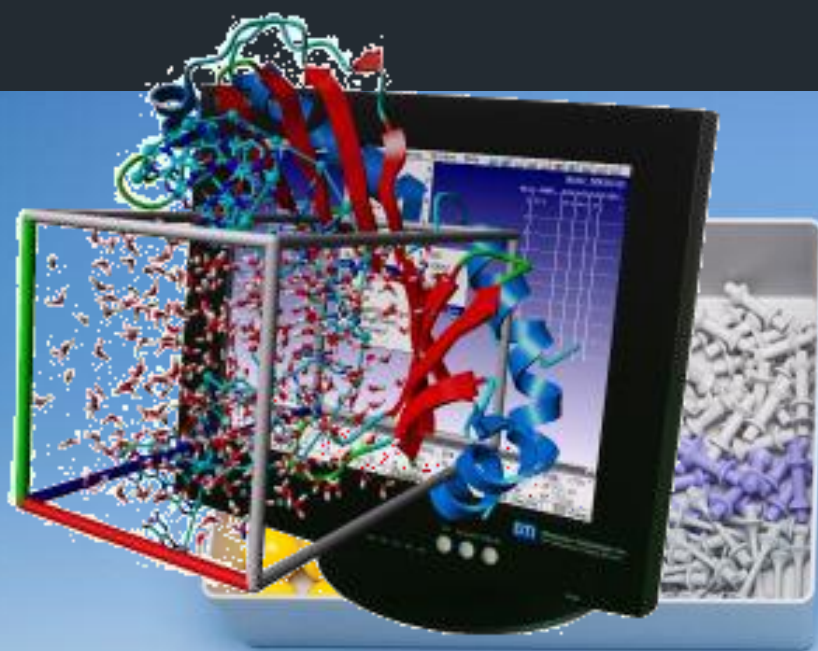
# Pemodelan Molekul



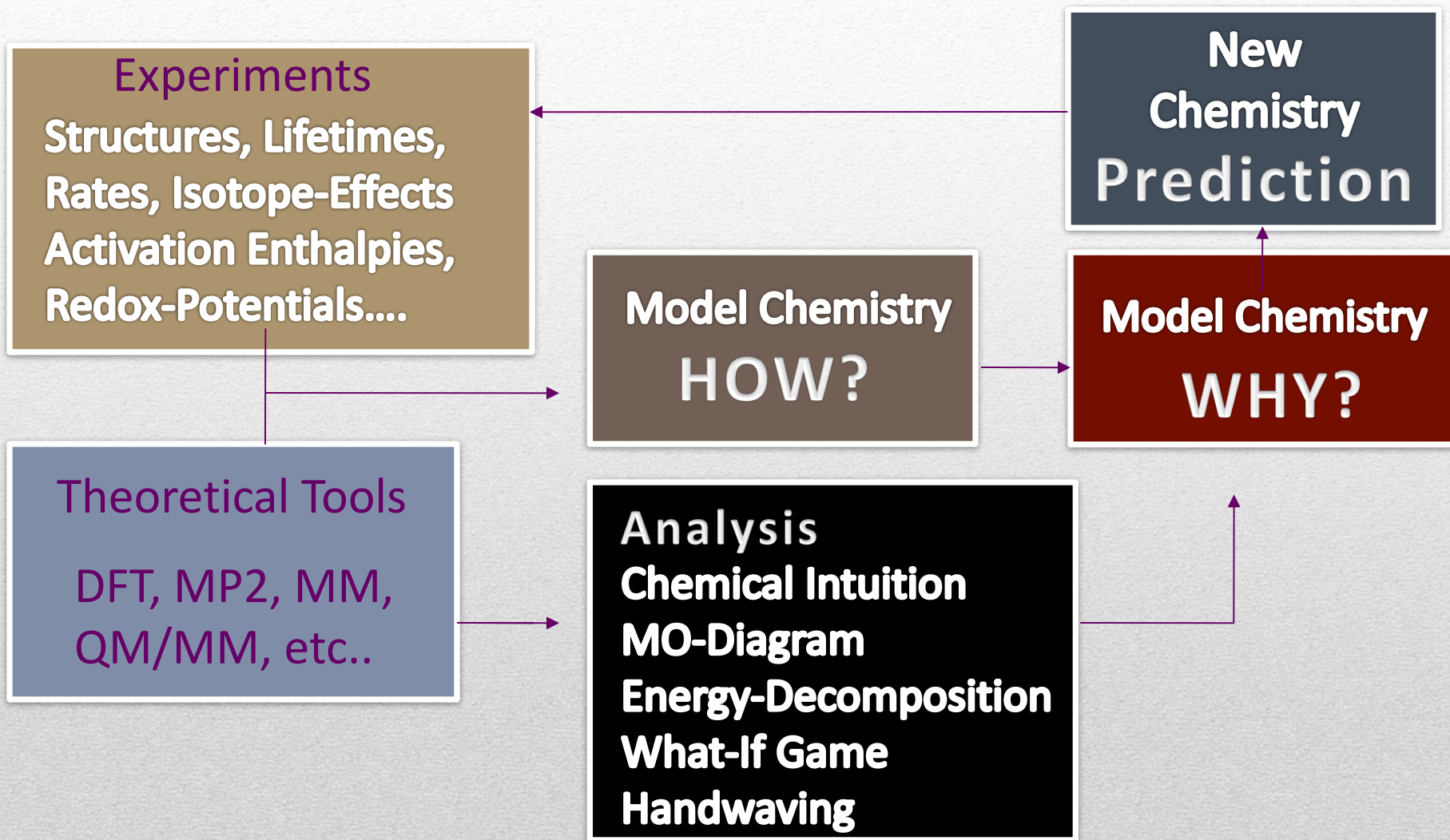
- Pemodelan molekul mencakup semua metode teoritis dan teknik komputasi yang digunakan untuk model atau meniru perilaku molekul.
- Teknik yang digunakan dalam bidang kimia komputasi, desain obat, biologi komputasi dan ilmu material untuk mempelajari sistem molekul mulai dari sistem kimia kecil ke besar molekul biologis dan rakitan materi.
- Fitur umum dari teknik pemodelan molekul adalah penjelasan tingkat atomistik dari sistem molekuler, termasuk memperlakukan atom sebagai unit terkecil individu (pendekatan mekanisme molekuler), atau secara eksplisit pemodelan elektron dari setiap atom (pendekatan kimia kuantum).

# Pemodelan Molekul

Teknik untuk mempelajari sistem molekul mulai dari sistem kimia kecil ke besar yang mencakup semua metode teoritis dan teknik komputasi yang digunakan untuk model atau meniru perilaku molekul dalam tingkat atomistik dari sistem molekuler.

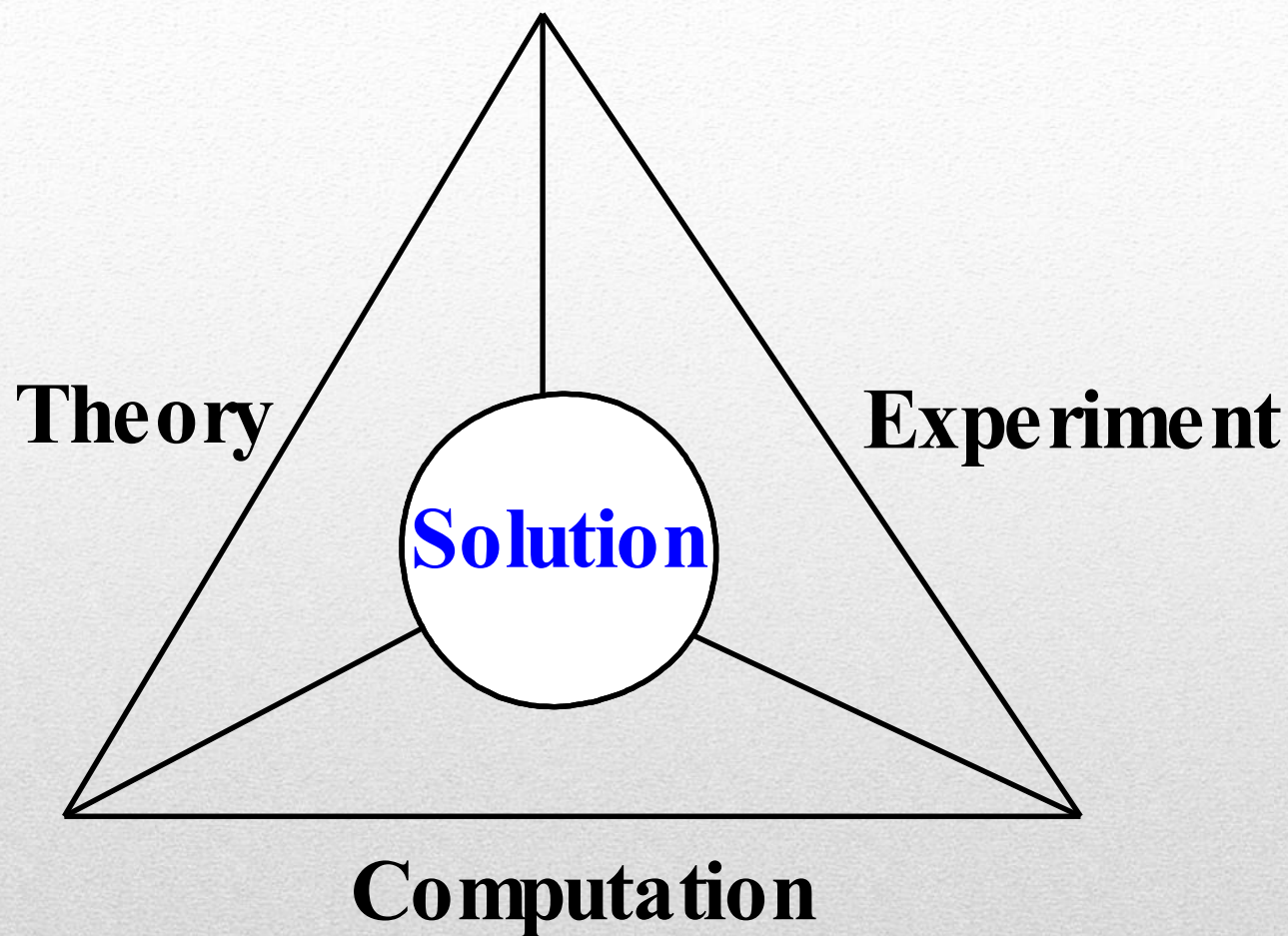


# General Research Philosophy



# Experimental Vs Theoretical

| EKSPERIMENTAL                                                                                                  | THEORETICAL                                                                                                                                                                                                                      |
|----------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <ol style="list-style-type: none"><li>1. Sistem diukur</li><li>2. Hasil pengukuran berbentuk numerik</li></ol> | <ol style="list-style-type: none"><li>1. Model sistem disusun sebagai himpunan persamaan matematik</li><li>2. Ada simplisitas sehingga model teoritis ini tidak dapat menjelaskan bentuk nyata dari sistem makroskopis</li></ol> |
| Deskripsi baru sistem kimia → eksperimen komputer                                                              |                                                                                                                                                                                                                                  |
| <i>COMPUTER EXPERIMENT</i>                                                                                     |                                                                                                                                                                                                                                  |



**Computational Chemistry**

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# COMPUTER EXPERIMENT

masih tetap menggunakan hasil dari pakar kimia teoritis, tetapi perhitungan dilakukan dengan komputer berdasar atas suatu "resep" algoritma yang dituliskan dalam bahasa pemrograman.

Model



Keuntungan

dimungkinkannya  
menghitung sifat molekul  
yang kompleks dan hasil  
perhitungannya berkorelasi  
secara signifikan dengan  
data eksperimen

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# COMPUTER EXPERIMENT

Perkembangan eksperimen komputer mengubah secara substansial hubungan tradisional antara teori dan eksperimen.



Simulasi komputer membutuhkan suatu metode yang akurat dalam memodelkan sistem yang dikaji.



Simulasi sering dapat dilakukan dengan kondisi yang sangat mirip dengan eksperimen sehingga hasil perhitungan kimia komputasi dapat dibandingkan secara langsung dengan eksperimen.

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# COMPUTER EXPERIMENT

## Modern

### Simulasi komputer bersifat sebagai:

- Alat untuk memahami dan menginterpretasi data eksperimen dalam tingkat mikroskopik,
- Alat mengkaji bagian yang tidak dapat dijangkau secara eksperimen, seperti reaksi pada kondisi tekanan yang sangat tinggi atau reaksi yang melibatkan gas berbahaya → instrumen penghasil data pelengkap eksperimen laboratorium

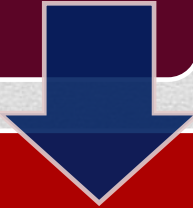
# COMPUTER EXPERIMENT

## Modern

Penelitian kimia dengan alat komputer pada era 1950-an dimulai dengan kajian hubungan struktur kimia dengan aktivitas fisiologi dari senyawa



John Pople berhasil mengkonversi teori-teori fisika dan matematika ke dalam kimia melalui program komputer



Metode kimia komputasi memungkinkan para kimiawan melakukan penentuan struktur dan sifat suatu sistem kimia dengan cepat.

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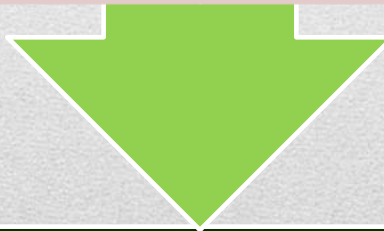
# Penerima Hadiah Nobel Tahun 1998

Walter Kohn:

Teori Fungsional Kerapatan  
(*Density Functional Theory*,  
*DFT*)

John A. Pople:

Berjasa dalam mengembangkan  
metode komputasi dalam kimia  
kuantum.

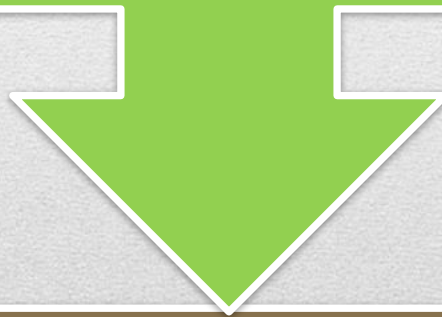


Mereka telah memberi peluang para kimiawan mempelajari  
sifat molekul dan interaksi antar molekul.

John Pople:

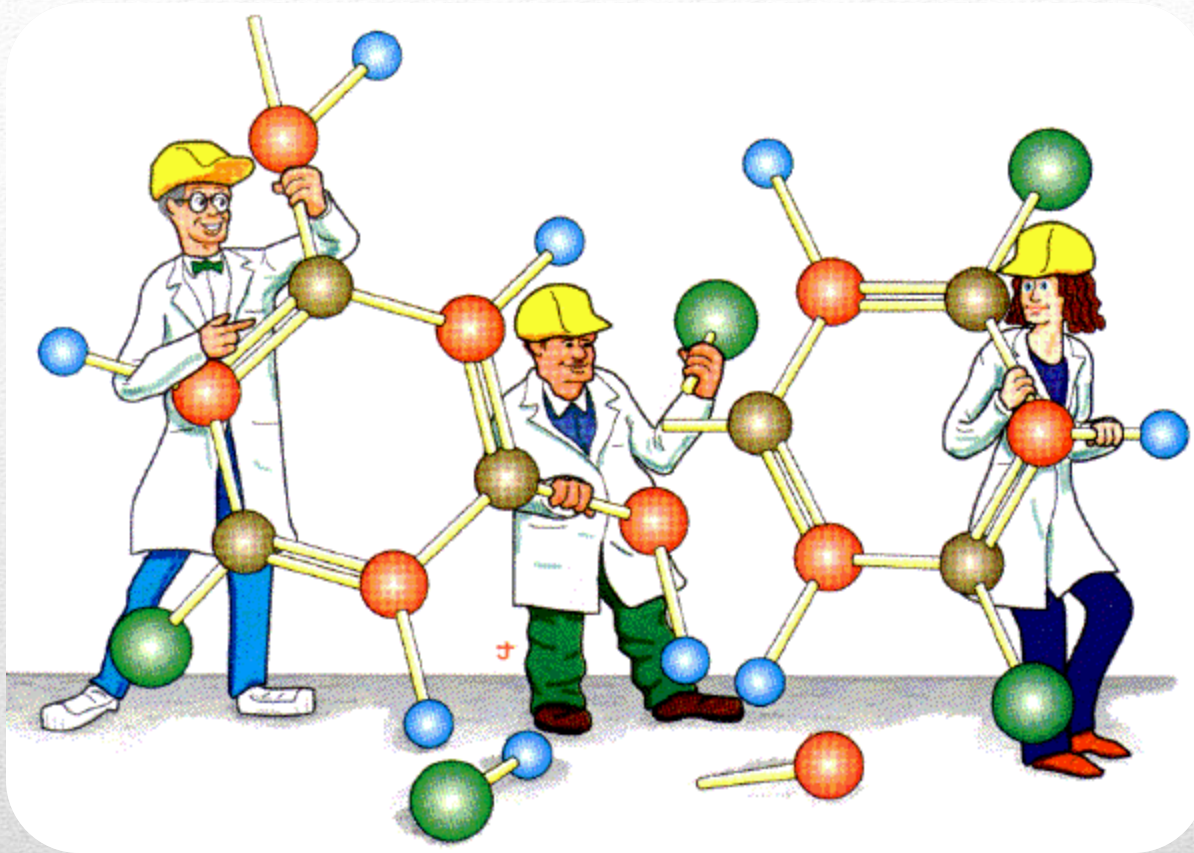
Mengembangkan kimia kuantum sebagai suatu metode yang dapat digunakan oleh hampir semua bidang kimia

Membawa kimia ke dalam era baru yaitu eksperimen dan teori bergabung dalam mengeksplorasi sifat sistem molekular



Salah satu produk program komputasi kimia yang dihasilkan Pople adalah GAUSSIAN

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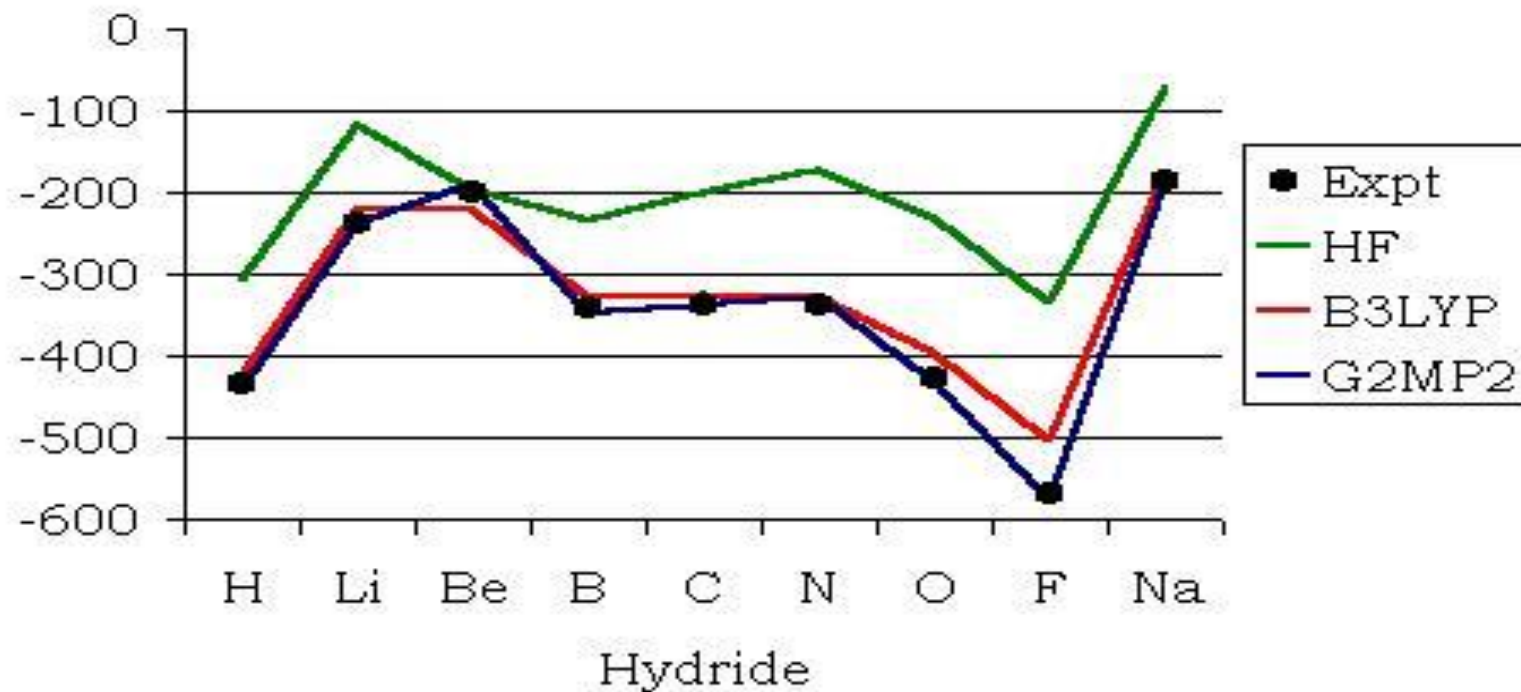


Makin banyak peneliti terapan yang memasuki penelitian teoretis molekuler

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# Experimental Vs theoretical

Bond Enthalpies [kJ/mol]



# NMR CHEMICAL SHIFT CALCULATIONS

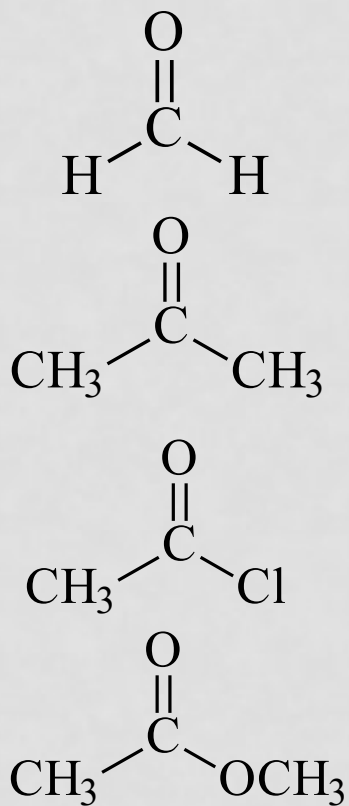
|                                                                 | <u>calc. (in ppm)</u>           | <u>expt.*</u> |
|-----------------------------------------------------------------|---------------------------------|---------------|
|                                                                 | * in CDCl <sub>3</sub> solution |               |
| CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> |                                 |               |
| C <sub>1</sub>                                                  | 15.9                            | <b>13.4</b>   |
| C <sub>2</sub>                                                  | 23.7                            | <b>25.2</b>   |
| CH <sub>3</sub> CH=CHCH <sub>3</sub>                            |                                 |               |
| C <sub>1</sub>                                                  | 18.4                            | <b>17.6</b>   |
| C <sub>2</sub>                                                  | 124.7                           | <b>126.0</b>  |
| benzene (C <sub>6</sub> H <sub>6</sub> )                        | 128.9                           | <b>130.9</b>  |

# NMR: EFFECT OF BASIS SET

Calculated chemical shifts (ppm) and difference from gas phase experimental values as a function of basis set

|                 | <u>Shift</u> | <u>Diff.</u> |
|-----------------|--------------|--------------|
| HF/6-31G(d)     | 127.3        | -3.6         |
| HF/6-31G(d,p)   | 128.4        | -2.5         |
| HF/6-31++G(d,p) | 128.9        | -2.0         |
| (observed)      | 130.9        | --           |

# IR FREQUENCIES ( $\text{CM}^{-1}$ , GAS PHASE)



Scaled Freq.

