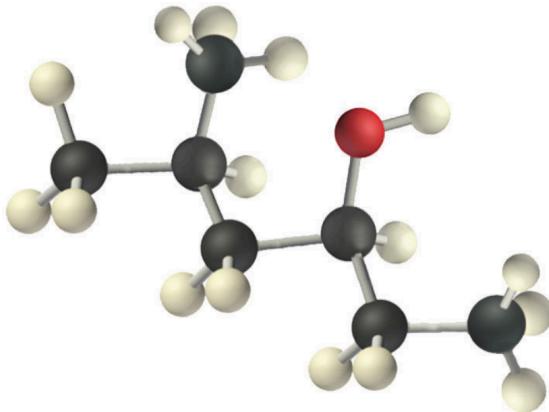
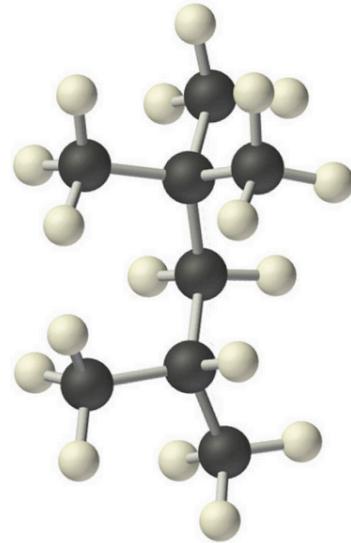
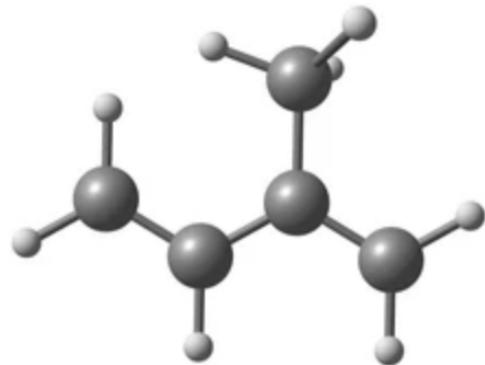