Expt.

**1805**

**1746**

**1799**

**1737**

**1850**

**1822**

**1797**

**1761**

# DIPOLE MOMENT

(in Debyes)

|                                      | <u>MMFF</u> | <u>AM1</u> | <u>HF /<br/>PM3</u> | <u>HF /<br/>3-21G*</u> | <u>MP2 /<br/>6-311+G**</u> | “    | Expt.       |
|--------------------------------------|-------------|------------|---------------------|------------------------|----------------------------|------|-------------|
| <b>NH<sub>3</sub></b>                | 2.04        | 1.85       | 1.55                | 1.75                   | 1.68                       | 1.65 | <b>1.47</b> |
| <b>H<sub>2</sub>O</b>                | 2.46        | 1.86       | 1.74                | 2.39                   | 2.12                       | 2.08 | <b>1.85</b> |
| <b>P(CH<sub>3</sub>)<sub>3</sub></b> | 2.06        | 1.52       | 1.08                | 1.28                   | 1.44                       | 1.31 | <b>1.19</b> |
| <b>thiophene</b>                     | 1.32        | 0.34       | 0.67                | 0.76                   | 0.80                       | 0.47 | <b>0.55</b> |

(note that none are very accurate; this reflects two factors: equilibrium geometry is only one of several, even many, in an ensemble of conformations, and charges are ill-defined.

# Conformational Energy Difference

(in kcal/mol)

Generally poor:

Good:

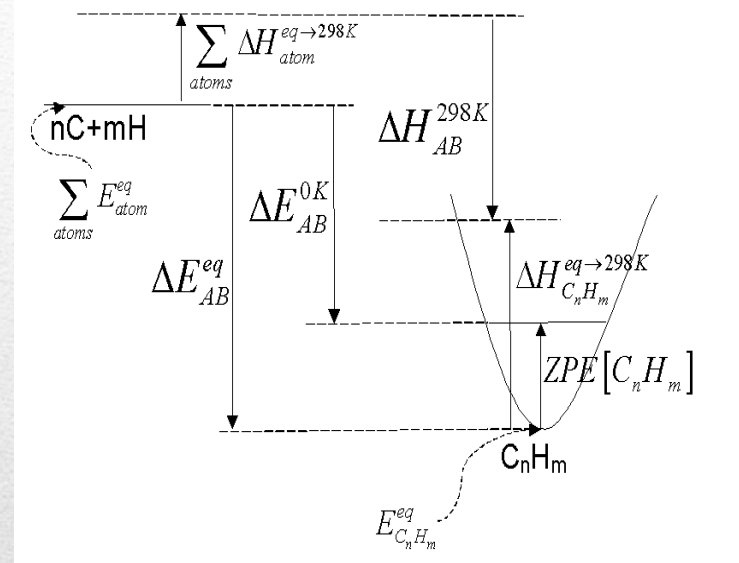
|                                         | <u>Sybyl</u> | <u>MMFF</u> | <u>AM1</u> | <u>HF /<br/>PM3</u> | <u>HF /<br/>3-21G*</u> | <u>MP2 /<br/>6-311+G**</u> | <u>“</u> | <u>Expt.</u> |
|-----------------------------------------|--------------|-------------|------------|---------------------|------------------------|----------------------------|----------|--------------|
| <b>acetone</b><br>(trans/gauche)        | 0.6          | 0.8         | 0.7        | 0.5                 | 0.8                    | 1.0                        | 0.6      | 0.8          |
| <b>N-Me formamide</b><br>(trans/cis)    | -1.8         | 2.6         | 0.4        | -0.5                | 3.9                    | 2.7                        | 2.7      | 2.5          |
| <b>1,2-diF ethane</b><br>(gauche/anti)  | 0.0          | -0.6        | -0.5       | 1.4                 | -0.9                   | 0.3                        | 0.8      | 0.8          |
| <b>1,2-diCl ethane</b><br>(anti/gauche) | 0.0          | 1.2         | 0.8        | 0.6                 | 1.9                    | 1.9                        | 1.3      | 1.2          |

# EQUILIBRIUM BOND LENGTH

(in Å)

|                                      | <u>Sybyl</u> | <u>MMFF</u> | <u>AM1</u> | <u>PM3</u> | <u>HF /</u><br><u>3-21G*</u> | <u>HF /</u><br><u>6-311+G**</u> | <u>MP2</u><br>“ | <u>Expt.</u> |
|--------------------------------------|--------------|-------------|------------|------------|------------------------------|---------------------------------|-----------------|--------------|
| <b>propane</b><br>(C-C single)       | 1.551        | 1.520       | 1.501      | 1.512      | 1.541                        | 1.525                           | 1.526           | 1.526        |
| <b>propene</b><br>(C=C double)       | 1.334        | 1.334       | 1.331      | 1.328      | 1.316                        | 1.316                           | 1.336           | 1.318        |
| <b>1,3-butadiene</b><br>(C=C double) | 1.338        | 1.338       | 1.335      | 1.331      | 1.320                        | 1.320                           | 1.342           | 1.345        |
| <b>propyne</b><br>(C≡C triple)       | 1.204        | 1.201       | 1.197      | 1.192      | 1.188                        | 1.181                           | 1.214           | 1.206        |

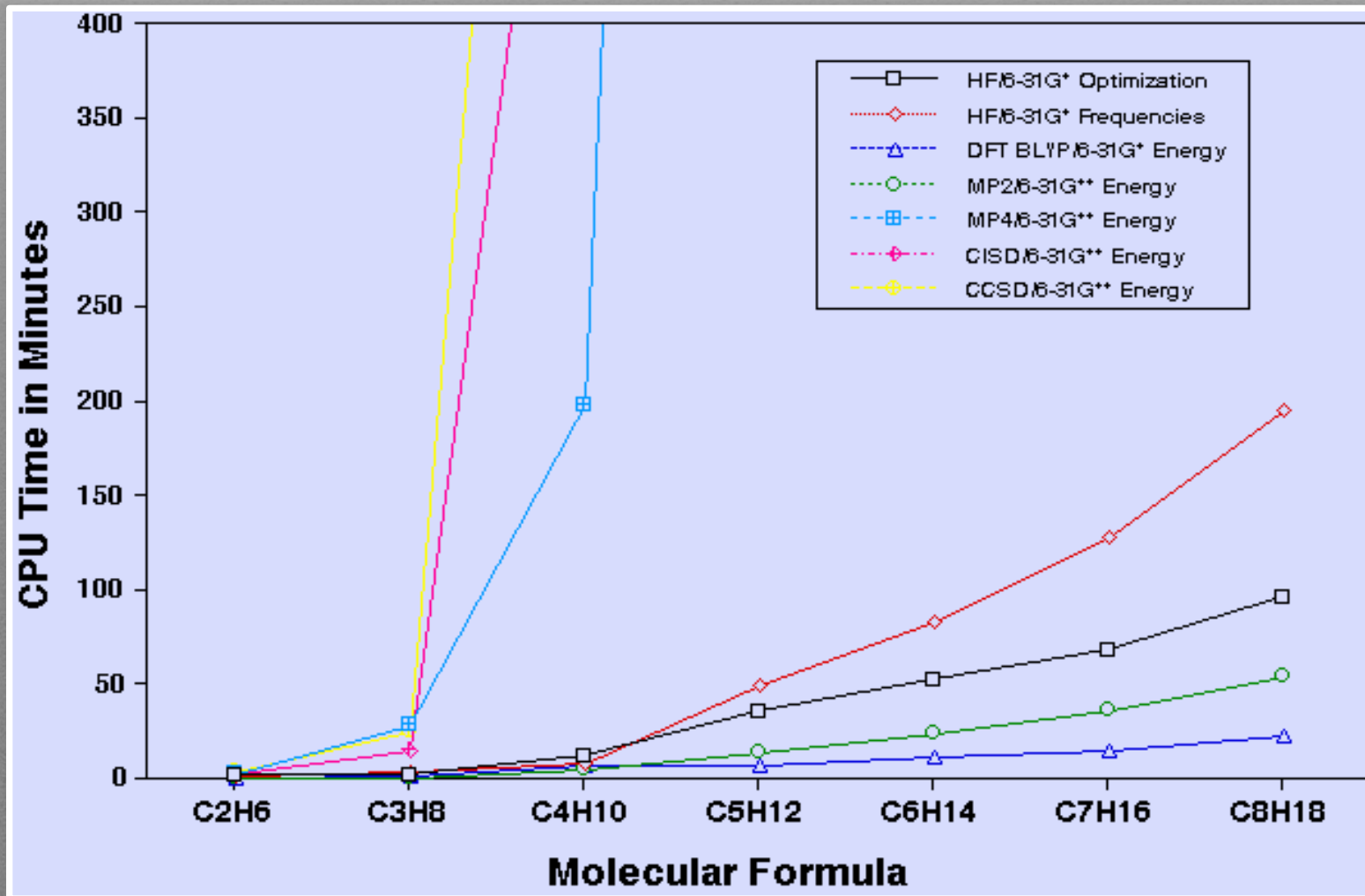
| species                       | Method          | Eeq<br>(H)              | $\Delta H_f^{298K}$<br>(kcal/mol) |
|-------------------------------|-----------------|-------------------------|-----------------------------------|
| CH <sub>4</sub>               | PM3             |                         | -13.0                             |
|                               | HF/6-31G*       | -40.19517               | +77.51                            |
|                               | HF/CBSB3        | -40.21237               | +76.04                            |
|                               | MP2/aug-cc-pVDZ | -40.367727              | +23.1                             |
|                               | G2              | -40.4535 <sup>a</sup>   | -18.50                            |
|                               | W2              |                         | -18.05                            |
|                               | G3              | -40.5003 <sup>a</sup>   | -18.04                            |
|                               | exp.            |                         | -17.89                            |
|                               | B3LYP/6-31G*    | -40.51838 <sup>b</sup>  | -17.95                            |
| C <sub>2</sub> H <sub>2</sub> | PM3             |                         | +50.7                             |
|                               | HF/6-31G*       | -76.81783               | +173.18                           |
|                               | HF/CBSB3        | -76.84932               | +166.94                           |
|                               | MP2/aug-cc-pVDZ | -77.092997              | +63.14                            |
|                               | G2              | -77.2120 <sup>a</sup>   | +55.99                            |
|                               | W2              |                         | +54.48                            |
|                               | G3              | -77.3022 <sup>a</sup>   | +55.08                            |
|                               | exp.            |                         | +54.19                            |
|                               | B3LYP/6-31G*    | -77.325646 <sup>b</sup> | +63.11                            |



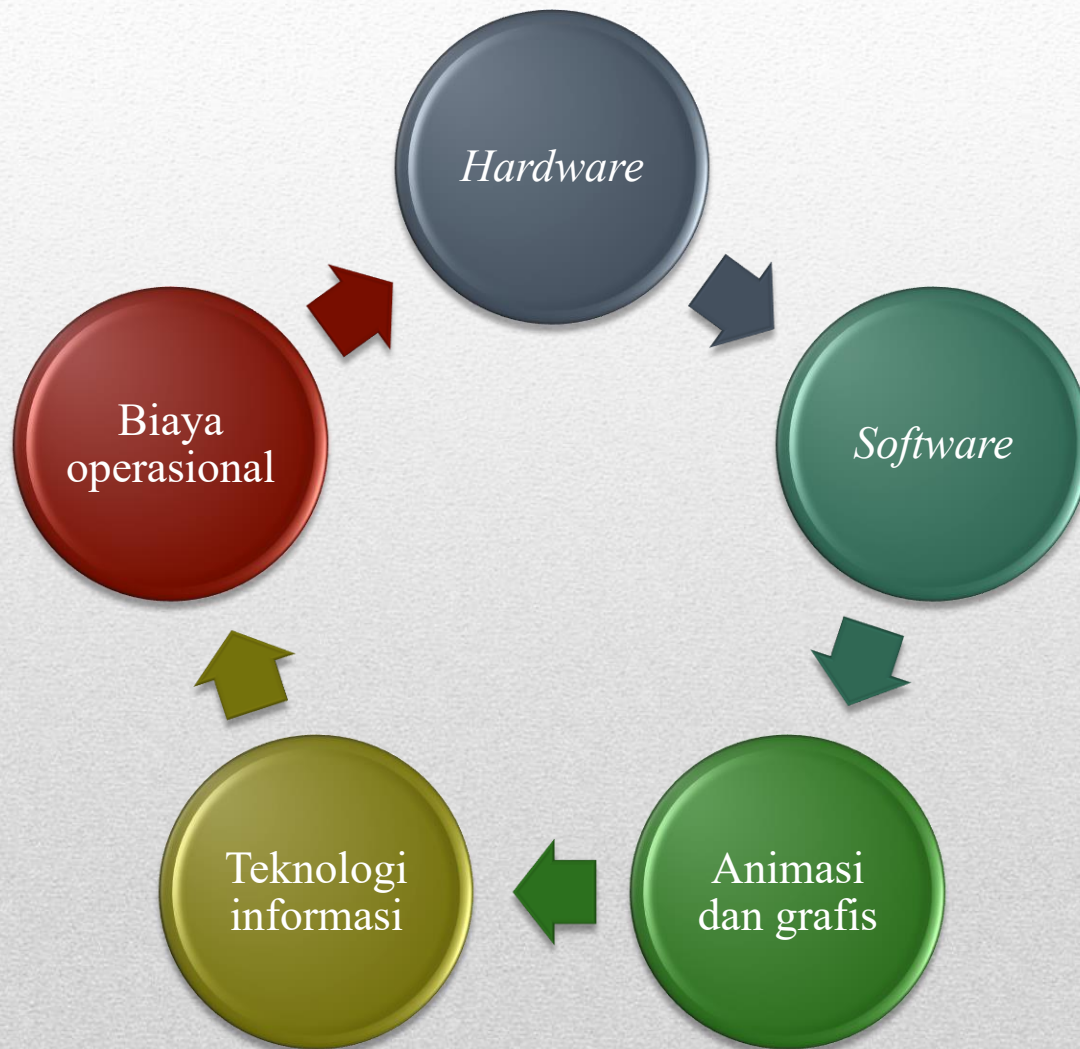
<sup>a</sup>estimated with harmonic approximation for vibrations, scaling factor of 0.8929 from a HF/6-31G\* calc.

<sup>b</sup>method not variational, an unknown electron-correlation term has been added to the real Hamiltonian

# CPU time vs Method



# DUKUNGAN PADA KIMIA KOMPUTASI



## 1. Dinamika molekular:

- Pengujian perilaku molekul atau sistem kimia sebagai fungsi waktu, seperti gerakan vibrasional atau gerakan Brownian
  - Penerapan pada sistem pelarut / zat terlarut memungkinkan perhitungan sifat sistem seperti koefisien difusi atau fungsi distribusi radial untuk digunakan dalam perhitungan mekanika statistik
  - Sangat berguna dalam mempelajari sistem molekular seperti molekul organik dalam larutan dan senyawa makromolekul dalam proses metabolisme.
  - Memungkinkan penggambaran struktur, sifat termodinamika dan sifat dinamis dari sistem pada fasa terkondensasi
-

## 2. Mekanika statistika:

- Cara matematika untuk mengekstrapolasi sifat termodinamika materi secara keseluruhan (*bulk*) berpijak pada gambaran molekular materi.
  - Masih dalam tataran metode kertas dan pensil, karena ahli mekanika kuantum belum dapat menyelesaikan persamaan Schroedinger secara eksak hingga sekarang sehingga ahli mekanika statistik tidak mempunyai titik awal untuk mengembangkan metode penyelesaiannya.
  - Perhitungan mekanika statistika sering dilakukan pada akhir perhitungan *ab initio* terhadap sifat fasa gas.
-

## 2. Mekanika statistika:

Salah satu metode mekanika statistika yang banyak digunakan dalam kimia komputasi adalah **Monte Carlo**. Metode Monte Carlo digunakan untuk mendapatkan gambaran tentang struktur dan energi dalam keseimbangan, tetapi tidak dapat memberikan gambaran dinamika atau sifat yang bergantung pada waktu.

---

## 3. Pemodelan keadaan padat

- Perhitungan *ab initio* dan semiempiris menghasilkan energi orbital, sehingga mereka dapat diterapkan pada perhitungan struktur pita.
  - Perhitungan struktur pita telah dilakukan untuk sistem yang sangat kompleks, namun software belum otomatis dan belum cukup cepat untuk menyelesaikan kasus-kasus struktur pita.
-

## 4. Termodinamika

Perhitungan kimia komputasi dapat membantu penyelesaian penghitungan besaran termodinamika, terutama untuk molekul-molekul yang besar.

---

## 5. Hubungan struktur dan sifat

- Pendefinisian empiris kualitatif atau kuantitatif antara struktur molekul dengan sifat yang teramati
- Pendekatan teoritis untuk menghitung secara kuantitatif hubungan antara aktivitas biologis terhadap perubahan struktur senyawa
- Hubungan diturunkan menggunakan software fitting kurva untuk mendapatkan kombinasi linear sifat-sifat molekuler yang dapat memprediksi sifat-sifat yang dimaksud.
- Sifat molekuler biasanya didapatkan dari perhitungan model molekuler.

## 5. Hubungan struktur dan sifat

- Jika sifat digambarkan sebagai sifat fisika, seperti titik didih, hal ini dikenal dengan hubungan kuantitatif antara Struktur dan Sifat (*Quantitative Structure-Property Relationship, QSPR*).
  - Jika sifat digambarkan sebagai aktivitas biologis – misalnya aktivitas obat- maka dikenal sebagai hubungan kuantitatif antara Struktur dan aktivitas (*Quantitative Structure-Activity Relationship, QSAR*).
-

## 5. Hubungan struktur dan sifat

- Perkembangan lanjut dari QSAR adalah **QSAR** tiga dimensi, CoMFA (*Comparative Molecular Field Analysis*).
  - Dalam metode CoMFA, efek sterik, elektrostatik, luas permukaan dari molekul dihubungkan pada deskripsi molekular spesifik (substituen).
-

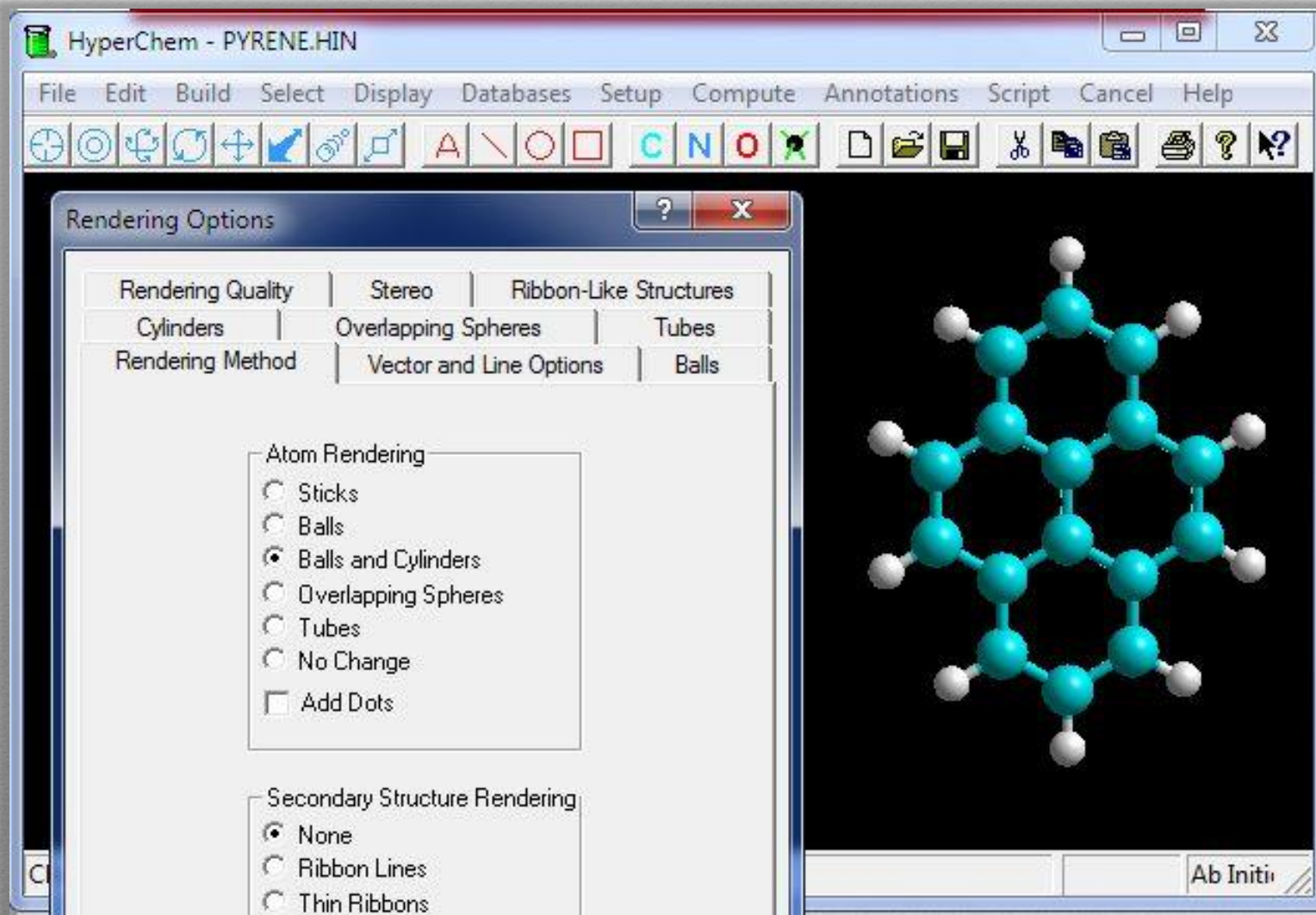
## 6. Perhitungan simbolik

- Perhitungan simbolik dikerjakan jika sistem sangat besar untuk digambarkan sebagai atom per atom sesuai dengan tingkat pendekatan yang ditetapkan
  - Perlakuan simbolik banyak digunakan pada komputasi bidang biokimia dan mikrobiologi
-

## 7. Inteligencia artificial

- Diterapkan pada kebanyakan kegiatan perancangan obat sehingga disebut *de Novo* atau rancangan obat rasional (*rational drug design*).
- Skenario umumnya adalah beberapa sisi fungsional diidentifikasi dan dilanjutkan dengan melihat struktur molekular yang akan berinteraksi dengan sisi tersebut agar dapat menentukan fungsi atau aktivitasnya.
- Hasil mekanika molekular diintegrasikan ke dalam program intelegensi artifisial yang mencoba sejumlah kecil kemungkinan yang beralasan secara otomatis

## 8. Visualisasi Molekul



## 9. Kajian konformasi dan struktur molekul

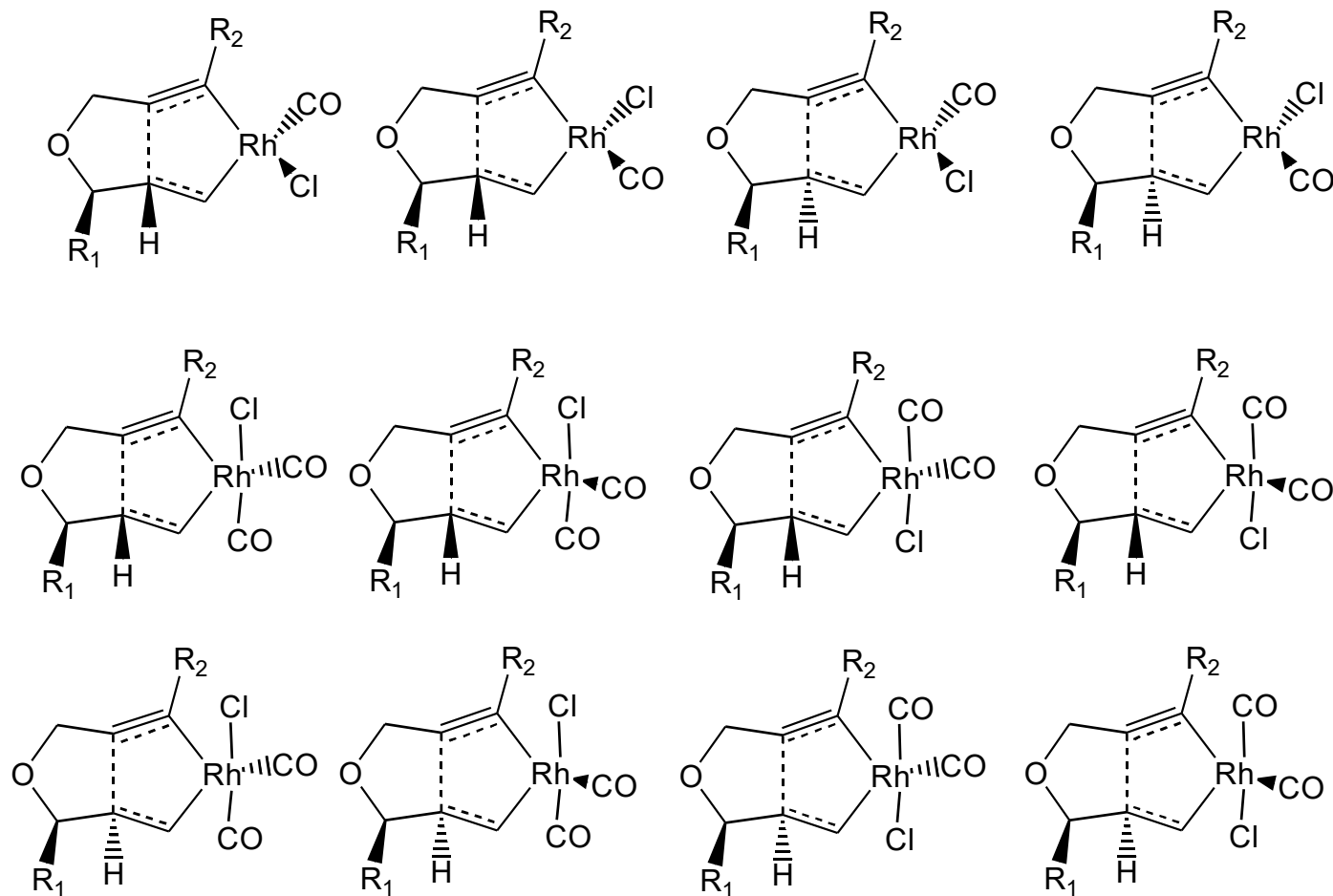
Penggambaran *side-chain* pada satu orientasi daripada yang lain, bentuk kursi dan perahu dan penggambaran ikatan hidrogen.

Semua masalah konformasi ini dapat diselesaikan dengan pemodelan molekul.

Hal ini menjadi penting karena konformasi akan mempengaruhi sifat dan energi molekul.

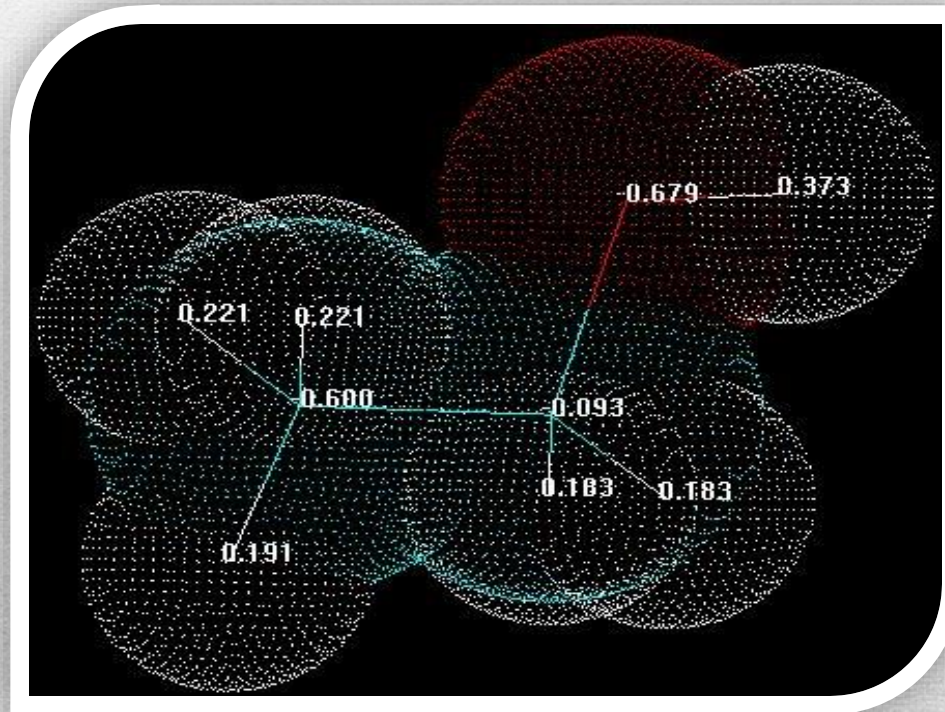
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# What about Structural Alternatives?

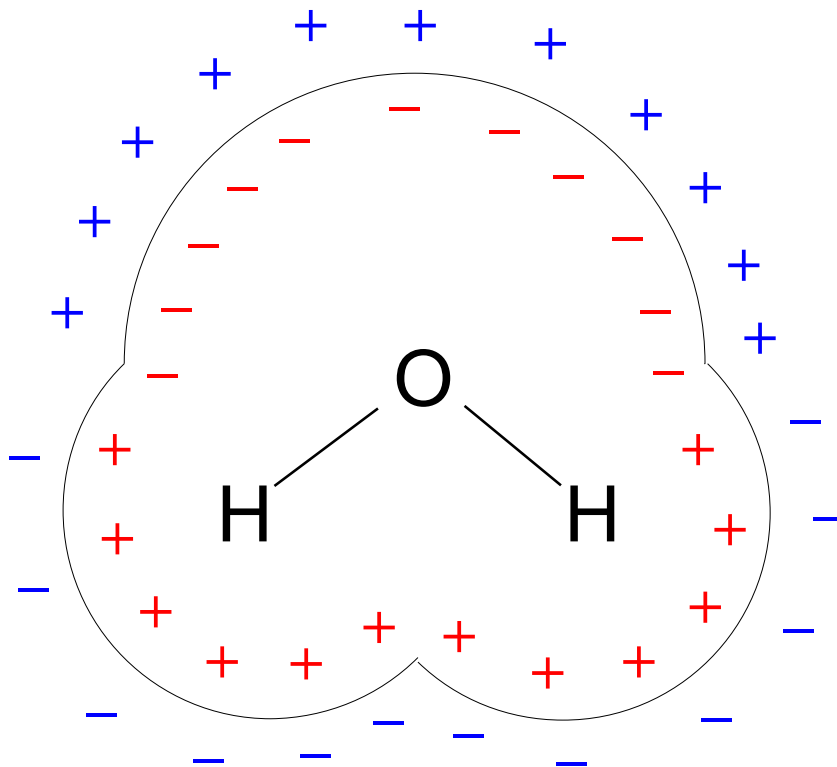
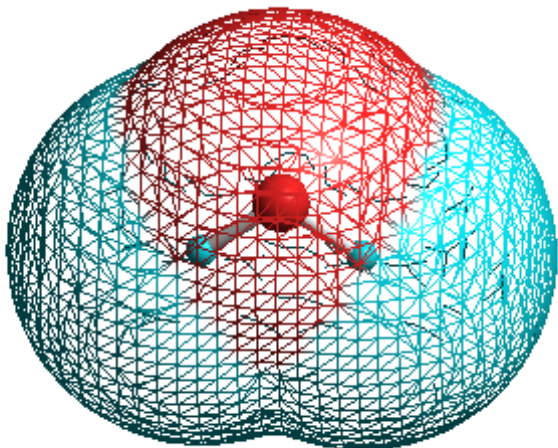


## 10. Kajian sifat molekul

Misal untuk mengetahui distribusi elektron yang berkaitan dengan perilaku molekul.



# Continuum Solvation Model



$$\hat{h}_i = \hat{h}_i^{gas} + \sum_k^M \frac{q_k}{|\mathbf{r}_k - \mathbf{r}_i|}$$

$$E^{ElSt.} = \int_S \sum_A \frac{Z_A \rho_S(r_S)}{|\mathbf{R}_A - \mathbf{r}_S|} d\mathbf{r}_S + \iint_S \frac{\rho_S(r_S) \rho_S(r'_S)}{|\mathbf{r}_A - \mathbf{r}'_S|} d\mathbf{r}_S d\mathbf{r}'_S$$

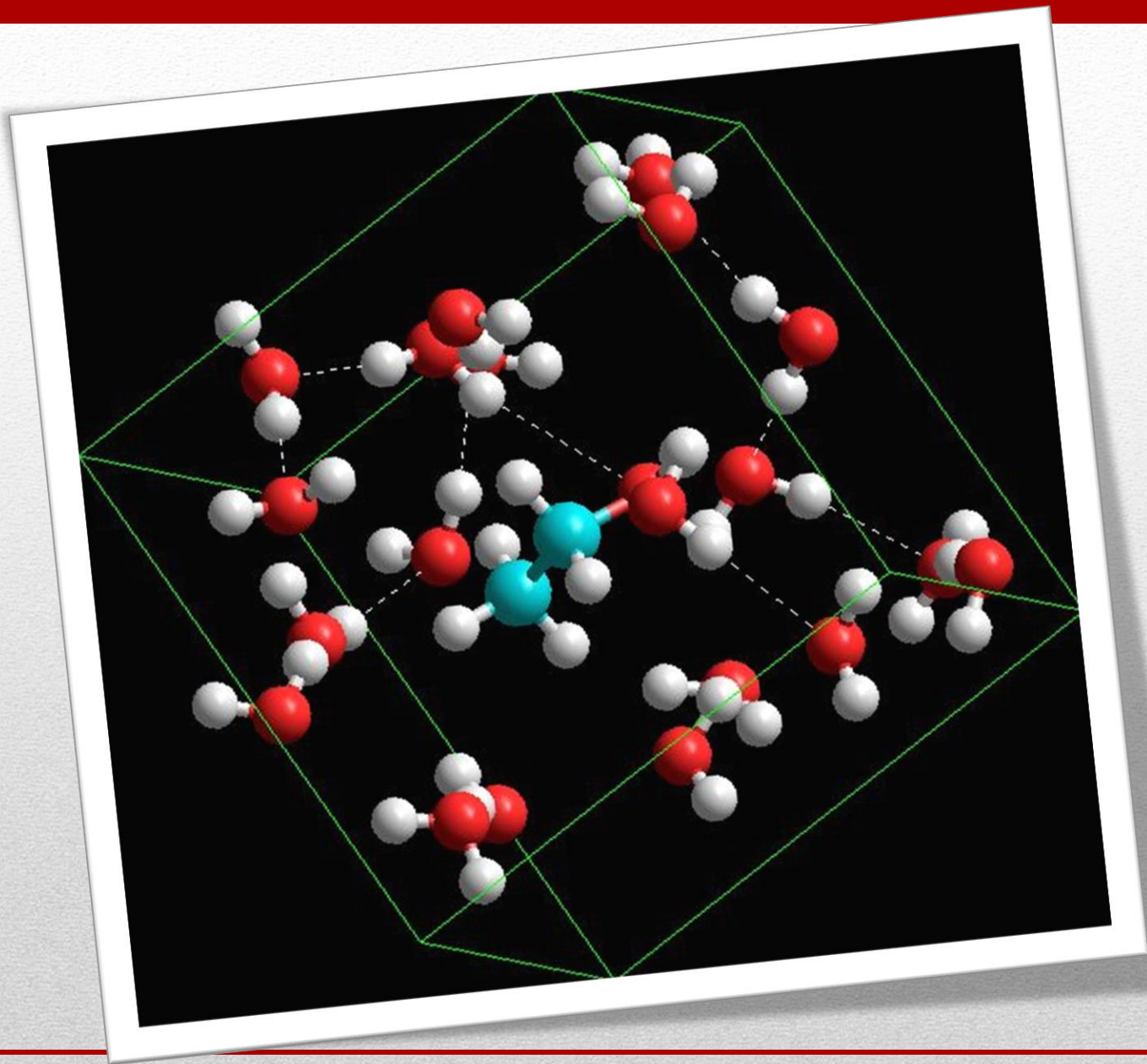
$$+ \iint_S \frac{\rho(r) \rho_S(r_S)}{|\mathbf{r} - \mathbf{r}_S|} d\mathbf{r}_S d\mathbf{r}$$

## 11. Membandingkan molekul

- Kajian ini meliputi kemiripan senyawa dan sifatnya.
  - Sifat dua senyawa yang berbeda penataan heteroatomnya dalam molekul, atau kemiripan volume senyawa dengan perbedaan sifat kimia.
-

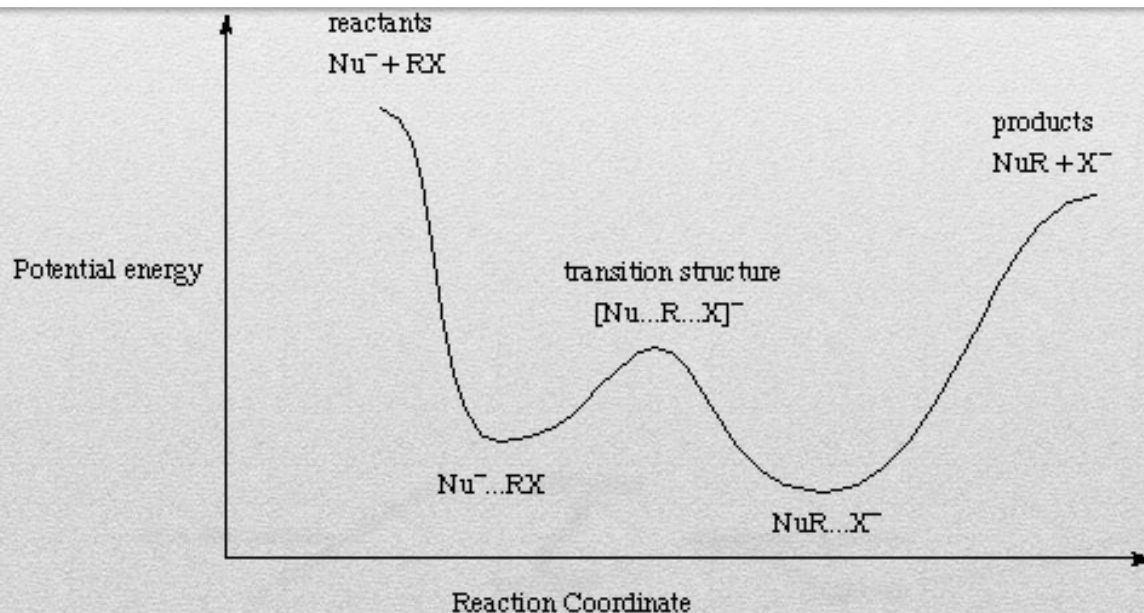
## 12. Kajian interaksi antar molekul

- Apakah sifat sejumlah molekul yang sama berbeda dengan molekul tunggal.
  - Apakah sifat molekul dipengaruhi oleh molekul yang ada di sekitarnya.
  - Simulasi komputer sangat membantu dalam menentukan model interaksi antar molekul.
-

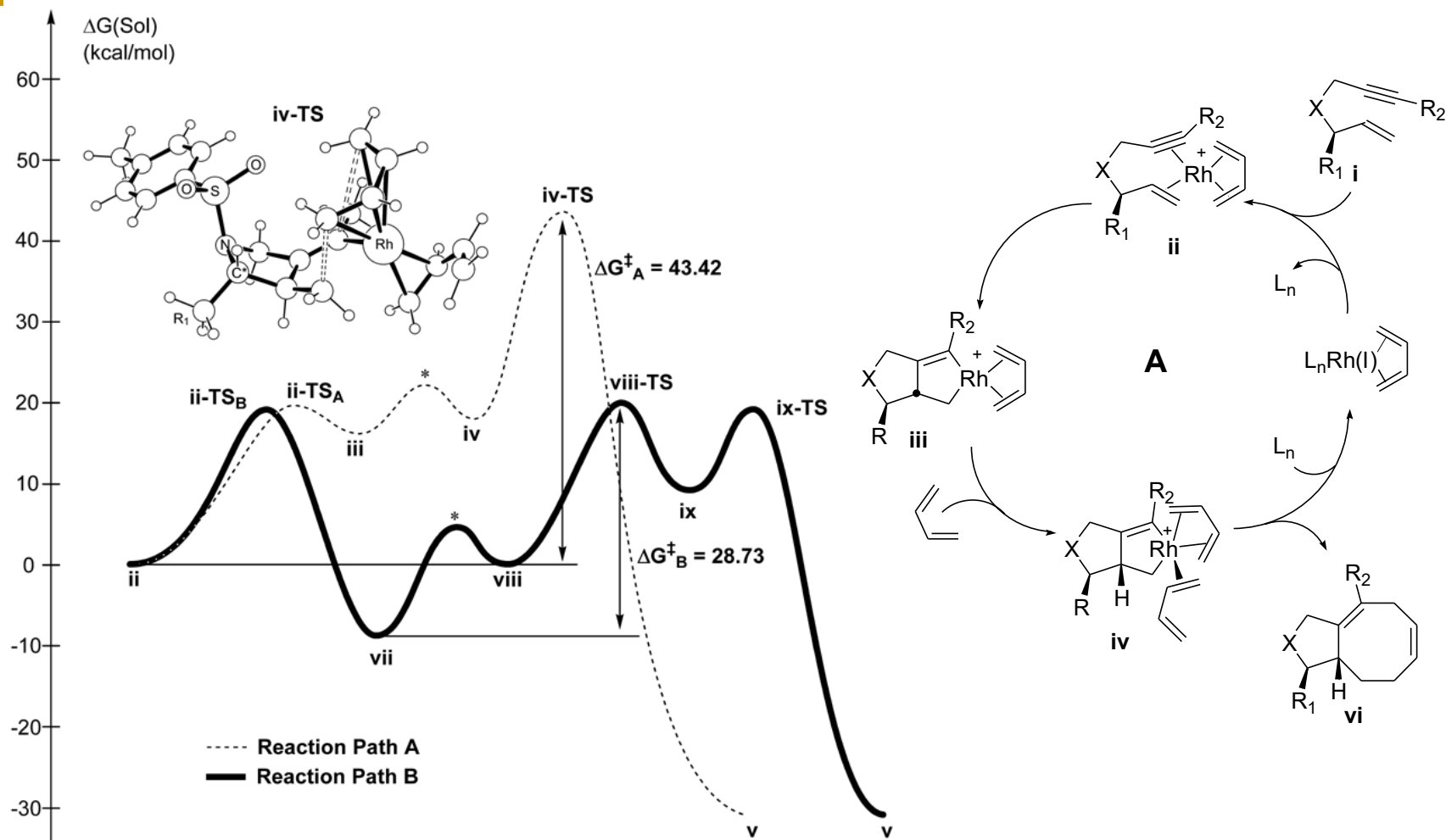


## 13. Kajian mekanisme reaksi.

Menyangkut kajian molekul pada keadaan khusus, seperti keadaan transisi yang mungkin mempunyai sifat berbeda dari molekul dalam keadaan normal.