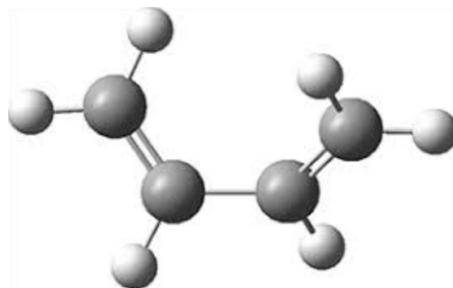
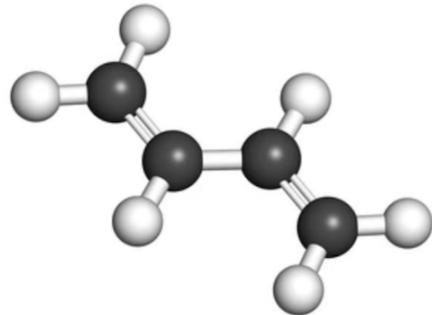
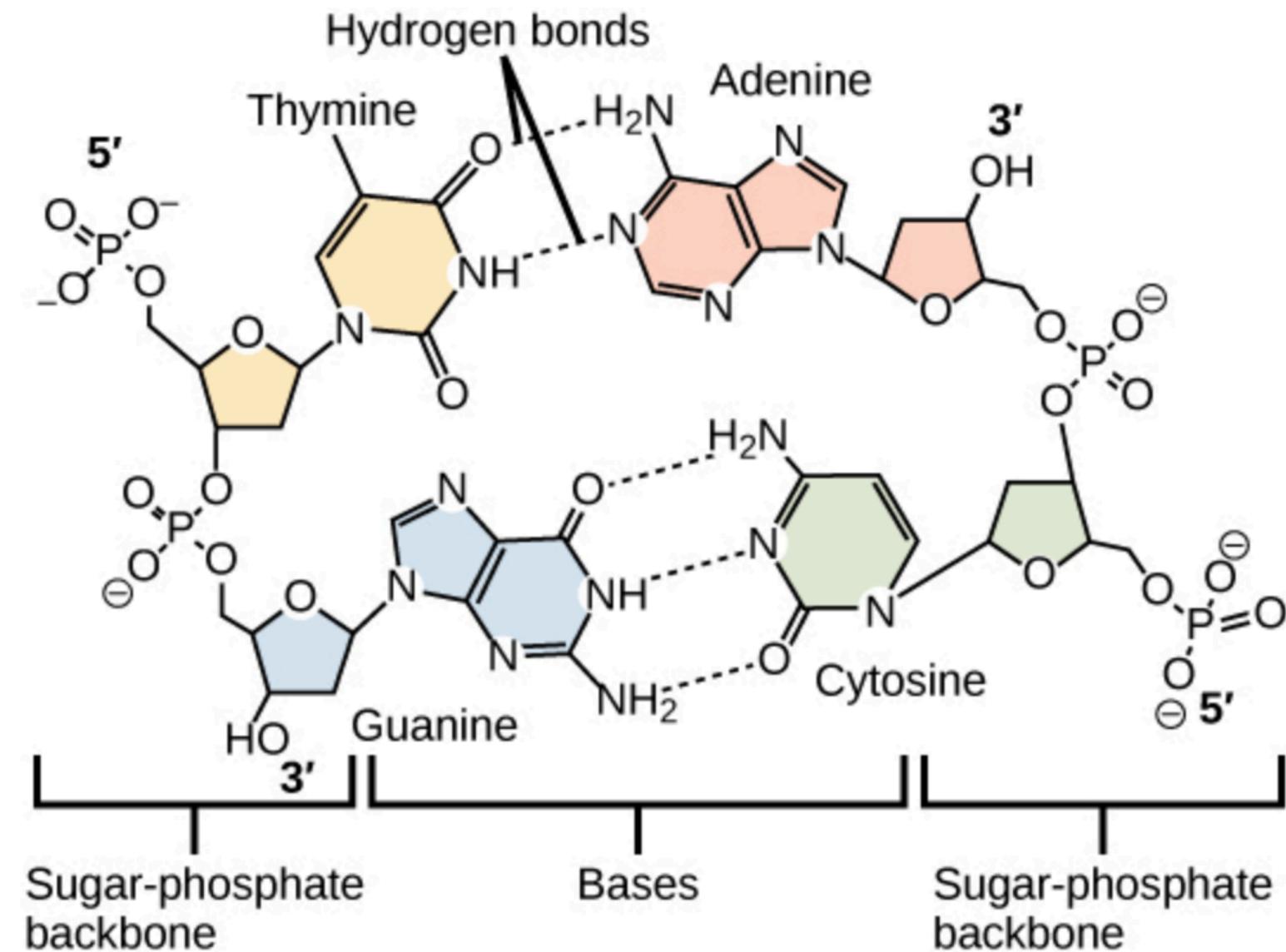
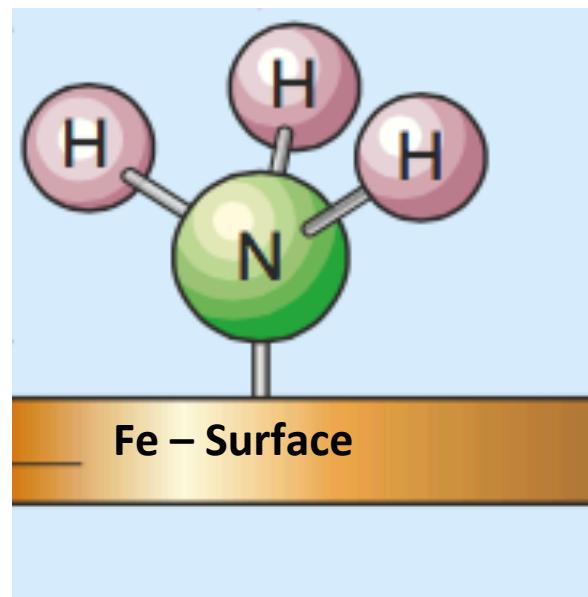