# Computed Reaction Energy Profiles



## Peran penting pemodelan molekul:

1. Model merupakan sesuatu yang kita ajarkan. Model memberikan gambaran yang paling baik dan secara langsung dari dunia molekul.
  2. Model adalah cara yang baik untuk mengubah teori ke dalam prediksi kimia. Metode komputasi modern memberikan hasil pengujian yang jauh lebih baik dari prediksi teoritis.
  3. Model mudah untuk digunakan, tidak mahal dan aman.
-

# PENELITIAN KIMIA KOMPUTASI

## Problem penelitian kimia komputasi :

- Apa yang ingin kita diketahui?
- Metode/pendekatan komputasi apa yang tepat?
- Bagaimana keakuratan perhitungannya?
- Adakah support hardware yang diperlukan?
- Software apa yang tepat?
- Bagaimana cara menggunakan software?
- Bagaimana cara menguji validitas software dan hasil perhitungannya?
- Adakah dukungan data hasil eksperimen?
- Adakah jurnal penelitian yang terkait?

- Valid
- Akurat
- Efisien

# ● ● ● Conducting a Computational Project

1. These questions should be answered
  - What do you want to know?
  - How accurate does the prediction need to be?
  - How much time can be devoted to the problem?
  - What approximations are being made?
2. The answers to these questions will determine the type of calculation, model and basis set to be used.

# PENELITIAN KIMIA KOMPUTASI

## Akurasi prediksi hasil komputasi:

- Dengan eksperimen komputasi, melakukan perhitungan untuk hal yang sama dengan metode yang sama akan selalu memberikan hasil secara eksak sama.
  - Cara untuk mengukur keakuratan hasil adalah memperkirakan kesalahan perhitungan dengan membandingkan sejumlah perhitungan serupa dengan data eksperimen → harus tersedia artikel dan kompilasi data.
  - Jika data eksperimen tidak ada, maka harus menggunakan metode yang *reasonable*.
-

# What area of chemistry is most interesting?

1. Organic chemistry
  - Structures and mechanisms
2. Medicinal chemistry
  - Comparison of energies of lead drugs
3. Environmental chemistry
  - Rates of hydroxyl radical degradation in the atmosphere
4. Inorganic chemistry
  - Excitation states of coordination complexes
5. Reaction chemistry
  - Prediction of kinetics, thermodynamics, transition states

# Is there a particular category of computations that is of most interest?

## 1. Structure:

- Geometry optimizations based on model chemistry
- Comparison of computational results to experimental results
- Transition state geometries

## 2. Property:

- Determination of spectra
- Calculation of quantum descriptors (QSPR)

## 3. Activity:

- Reaction mechanisms
- QSAR-types of problems

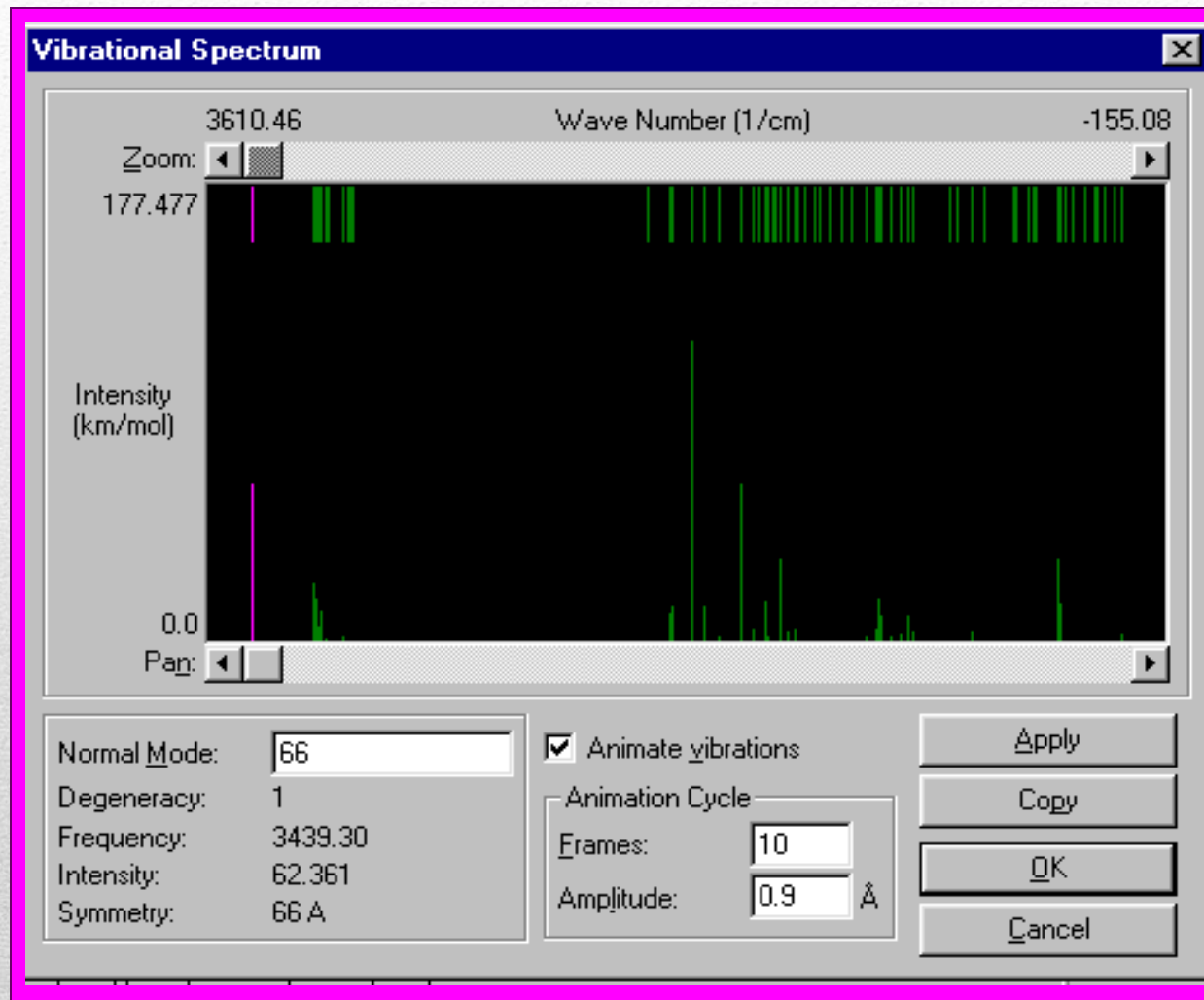
# RUANG LINGKUP KIMIA KOMPUTASI

- Energi, konformasi dan struktur molekul
  - Visualisasi Molekul
  - Spektroskopi
  - Mekanisme reaksi
  - Termodinamika/Termokimia
  - Sifat Molekul: muatan, momen dipol, sifat spektra UV, IR-NMR
  - Muatan Atomik dan Potensial Elektrostatik
-

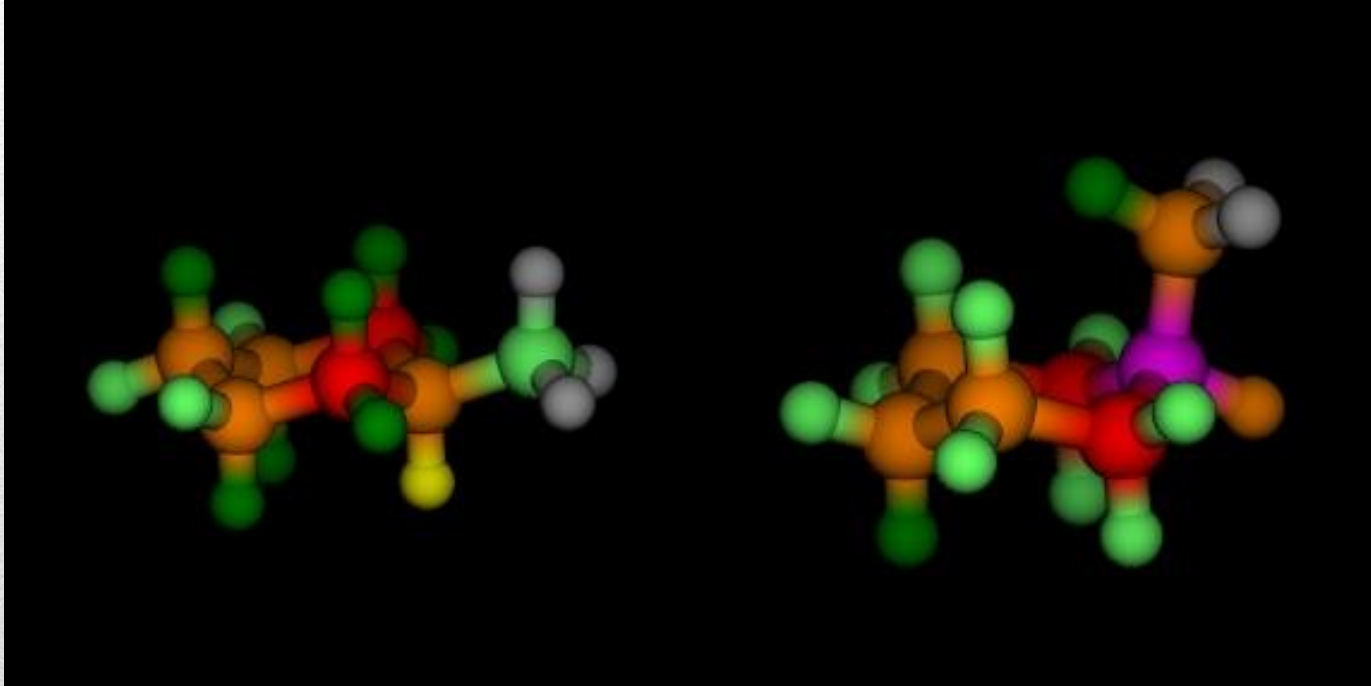
- Pembandingan molekul: membandingkan kemiripan senyawa dan sifatnya
  - Kajian Interaksi antar Molekul: teknik simulasi penentuan ttg model interaksi antar molekul (ikatan VdW, ik hidrogen, Coulombik, interaksi dipol-dipol)
  - Pemodelan Keadaan Padat (kristal), didefinisikan dg *band structure plot*
-

- QSAR/QSPR (*Quantitative Structure and Activity/Property Relationships*)
  - Statistika Mekanika (Monte Carlo)
  - Dinamika Molekular, sistem kimia vs waktu dg metode simulasi
  - Perhitungan simbolik, bidang biokimia dan mikrobiologi
-

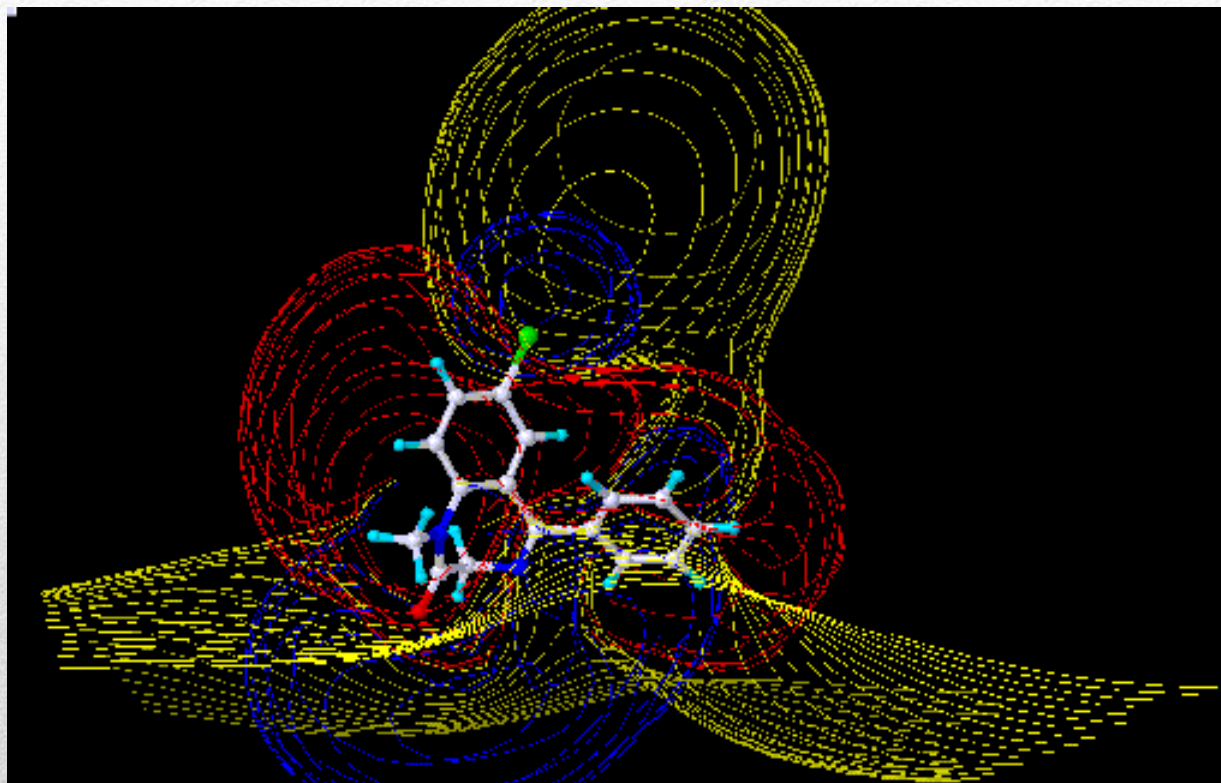
# Spektrum Vibrasi



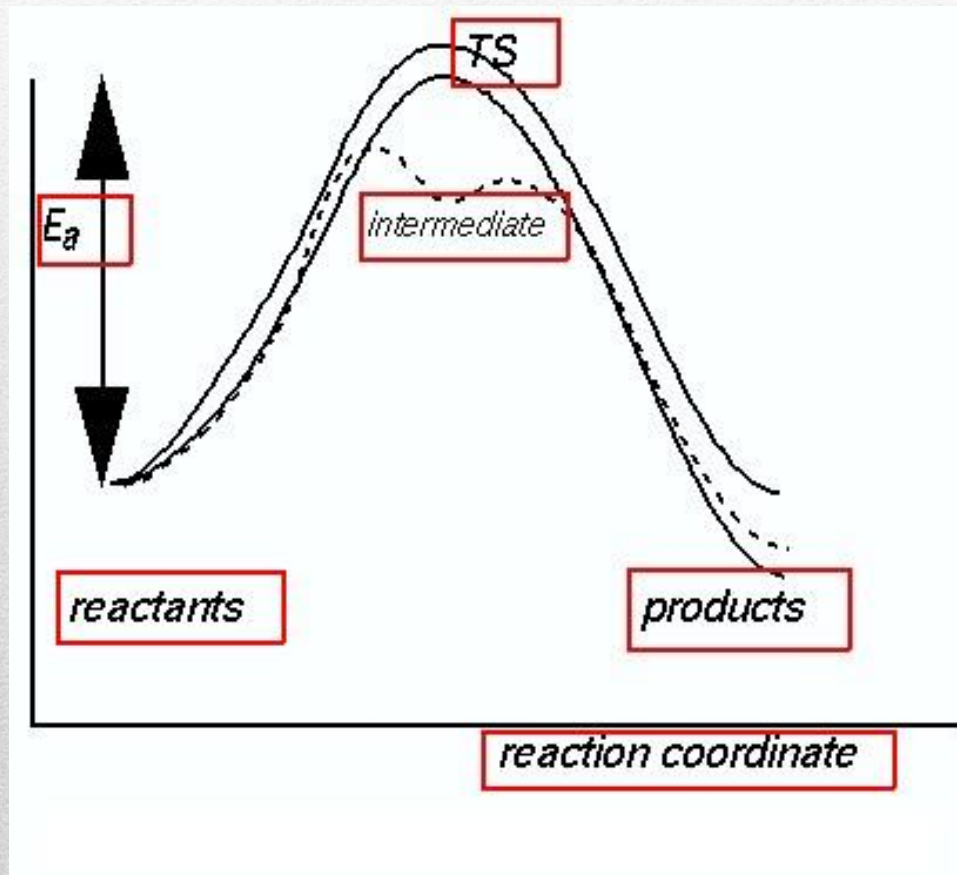
# Konformasi



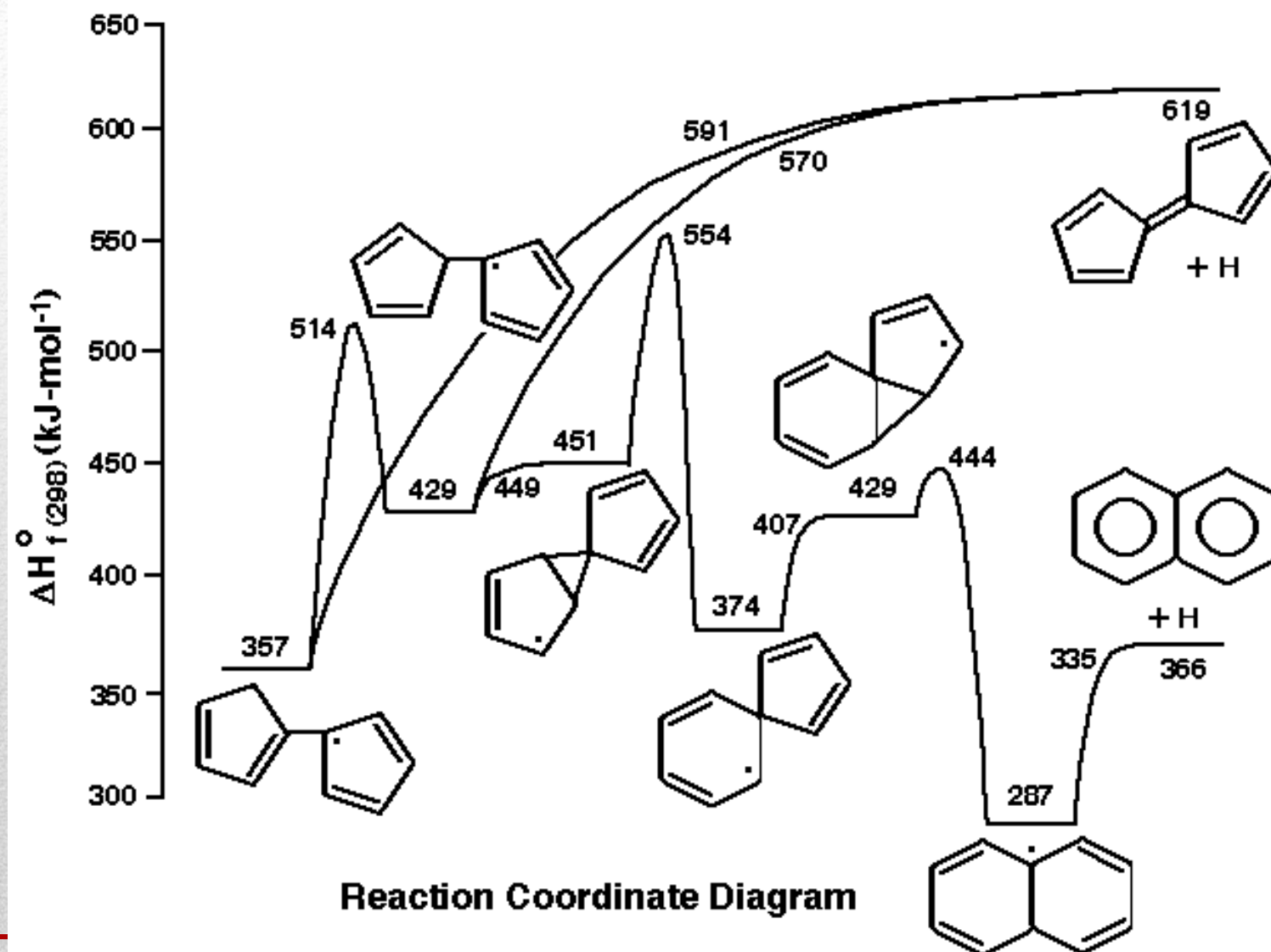
# Electrostatic potential



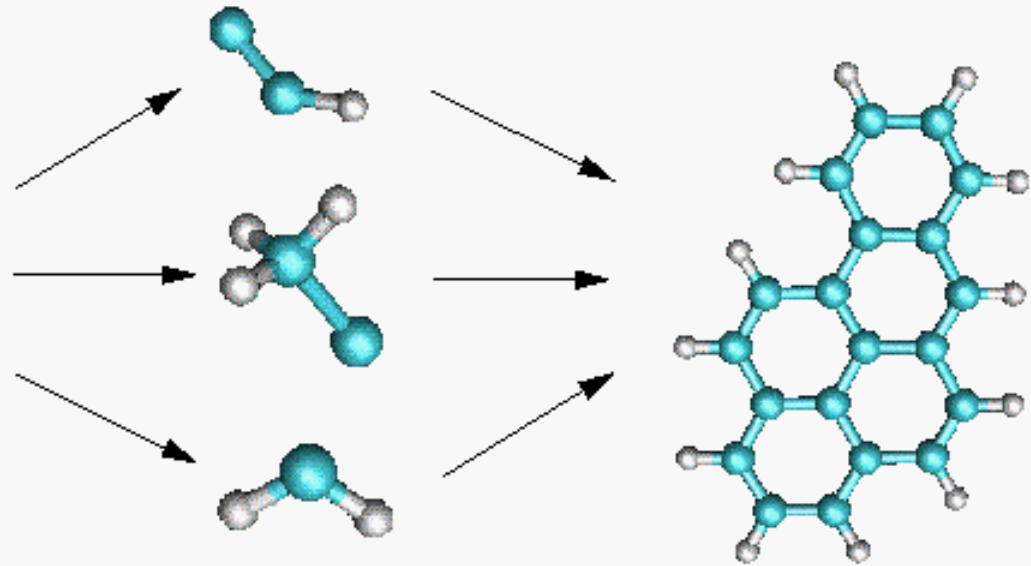
# Kadaan transisi



# Reaction of $C_{10}H_9 \rightarrow$ Naphthalene + H



## Pyrolysis Reaction Pathways

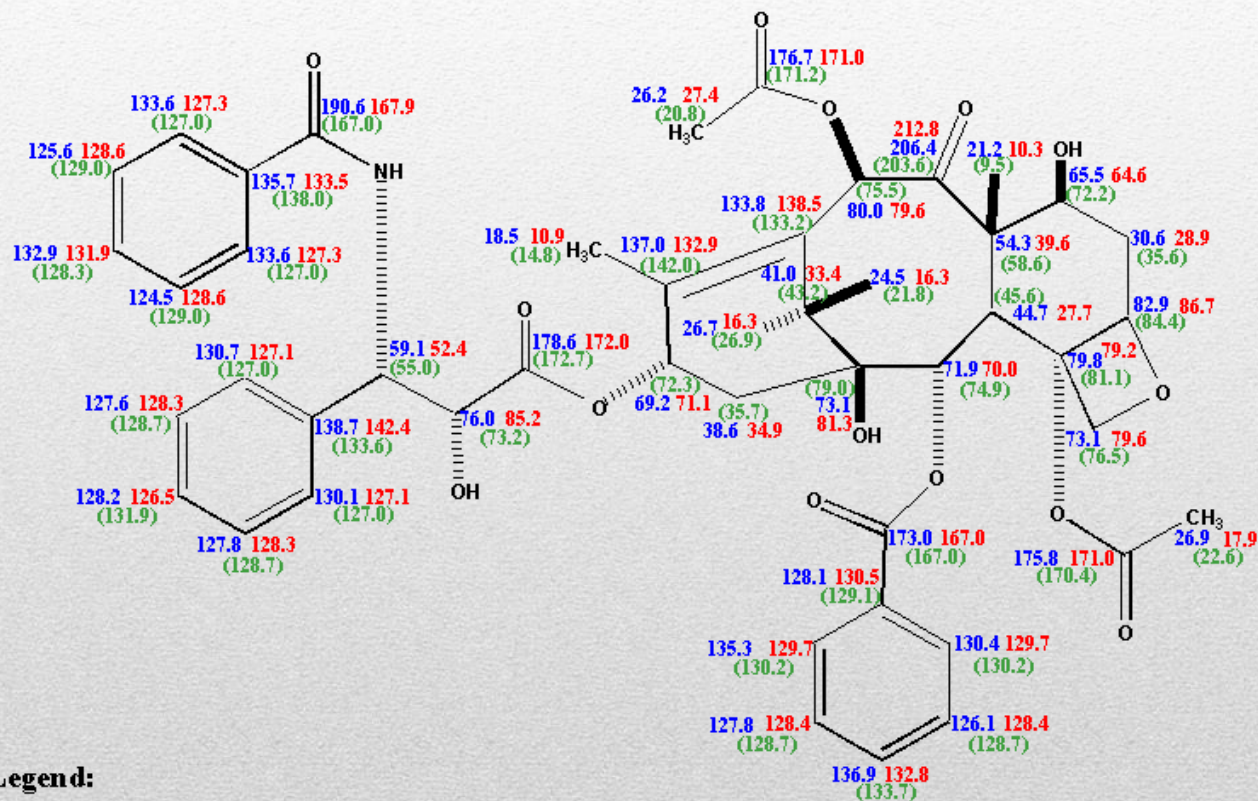


Benz[a]pyrene

Hydrocarbon Flame ———▶ Metastable Radicals ———▶ Stable Mutagens

# Spectroscopy

## Observed and Predicted $^{13}\text{C}$ Chemical Shifts for Taxol



### Legend:

Gaussian 98 Shift CS ChemNMRPro Shift  
(Observed Shift)

Layout occasionally modified due to space constraints.

Chemical shifts are with respect to TMS.

# Basis Set Effect

## Effective Core Potentials

ECP's are functions that are used to replace the core orbitals. They can greatly speedup calculations and can be used to approximate some relativistic effects; however, ECP's introduce another layer of approximation into the calculations.

**Example:  $\text{Si}_2\text{H}_4\text{Cl}_2$**

**HF/DZ (80 bfs):**

Optimization: 18 min. 41 sec.

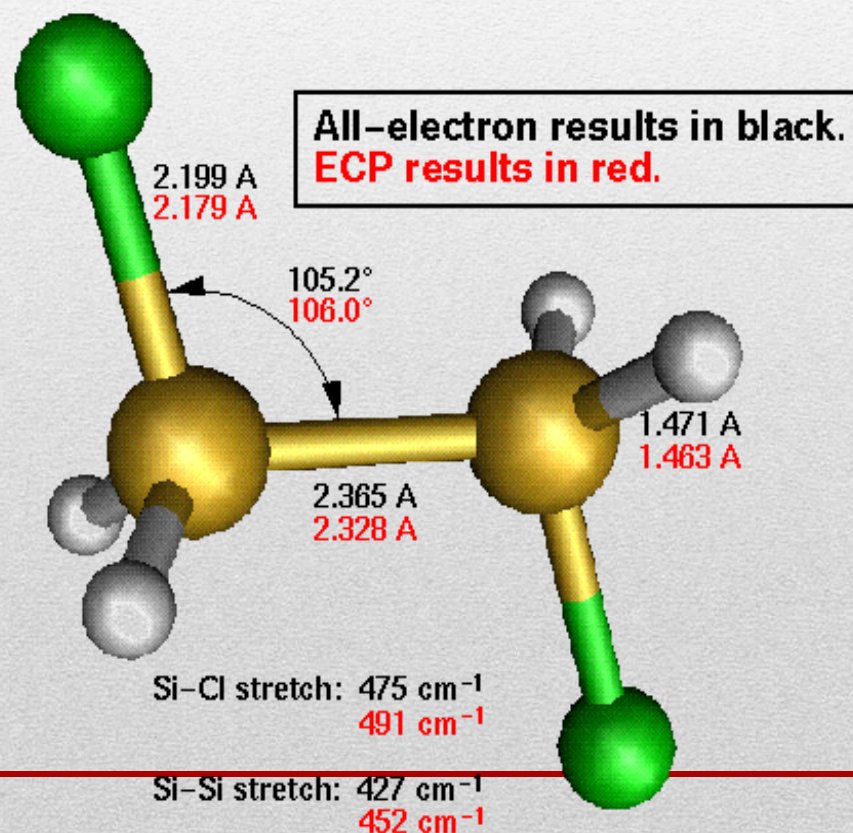
Frequencies: 10 min. 21 sec.

**HF/DZ+LANL2 ECP (40 bfs):**

Optimization: 5 min. 10 sec.

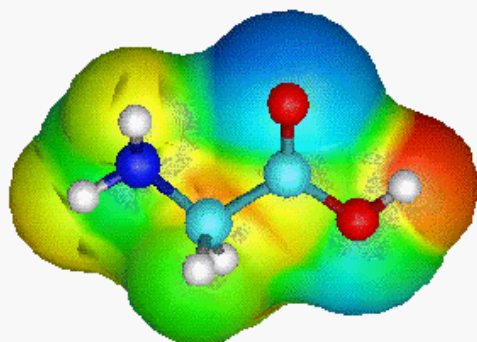
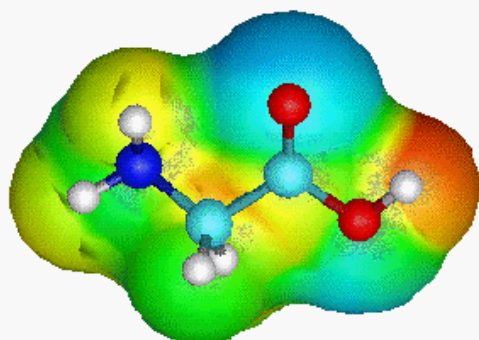
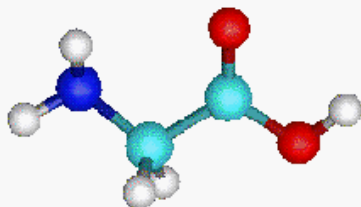
Frequencies: 31 min. 10 sec.\*

(\*By finite differences)

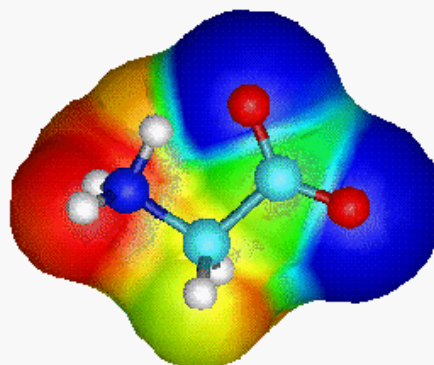
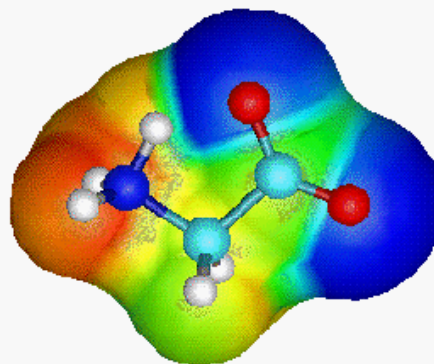
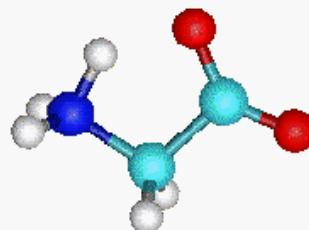


# Polarizable Continuum Solvation Model

Neutral



Zwitterion



Relative Energies

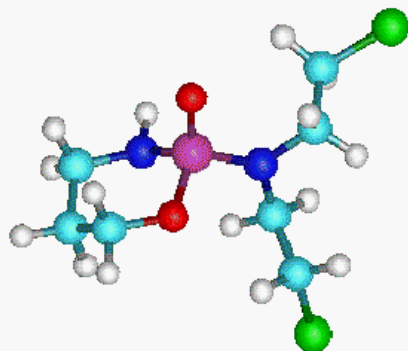
neutral – zwitterion  
(kcal/mol)

Gas Phase: -22.0

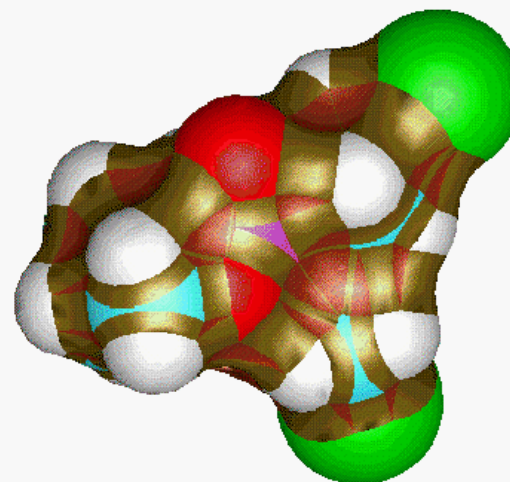
Zeroth order  
reaction field: -4.9

Self-consistent  
reaction field: +13.5

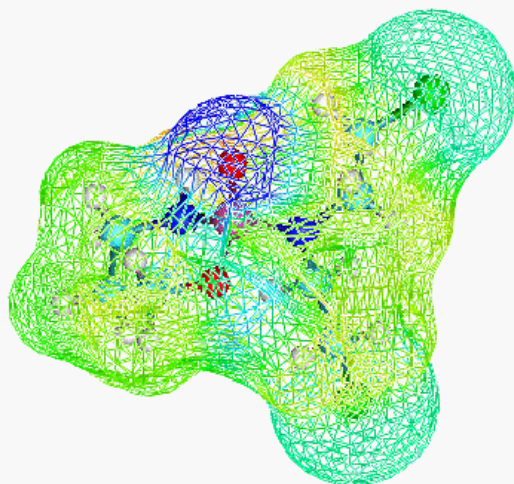
Comparison of induced surface charges on glycine neutral and zwitterion. Relaxation of the wavefunction lowers the zwitterion solvation energy by nearly 20 kcal/mole relative to the neutral. The increased charge separation is evident in the surface charges of the zwitterion.



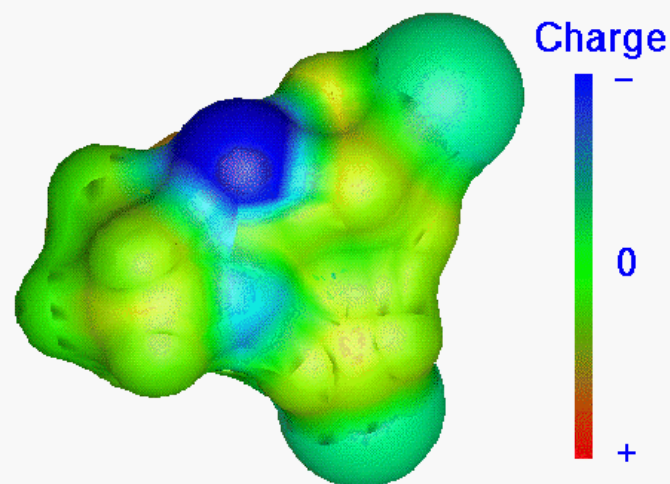
Molecular structure  
Cyclophosphamide



Solvent accessible surface



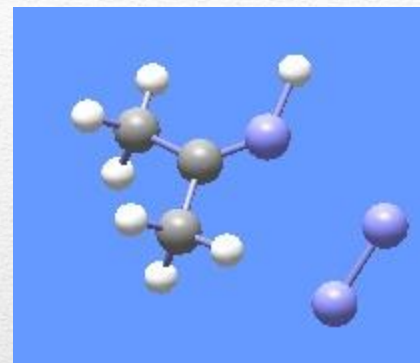
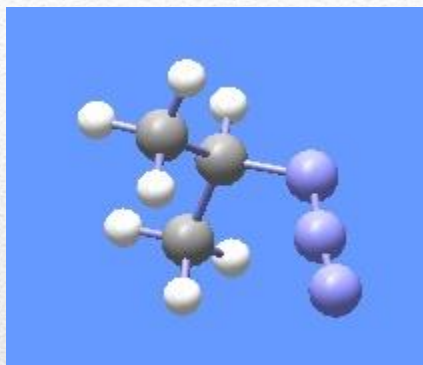
Surface mesh



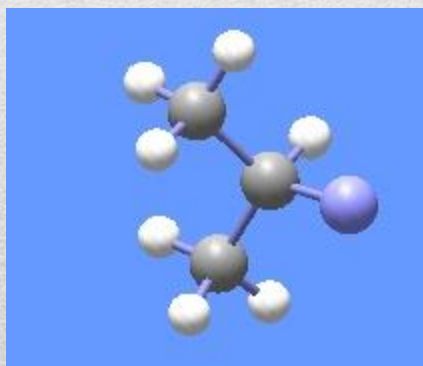
Surface charge

Steps in computing the induced charges at the solvent accessible surface. First the gas phase equilibrium structure is calculated (upper left). Then a solvent accessible surface is computed (upper right). A mesh is formed at the solvent accessible surface (lower left). Finally, the induced surface charge is computed on this mesh (lower right).

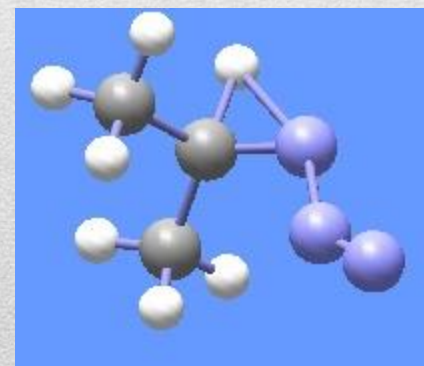
## ELIMINASI N<sub>2</sub> DAN MIGRASI H



Zat antara yang mungkin ?



Zat antara nitrena

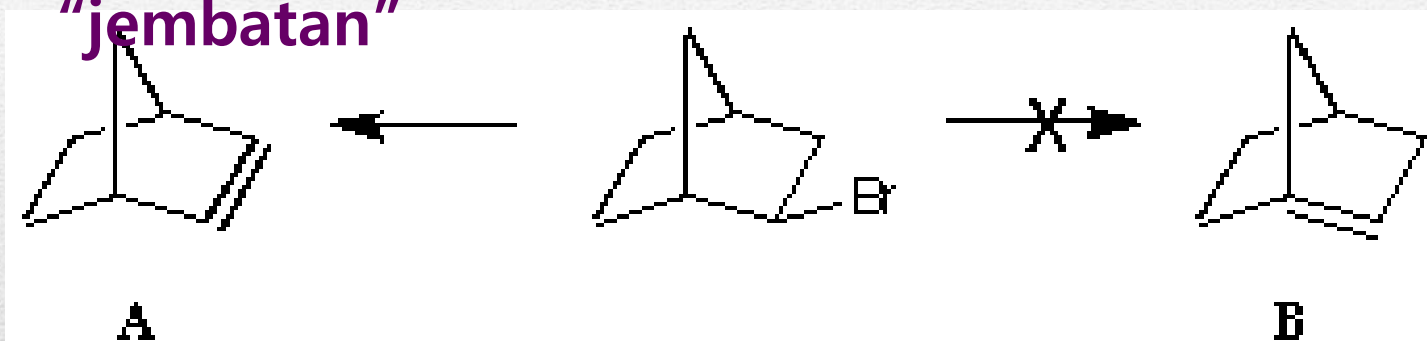


Reaksi serempak

---

# ATURAN BREDDT

Eliminasi tidak akan terjadi pada atom c yang menjadi "jembatan"



- Optimasi struktur A dan B
- Penentuan beda energi

# Enthalpy of Formation via QM

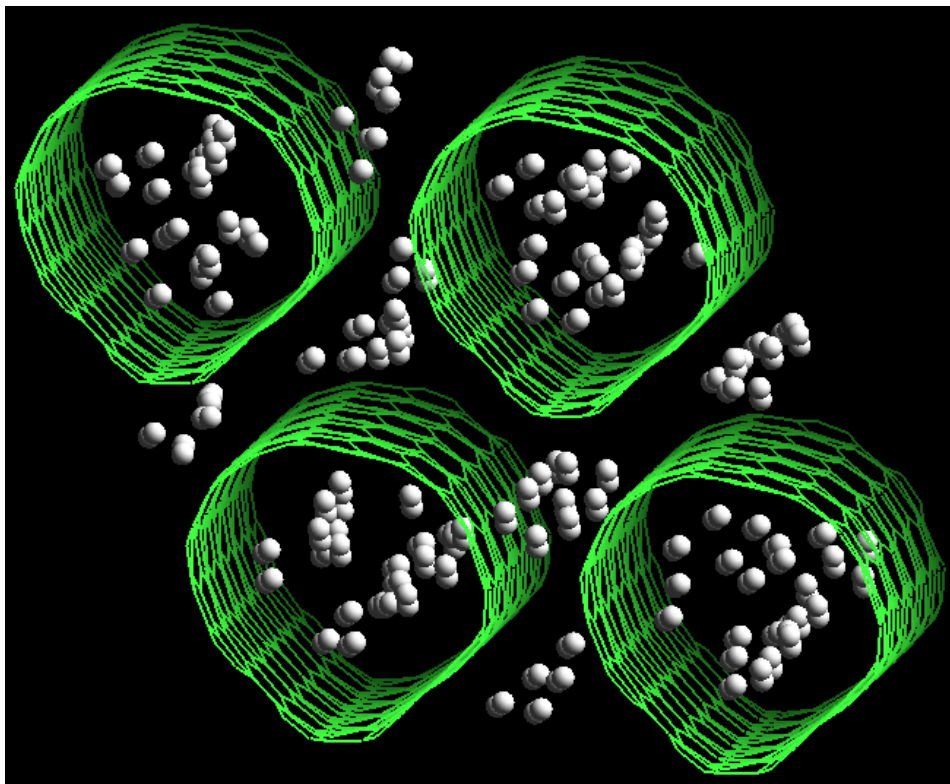
| Molecule                                | G2 Theory<br>(kcal/mol) | Literature<br>(kcal/mol) |
|-----------------------------------------|-------------------------|--------------------------|
| ethylene                                | 12.9                    | 12.5                     |
| cyclopropane                            | 13.8                    | 12.7                     |
| bicyclobutane                           | 55.2                    | 51.9                     |
| ammonia                                 | -10.8                   | -11.0                    |
| phosgene $\text{Cl}_2\text{C}=\text{O}$ | -54.9                   | -51.9, -52.4             |
| methyl fluoride                         | -58.3                   | -59                      |
| aminotriazole                           | 45.2                    | 47.6                     |
| tetraHpyrimidine                        | 18.9                    | 13.2                     |
| acrylonitrile                           | 46.2                    | 43.2                     |

D. Frurip et al., ACS SS 677, 1998

- Heats of reaction can be more accurate than heats of formation
- Can use QM to calculate group contributions for new groups
- Outliers are not always predictable a priori
- Many outliers are the result of experimental problems

# Example: Hydrogen Storage

## *ab initio* MD of H<sub>2</sub> in SWNT



- SWNT highly fluxional; large C-C-C bond angle deformations are observed.
- Adsorption energies much higher than previously published calculations using classical simulation methods: enhanced potential from curved carbon surface.
- Improved, curvature-dependent potentials were created.

H. Cheng, G. P. Pez, A. C. Cooper,  
*J. Am. Chem. Soc.* **123**, 5845 (2001).

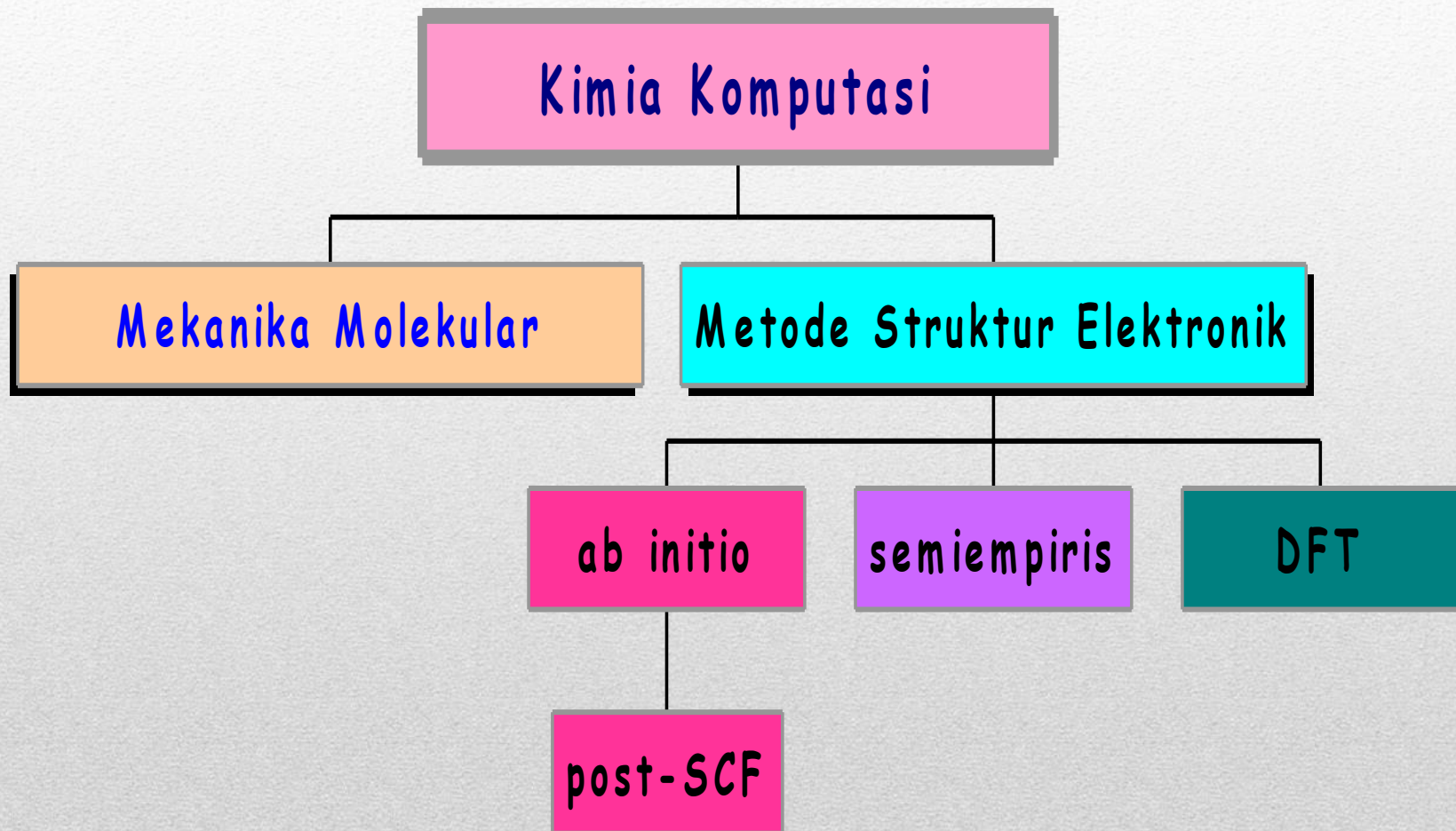
M. K. Kostov, H. Cheng, A. C. Cooper, G. P. Pez  
*Phys. Rev. Lett.* **89**, 6105 (2002)

| $\Delta H_{\text{Expt}}$ (kcal/mol) | $\Delta H_{\text{Sim}}$ (kcal/mol) |
|-------------------------------------|------------------------------------|
| (95% swnt, 7-14Å)                   | (7.8Å, 11.8Å)                      |
| 4 – 4.8                             | 4.8, 3.3                           |

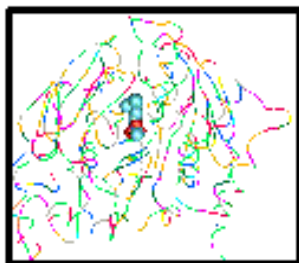
# Xenon binding to Proteins

- **Xenon/protein interactions are important...**
    - Xenon is an anesthetic
    - Xenon is a neuroprotectant
    - Xenon is used to prepare “heavy atom” derivatives for X-ray diffraction
    - $^{129}\text{Xe}$  is used in NMR studies of cavities
  - **Predictive methods for binding of xenon would enable better understanding of**  
...
    - the mechanisms of physiological activity
    - the behavior of xenon in NMR and XRD experiments
    - binding sites not visible by XRD (due to resolution, occupancy, disorder)
  - **The goal of this work was to show how grand canonical Monte Carlo Simulations (GCMC) coupled with a clustering algorithm can determine the positions, occupancy, and free energies of binding of small molecules.**
-

# METODE PERHITUNGAN KIMIA KOMPUTASI



# KARAKTER METODE KIMIA KOMPUTASI



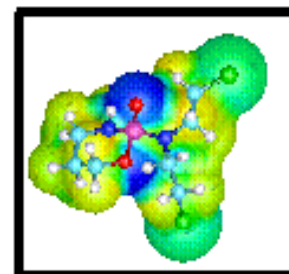
Molecular  
Mechanics

100,000  
atoms



Semi-Empirical  
Quantum Mechanics

1000  
atoms



*ab initio*  
Quantum Mechanics

100  
atoms



Use Empirically-Derived  
Potential Function

Solve Approximate  
Schrodinger Equation

Solve Exact  
Schrodinger Equation



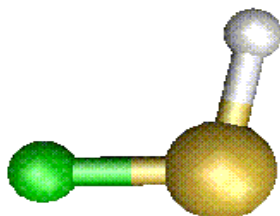
Empirical Parameters Needed



Computationally Demanding

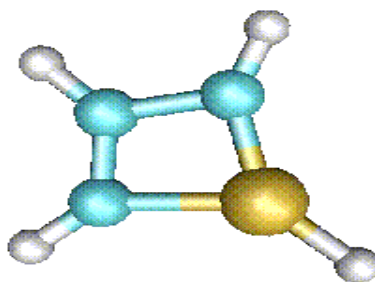
# PERKEMBANGAN KIMIA KOMPUTASI

1982:



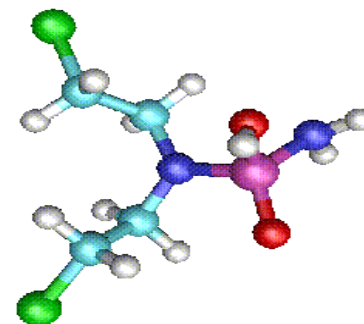
Fluorosilene

1985:



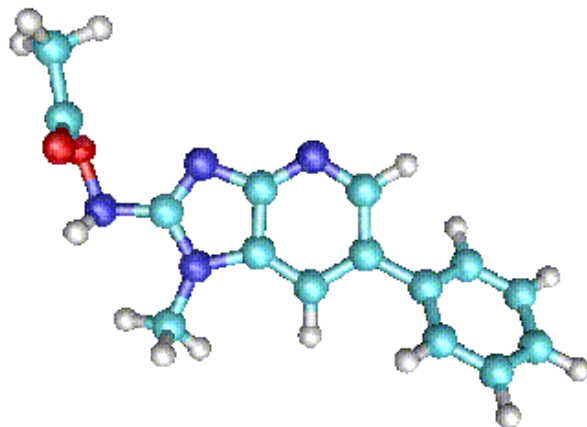
Silacyclobutadiene

1991:



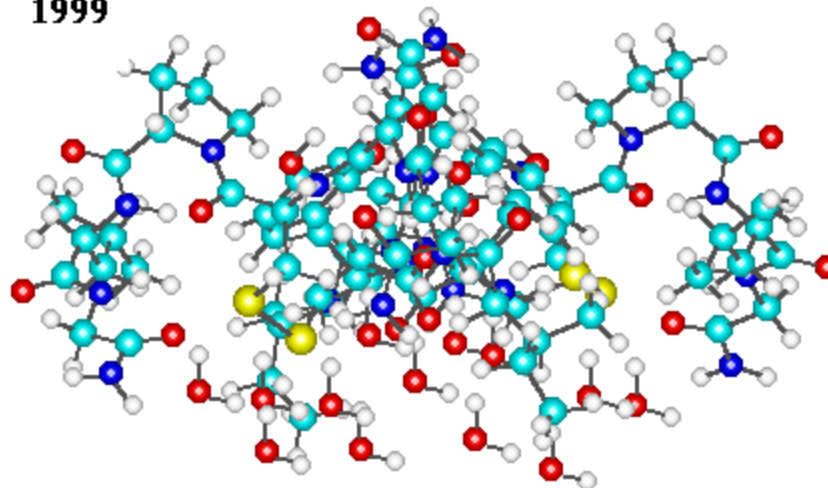
Phosphoramidate Mustard

1994:



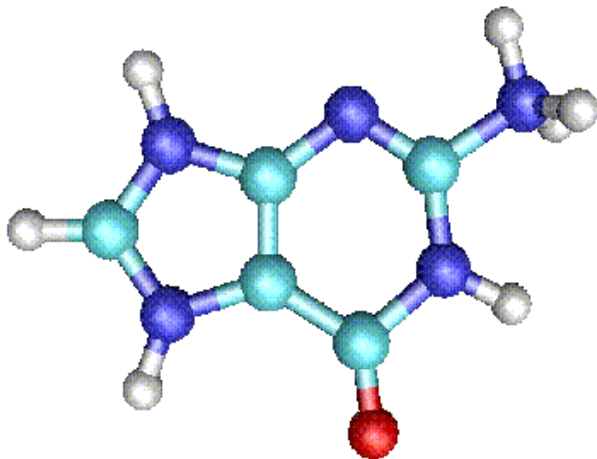
N-acetoxy-2-amino-3-methyl-6-phenylimidazo[4,5-b]pyridine

1999

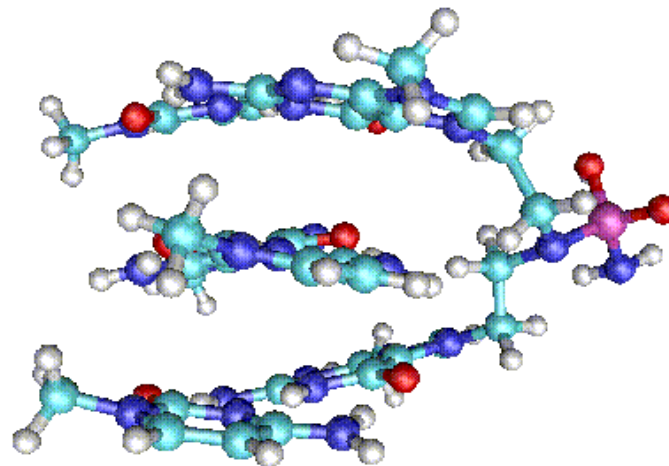


1-beta-mercaptopropionate-oxytocin

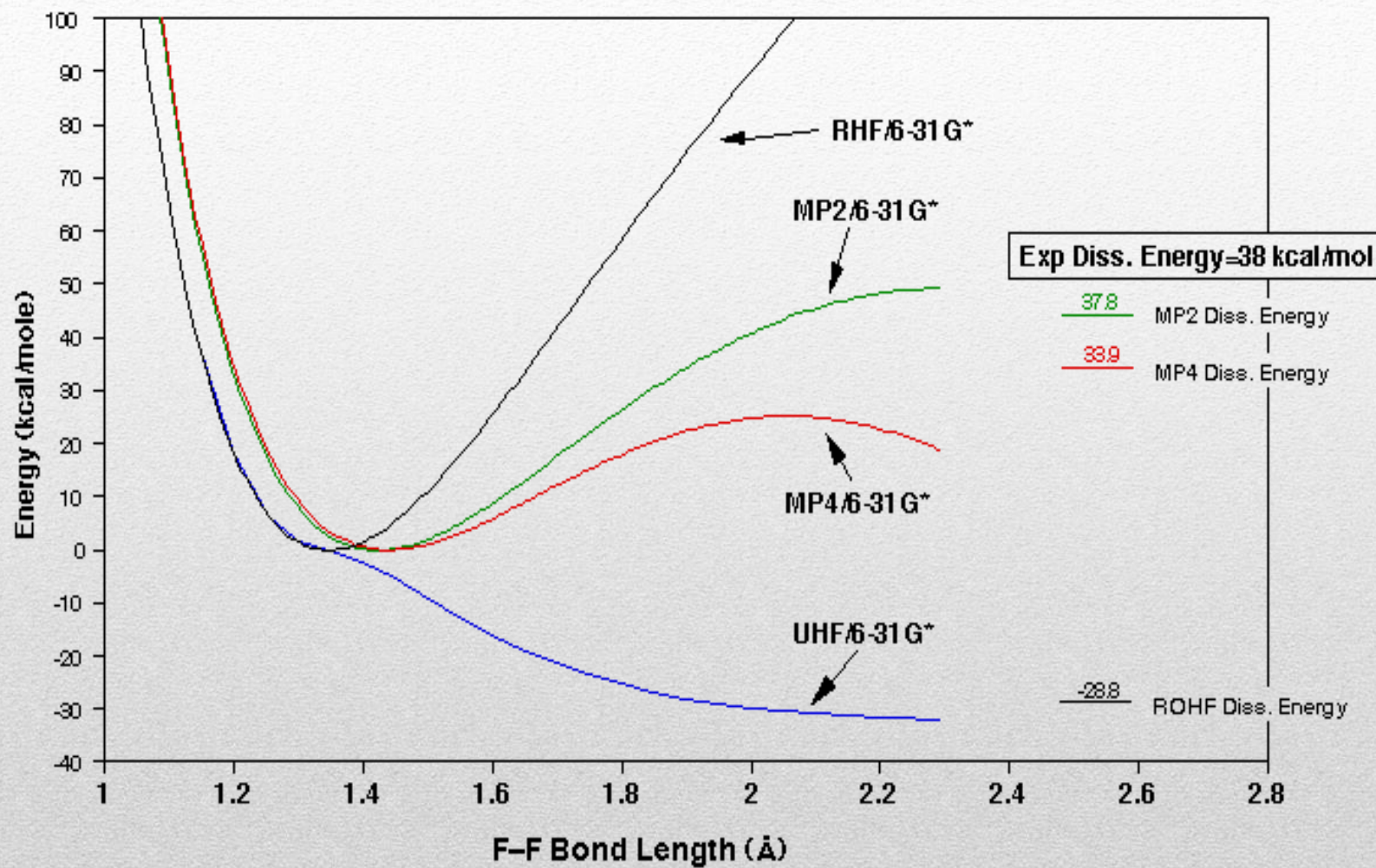
# JUMLAH ATOM VS CPU TIME



**Protonated Guanine**  
10 hours on workstation



**Crosslinked DNA Trimer**  
20 hours on parallel supercomputer



# METODE MEKANIKA MOLEKULER

Metode Klasik / Mekanika Newton

# Overview

- Simplest type of calculation
    - Used when systems are very large and approaches that are more accurate become too costly (in time and memory)
  - Does not use any quantum mechanics instead uses parameters derived from experimental or *ab initio* data
    - Uses information like bond stretching, bond bending, torsions, electrostatic interactions, van der Waals forces and hydrogen bonding to predict the energetics of a system
    - The energy associated with a certain type of bond is applied throughout the molecule. This leads to a great simplification of the equation
-

- It should be clarified that the energies obtained from molecular mechanics do not have any physical meaning, but instead describe the difference between varying conformations (type of isomer). Molecular mechanics can supply results in heat of formation if the zero of energy is taken into account.
- Employs classical (Newtonian) physics
- Assumes Hooke's Law forces between atoms (like a spring between two masses)

$$E_{\text{stretch}} = k_s (l - l_o)^2$$

---

# Properties calculated by MM:

- SIMILAR CALCULATIONS FOR OTHER DEVIATIONS FROM “NORMAL” GEOMETRY (BOND ANGLES, DIHEDRAL ANGLES)
  - BASED ON SIMPLE, EMPIRICALLY DERIVED RELATIONSHIPS BETWEEN ENERGY AND BOND ANGLES, DIHEDRAL ANGLES, AND DISTANCES
  - IGNORES ELECTRONS AND EFFECT OF  $\pi$  SYSTEMS!
  - VERY SIMPLE, YET GIVES QUITE REASONABLE, THOUGH LIMITED RESULTS, ALL THINGS CONSIDERED.
-

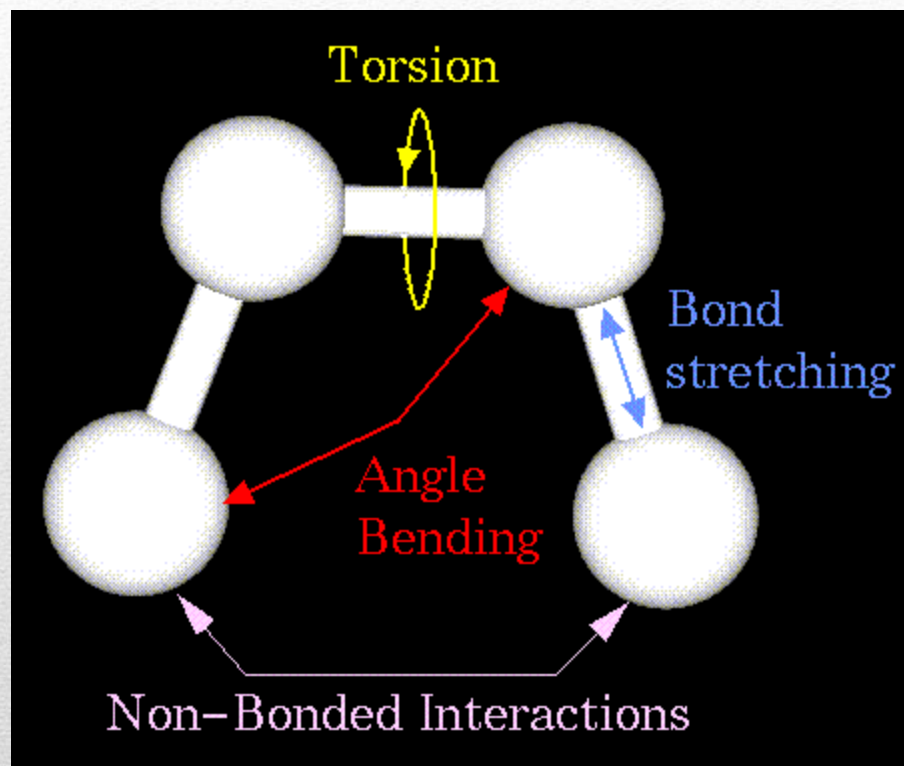
# Properties calculated by MM:

- “Steric” or Total energy = sum of various artificial energy components, depending on the program...not a “real” measurable energy.
  - Enthalpy of Formation (sometimes)
  - Dipole Moment
  - Geometry (bond lengths, bond angles, dihedral angles) of lowest energy conformation.
-

# Molecular Mechanics Forcefields

- MM2, MM3 (ALLINGER)
  - MMX (GILBERT, IN PCMODEL)
  - MM+ (HYPERCHEM'S VERSION OF MM2)
  - MMFF (MERCK PHARM.)
  - AMBER (KOLLMAN)
  - OPLS (JORGENSEN)
  - BIO+ (KARPLUS, PART OF CHARMM)
  - (OTHERS)
-

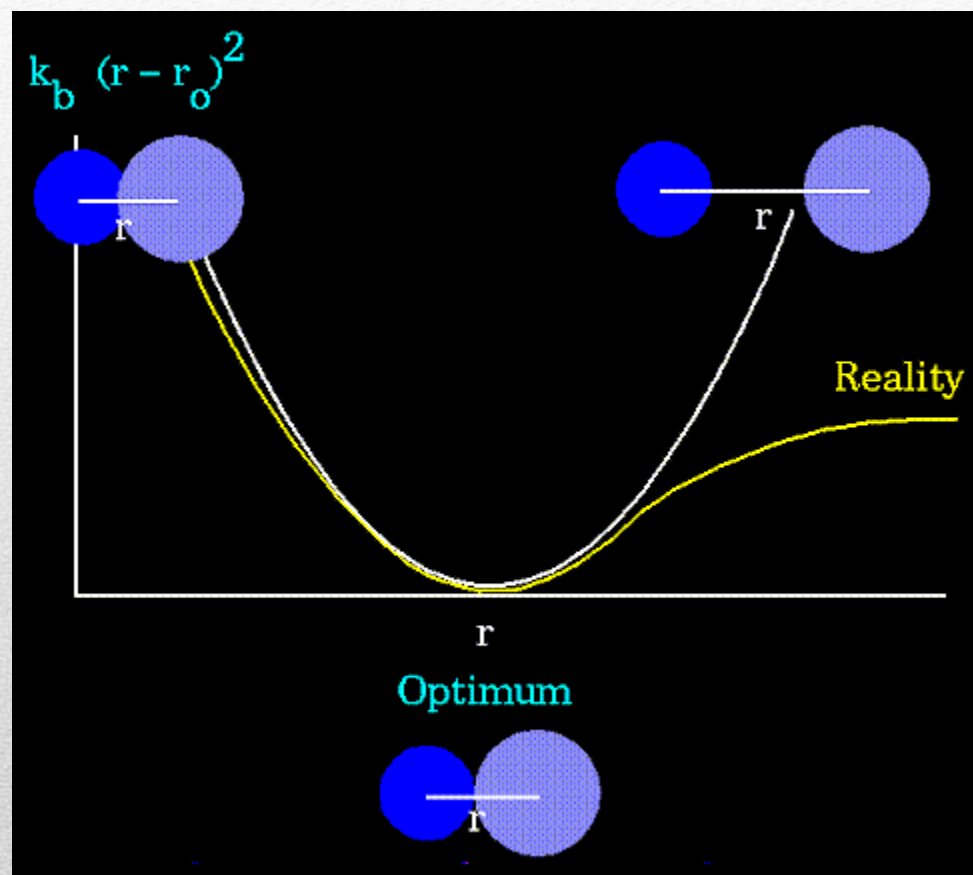
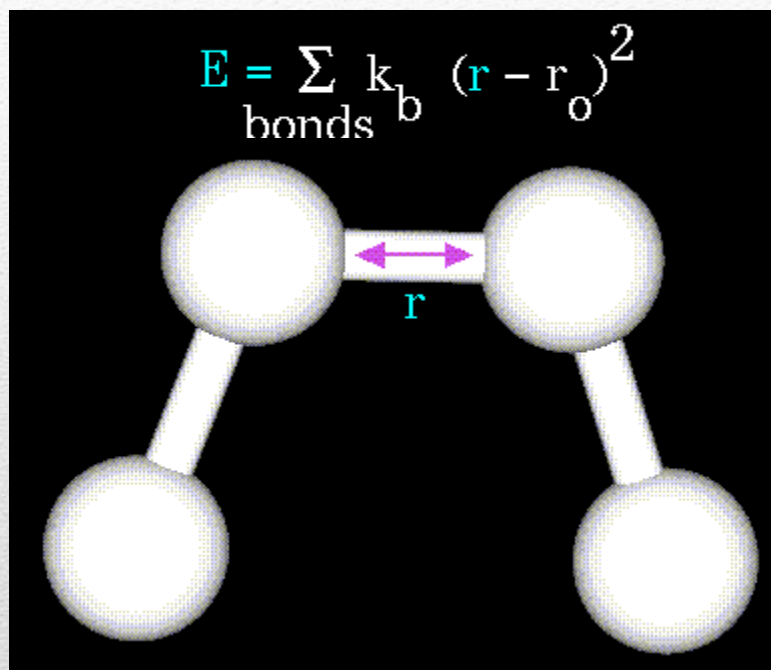
# Molecular Mechanics



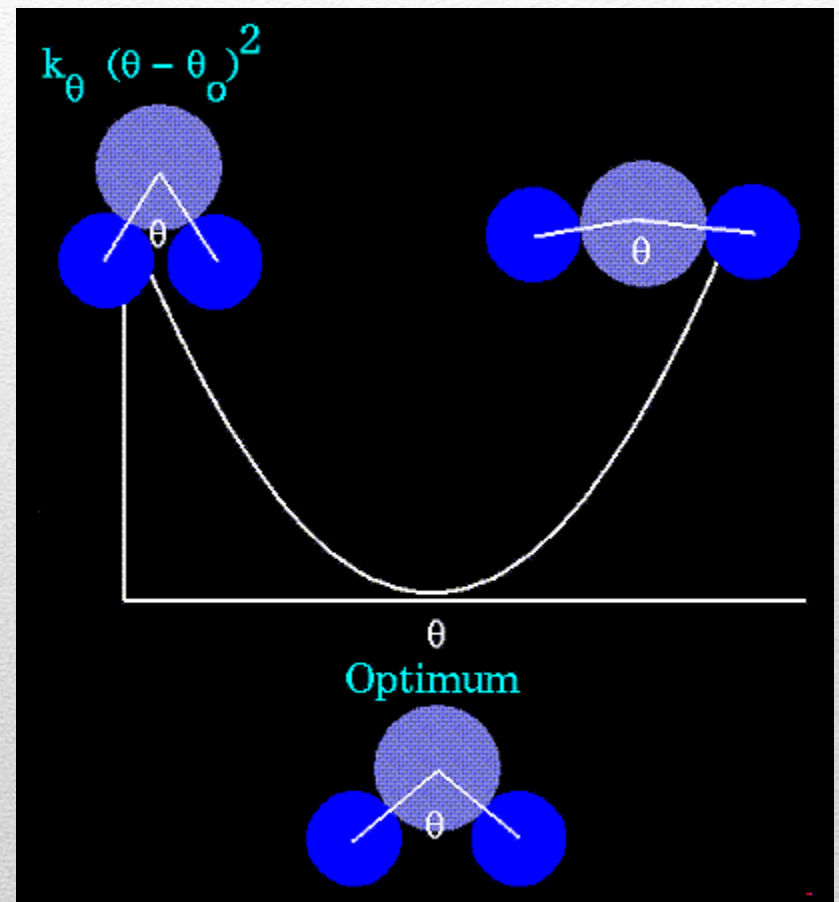
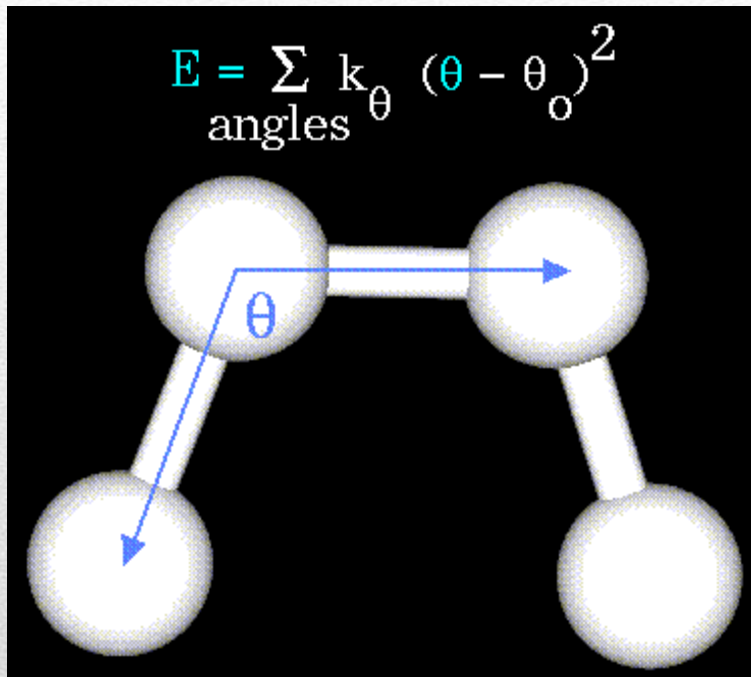
$$\text{Energy} = \text{Stretching Energy} + \text{Bending Energy} + \text{Torsion Energy} + \text{Non-Bonded Interaction Energy}$$

---

# Stretching Energy

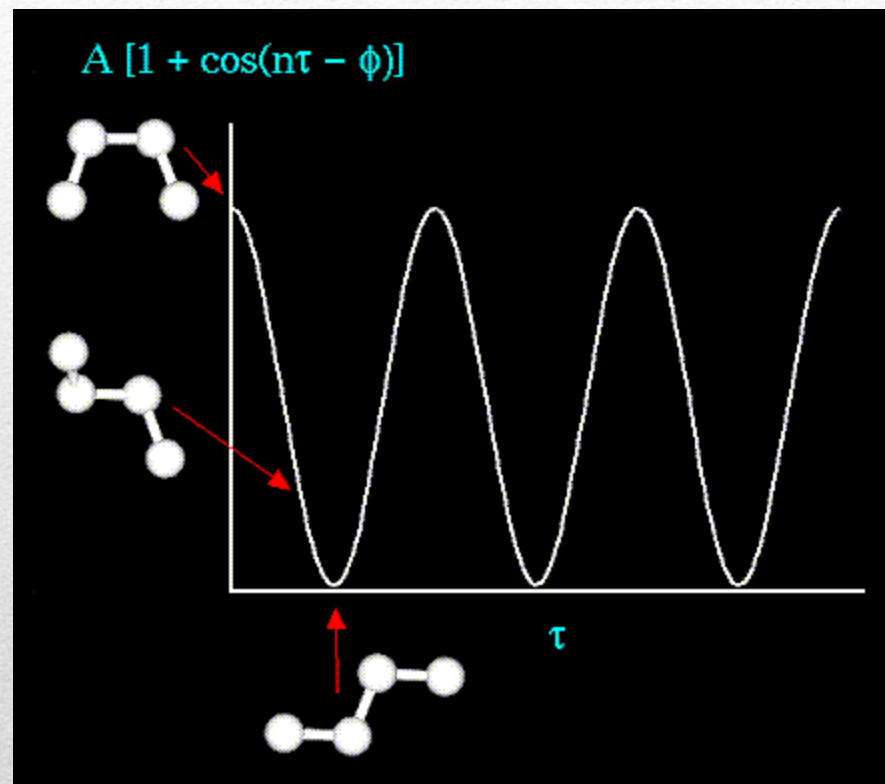
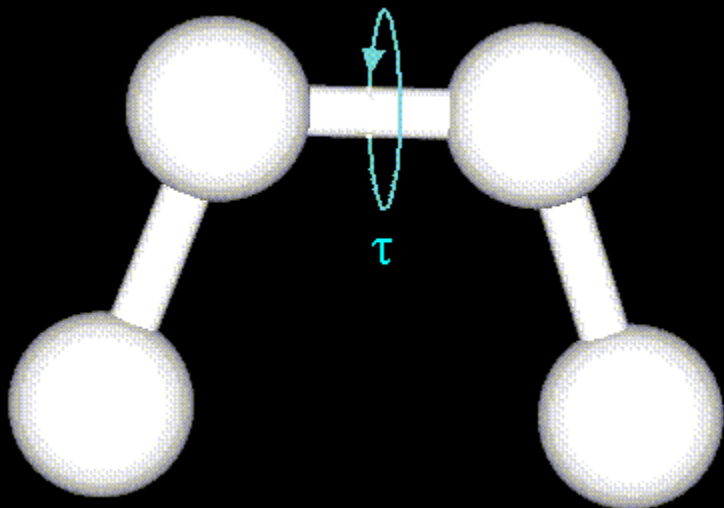


# Bending Energy



# Torsion Energy

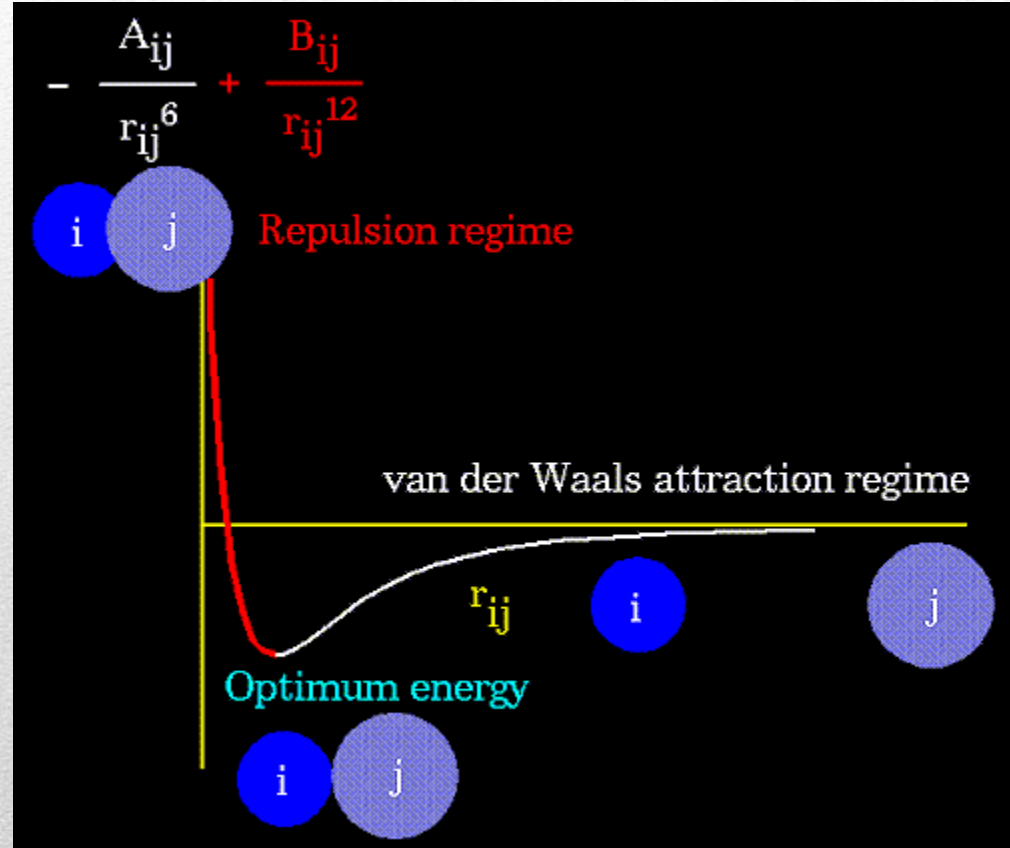
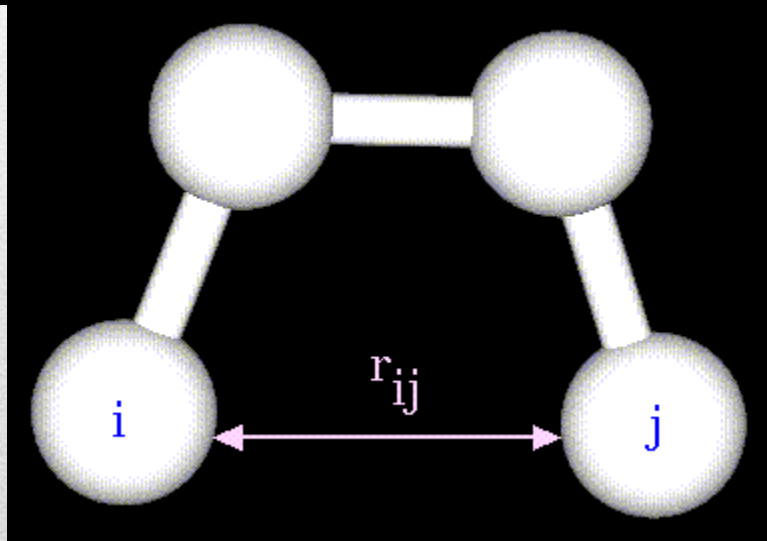
$$E = \sum_{\text{torsions}} A [1 + \cos(n\tau - \phi)]$$



# Non-Bonded Energy

$$E = \sum_i \sum_j \frac{-A_{ij}}{r_{ij}^6} + \frac{B_{ij}}{r_{ij}^{12}} + \sum_i \sum_j \frac{q_i q_j}{r_{ij}}$$

van der Waals term      Electrostatic term



# QUANTUM MECHANICS/MOLECULAR MECHANICS(QM/MM)

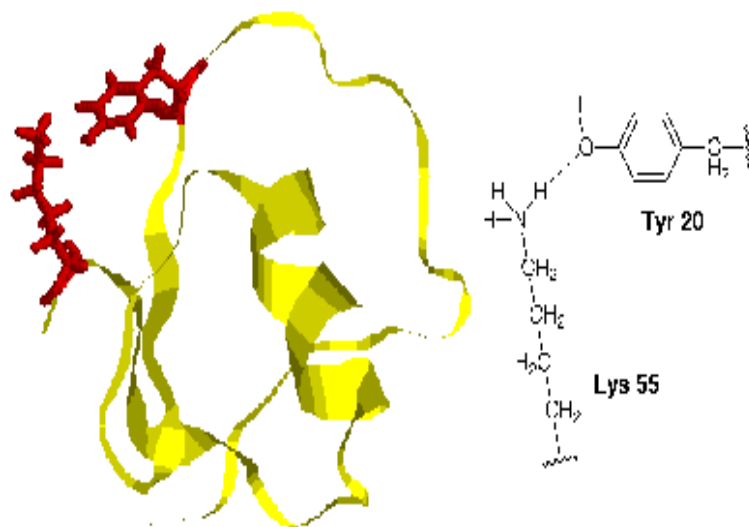


Figure 1. The active site in the turkey ovomucoid third domain serine protease inhibitor consisting of Lys55 interacting with Tyr20.

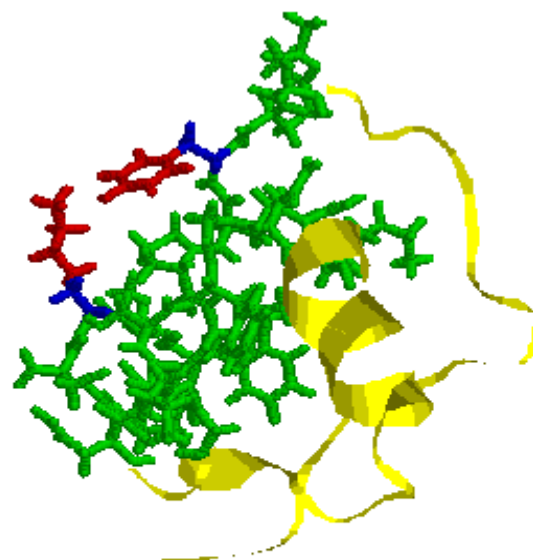


Figure 2. Setup of the QM/MM calculation: red = the *ab initio* region, green = the EFP region, and blue = the buffer region. The rest of the protein (yellow ribbon) is ignored.

# Quantum Mechanics

## Basic: Shroedinger Equation

- Where are the electrons and nuclei of a molecule in space?

*Configuration, conformation, size, shape, etc.*

- Under a given set of conditions, what are their energies?

*Heat of formation, conformational stability, chemical reactivity, spectral properties, etc.*

---

# Schrodinger's Equation for a Multi-Electron Atom

$$H = \overset{T_{\text{electron}}}{\left[ \left( -\frac{h^2}{8\pi^2 m_e} \right) \sum_{i=1,k} \nabla_i^2 \right]} - \overset{V_{\text{electron-nucleus}}}{\sum_{i=1,k} \frac{Z}{r_i}} + \overset{V_{\text{electron-electron}}}{\sum_{i=1,k-1} \sum_{j=1+1,k} \frac{1}{r_{ij}}}$$


---

# The Schrodinger Equation for a Molecule

$T_{\text{electron}}$

$V_{\text{electron-nucleus}}$

$$H = [(-h^2/8\pi^2m_e) \sum_{i=1,k} \nabla^2 - \sum_{j=1,N} \sum_{i=1,k} Z_j/r_{ji}]$$

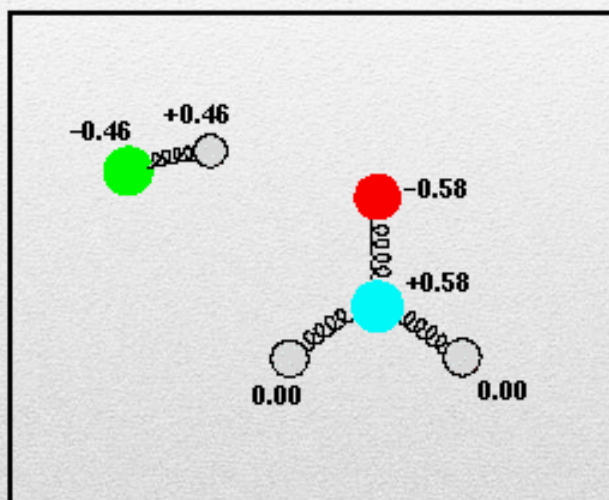
$$+ \sum_{i=1,k-1} \sum_{l=1+1,k} 1/r_{il} + \sum_{j=1,N-1} \sum_{m=j+1,N} Z_j Z_m/R_{jm}$$

$V_{\text{electron-electron}}$

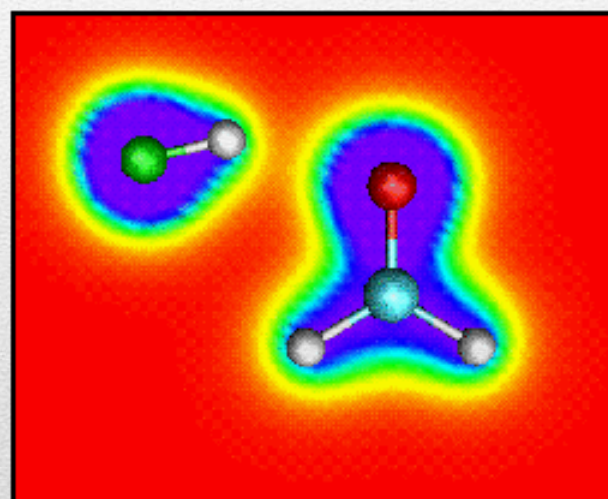
$V_{\text{nucleus-nucleus}}$

## Molecular Mechanics versus Quantum Mechanics

Formaldehyde Hydrogen Bonded to Hydrogen Fluoride

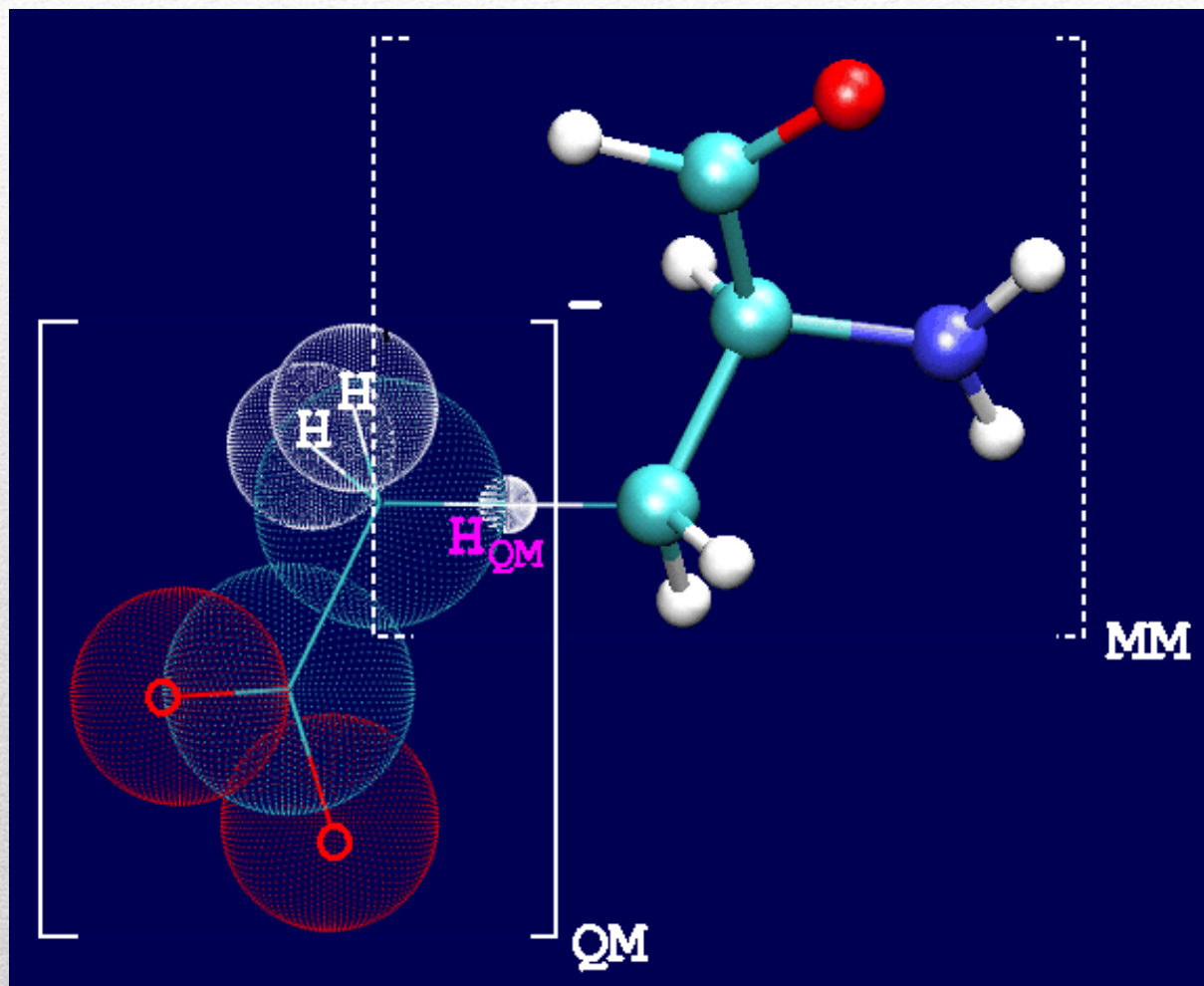


Energy Calculated from  
Empirical Spring Constants  
and Atomic Charges



Properties Calculated  
from First-Principles  
Prediction of Electron Density

# QUANTUM MECHANICS/MOLECULAR MECHANICS(QM/MM)



# QUANTUM MECHANICS/MOLECULAR MECHANICS(QM/MM)

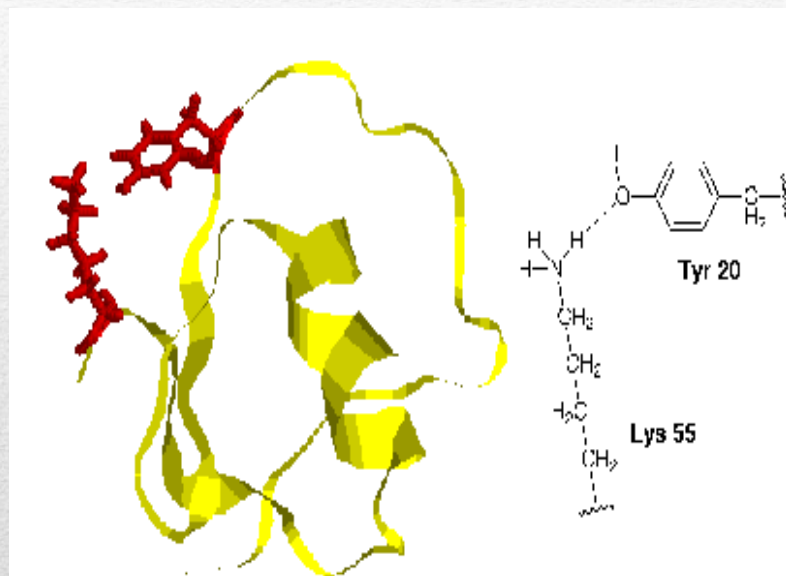


Figure 1. The active site in the turkey ovomucoid third domain serine protease inhibitor consisting of Lys55 interacting with Tyr20.

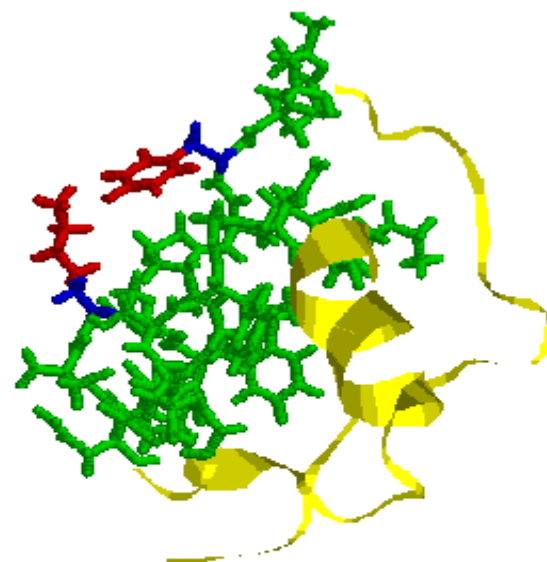


Figure 2. Setup of the QM/MM calculation: red = the *ab initio* region, green = the EFP region, and blue = the buffer region. The rest of the protein (yellow ribbon) is ignored.

# Schrödinger's Equation: $H\psi = E\psi$

- The Schrödinger equation is the basis of quantum mechanics and gives a complete description of the electronic structure of a molecule. If the equation could be fully solved all information pertaining to a molecule could be determined.
    - Complex mathematical equation that completely describes the chemistry of a molecular system.
    - Not solvable for systems with many atoms.
    - Due to the difficulty of the equation computers are used in conjunction with simplifications and parameterizations to solve the equation.
  - Describes both the wave and particle behavior of electrons.
    - The wavefunction is described by  $\psi$  while the particle behavior is represented by  $E$ .
    - In systems with more than one electron, the wavefunction is dependent on the position of the atoms; this makes it important to have an accurate geometric description of a system.
-

# Schrödinger Cont...

- Development of the Schrödinger equation from other fundamental laws of physics.**

$$\text{Kinetic Energy} + \text{Potential Energy} = E$$

Classical  
Conservation of  
Energy  
Newton's Laws

$$\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = E$$

Harmonic oscillator  
example.

$$F = ma = -kx$$

Quantum  
Conservation of  
Energy  
Schrödinger  
Equation

In making the  
transition to  
a wave equation,  
physical variables  
take the form of  
"operators".

The energy becomes the Hamiltonian operator

$$H\Psi = E\Psi$$

Wavefunction

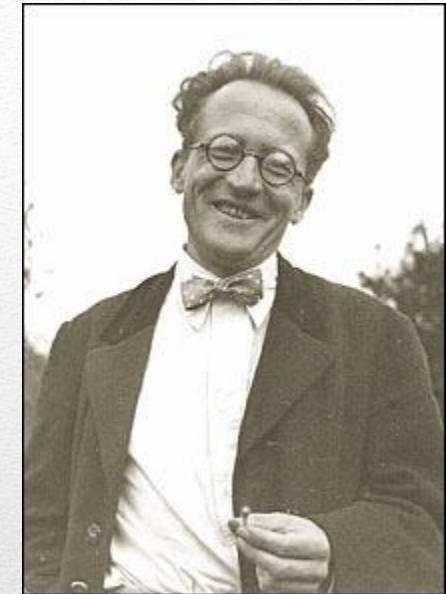
Energy "eigenvalue" for the system.

The form of the Hamiltonian operator for a quantum harmonic oscillator.

$$H \rightarrow \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$$

$p \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}$   
 $x \rightarrow x$

$\frac{p^2}{2m} + \frac{1}{2}kx^2$



Erwin Schrödinger,  
1927

- *"Anyone can do calculations nowadays.*
- *Anyone can also operate a scalpel.*
- *That doesn't mean all our medical problems are solved."*

**Karl Irikura**

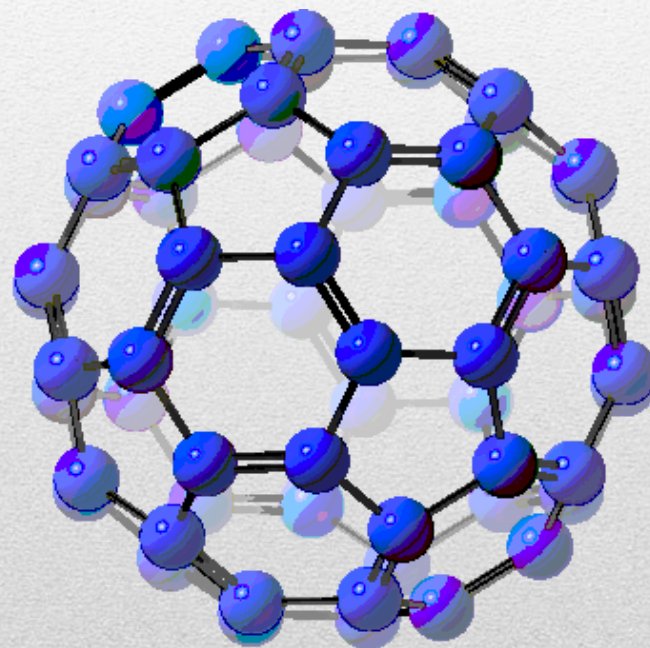
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# Conducting a Computational Project

- These questions should be answered
    - What do you want to know?
    - How accurate does the prediction need to be?
    - How much time can be devoted to the problem?
    - What approximations are being made?
  - The answers to these questions will determine the type of calculation, model and basis set to be used.
-

# Types of Calculations

- There are three basic types of calculations.  
From these calculations, other information can be determined.
- Single-Point Energy: predict stability, reaction mechanisms
- Geometry Optimization: predict shape
- Frequency: predict spectra



**Atomic model of a  
Buckyball (C<sub>60</sub>)**

---

# Computational Models

- A model is a system of equations, or computations used to determine the energetics of a molecule
  - Different models use different approximations (or levels of theory) to produce results of varying levels of accuracy.
  - There is a trade off between accuracy and computational time.
  - There are two main types of models; those that use Schrödinger's equation (or simplifications of it) and those that do not.
-

# Computational Models

- Types of Models

(Listed in order from most to least accurate)

- ***Ab initio***

- uses Schrödinger's equation, but with approximations

- **Semi Empirical**

- uses experimental parameters and extensive simplifications of Schrödinger's equation

- **Molecular Mechanics**

- does not use Schrödinger's equation
-

# *Ab Initio*

- *Ab initio* translated from Latin means “*from first principles*.” This refers to the fact that no experimental data is used and computations are based on quantum mechanics.
  - Different Levels of *Ab Initio* Calculations
    - Hartree-Fock (HF)
      - The simplest *ab initio* calculation
      - The major disadvantage of HF calculations is that electron correlation is not taken into consideration.
    - The Møller-Plesset Perturbation Theory (MP)
    - Density Functional Theory (DFT)
    - Configuration Interaction (CI)
-

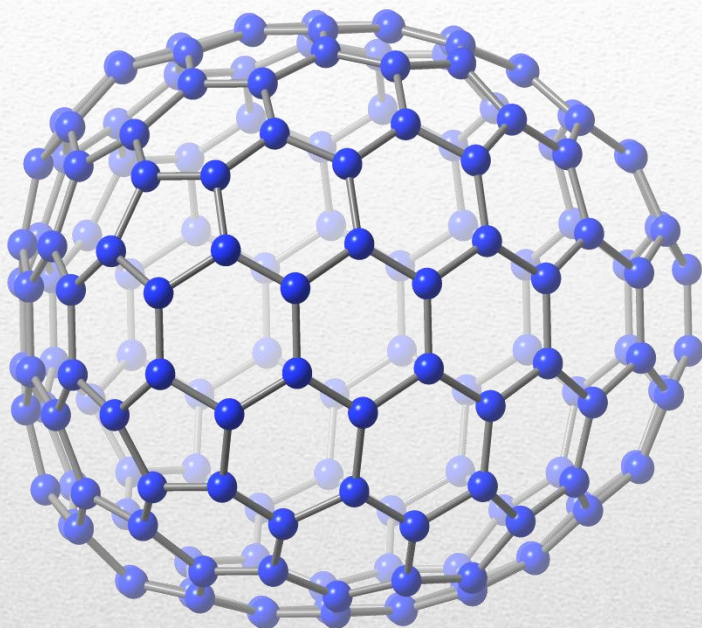
# *Ab Initio*

- Approximations used in some ab initio calculations
    - Central field approximation: integrates the electron-electron repulsion term, giving an average effect instead of an explicit energy
    - Linear combination of atomic orbitals (LCAO): is used to describe the wave function and these functions are then combined into a determinant. This allows the equation to show that an electron was put in an orbital, but the electron cannot be specified.
-

# Density Functional Theory

- Considered an *ab initio* method, but different from other *ab initio* methods because the wavefunction is not used to describe a molecule, instead the electron density is used.
  - Three types of DFT calculations exist:
    - local density approximation (LDA) – fastest method, gives less accurate geometry, but provides good band structures
    - gradient corrected - gives more accurate geometries
    - hybrids (which are a combination of DFT and HF methods) - give more accurate geometries
-

# DFT



DFT: -6139.46

HF: -6132.89

% Difference: 0.11% (units:a.u.)

- These types of calculations are fast becoming the most relied upon calculations for nanotube and fullerene systems.
- DFT methods take less computational time than HF calculations and are considered more accurate
- This (15,0) short zigzag carbon nanotube was simulated with two different models: Hartree-Fock and DFT. The differences in energetics are shown in the table.

# Semi Empirical

- Semi empirical methods use experimental data to parameterize equations
  - Like the *ab initio* methods, a Hamiltonian and wave function are used
    - much of the equation is approximated or eliminated
  - Less accurate than *ab initio* methods but also much faster
  - The equations are parameterized to reproduce specific results, usually the geometry and heat of formation, but these methods can be used to find other data.
-

# Molecular Mechanics

- Simplest type of calculation
    - Used when systems are very large and approaches that are more accurate become too costly (in time and memory)
  - Does not use any quantum mechanics instead uses parameters derived from experimental or *ab initio* data
    - Uses information like bond stretching, bond bending, torsions, electrostatic interactions, van der Waals forces and hydrogen bonding to predict the energetics of a system
    - The energy associated with a certain type of bond is applied throughout the molecule. This leads to a great simplification of the equation
  - It should be clarified that the energies obtained from molecular mechanics do not have any physical meaning, but instead describe the difference between varying conformations (type of isomer). Molecular mechanics can supply results in heat of formation if the zero of energy is taken into account.
-

# Basis Sets

- In chemistry a basis set is a group of mathematical functions used to describe the shape of the orbitals in a molecule, each basis set is a different group of constants used in the wavefunction of the Schrödinger equation.
  - The accuracy of a calculation is dependent on both the model and the type of basis set applied to it.
  - Once again there is a trade off between accuracy and time. Larger basis sets will describe the orbitals more accurately but take longer to solve.
  - General expression for a basis function =  $N * e^{(-\alpha * r)}$ 
    - where: N is the normalization constant,  $\alpha$  is the orbital exponent, and r is the radius of the orbital in angstroms.
-

# Examples of Basis Sets

- STO-3G basis set - simplest basis set, uses the minimal number of functions to describe each atom in the molecule
    - for nanotube systems this means hydrogen is described by one function (for the 1s orbital), while carbon is described by five functions (1s, 2s, 2px, 2py and 2pz).
  - Split valence basis sets use two functions to describe different sizes of the same orbitals.
    - For example with a split valence basis set H would be described by two functions while C would be described by 10 functions.
    - 6-31G or 6-311G (which uses three functions for each orbital, a triple split valence set).
  - Polarized basis sets - improve accuracy by allowing the shape of orbitals to change by adding orbitals beyond that which is necessary for an atom
    - 6-31G(d) (also known as the 6-31G\*) - adds a d function to carbon atoms
-

*“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 application of these laws leads to equations much too complicated to be soluble.”*

P.A.M. Dirac, 1929

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# Accuracy Comparison

Table 1. Comparison of the accuracy of different models and basis sets to experimental data.

| Method//Model/Basis Set           | Total Energy*<br>(kcal/mol) | Bond Length<br>(Å) |
|-----------------------------------|-----------------------------|--------------------|
| Mol. Mech.// MM2                  | 0.5 ( $\Delta H_f^\circ$ )  | 0.01               |
| Semi Emp.//AM1                    | 18.8                        | 0.048              |
| Semi Emp.//PM3                    | 17.2                        | 0.037              |
| <i>Ab Initio</i> //HF/STO-3G      | 93.3                        | 0.055              |
| <i>Ab Initio</i> //HF/6-31+G(d,p) | 46.7                        | -                  |
| DFT//B3LYP/6-31G(d)               | 7.9                         | 0.02               |
| DFT//B3LYP/6-31+G(d,p)            | 3.9                         | -                  |
| DFT//MP2/6-31+G(d,p)              | 11.4                        | -                  |

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\*mean absolute deviation

# Summary

- Schrödinger's equation is the basis of computational chemistry, if it could be solved all electronic information for a molecule would be known.
  - Since Schrödinger's equation cannot be completely solved for molecules with more than a few atoms, computers are used to solve approximations of the equation.
  - The level of accuracy and computational time of a simulation is dependent on the model and basis set used.
-

# Molecular Modeling & Chemical Engineering

- Molecular Modeling (Computational Chemistry, Computational Materials Science, “Theory”, “Modeling”) is the natural extension and limit of the reductionist approach to chemical engineering.
  - MM is broadly applicable because “everything” is made of atoms and molecules.
  - The power of MM is growing rapidly with the continuing development of computer power, new algorithms, and the availability of software.
  - Today MM can sometimes provide useful estimates of the properties and behavior of materials- even before they have been synthesized. (materials design)
  - Today MM can sometimes provide useful estimates of the parameters and behavior needed to do traditional chemical engineering process development & design.
  - Today MM is sometimes the most efficient way to obtain these estimates.
  - MM works best in partnership with experiments and with traditional estimation and design approaches.
-

# Molecular Modeling and the UG Chemical Engineering Curriculum

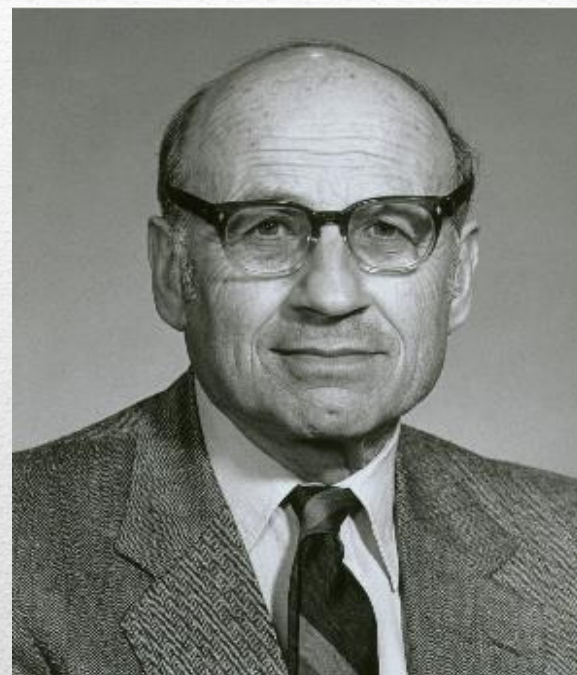
- Minimum: UG Chemical Engineers should be aware of the possibility that useful estimates of *some material properties* can be calculated for *some systems* and that the number of such properties and systems is continually increasing.
  - Optimum (?) : UG Chemical Engineers should have some familiarity with the techniques of MM and should be able to make informed guesses as to whether any given properties and materials are amenable to MM.
  - “Win/Win” MM techniques are wonderful pedagogical tools for understanding the fundamental physical processes which underlie thermodynamics, transport phenomena, and chemical kinetics. Much of the requisite familiarity could be obtained via the permeation, throughout the undergraduate curriculum, of computation and simulation as methods of understanding complementary to experiment and theory.
-

- Molecular Modeling will not replace all other scientists and engineers. Among other reasons, the techniques of computational chemistry and molecular modeling employ approximations. The validity of these approximations varies with the method and with the system considered. Therefore, one cannot blindly apply a given method to all systems and rationally expect useful answers.
  - Molecular Modeling can and does replace some unnecessary experimentation and it can lead to insights which initiate new experiments. Some approximations *are* quite valid for some systems and one can expect useful results when a suitable method is used to predict some subset of properties for those systems.
  - A given method will typically supply only some of the properties and information needed to solve a given problem. MM techniques are most useful when used in combination with each other and with experiment.
-

# PEMENANG HADIAH NOBEL TAHUN 1998 BIDANG KIMIA KOMPUTASI



**JOHN POPL**  
Dept. of Chemistry  
Northwestern University  
Illinois



**WALTER KOHN**  
Dept. of Physics  
Univ. of California,  
Santa Barbara

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# 1927 Solvay Conference



•Held in Belgium, the conference was attended by the world's most notable physicists to discuss the newly formulated quantum theory. Of the 12 individuals cited here in History of Quantum Mechanics, only the three mathematicians were not in attendance: William Hamilton was dead, John von Neumann did not publish his book until 1932, and David Hilbert ("physics far too difficult for physicists") probably wasn't invited.