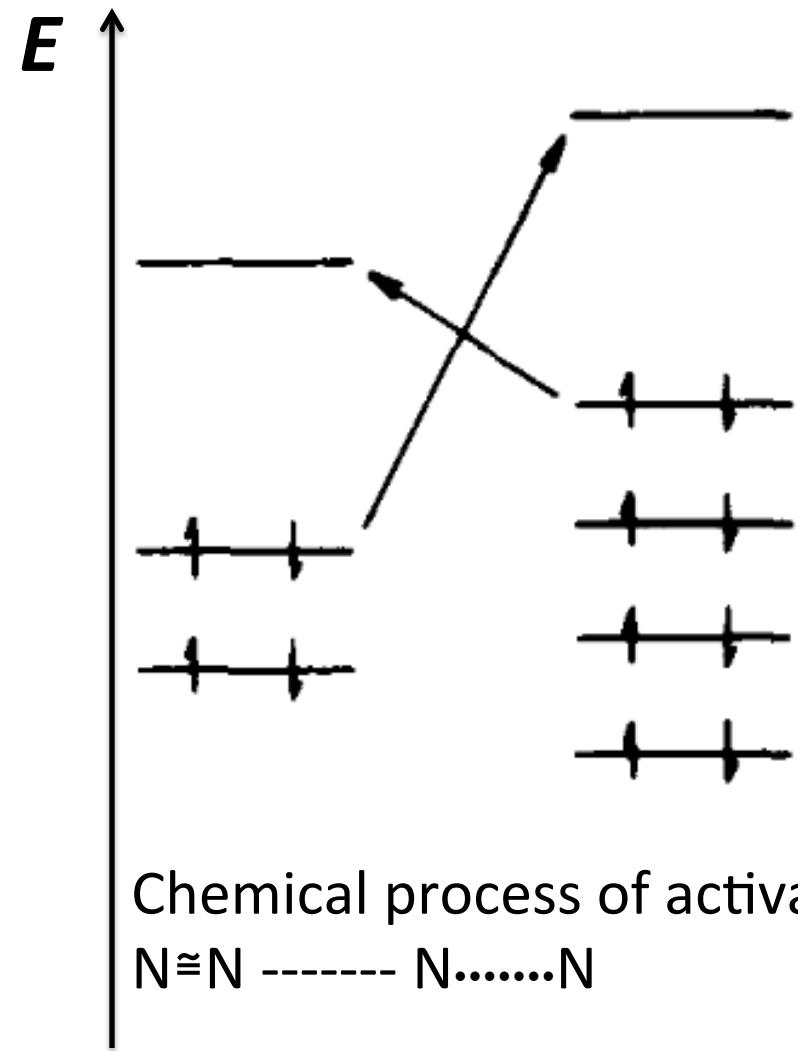


Chemical Reactivity.....

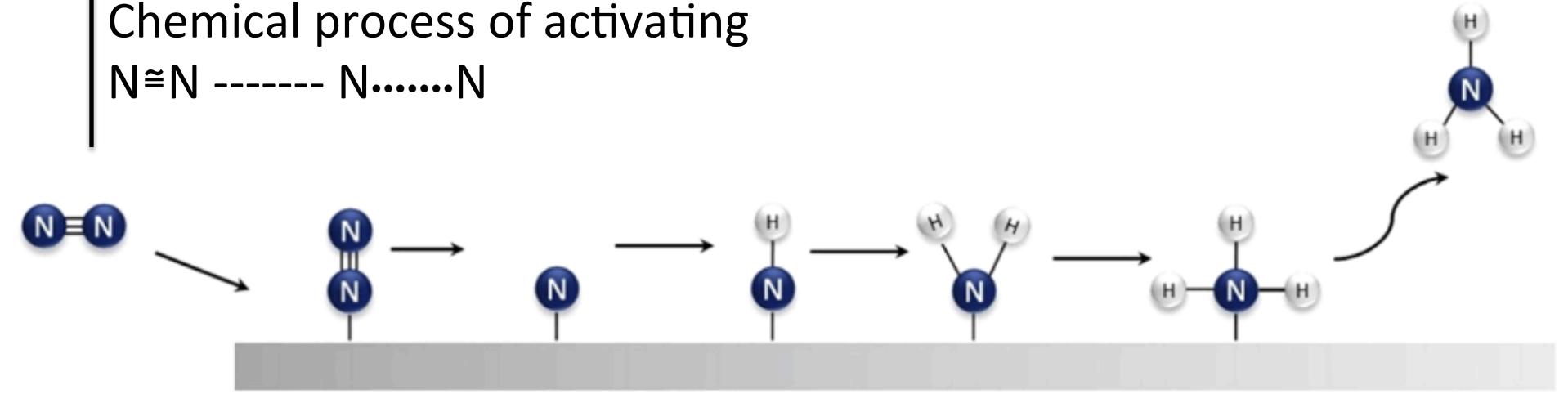


Chemical Reactivity.....

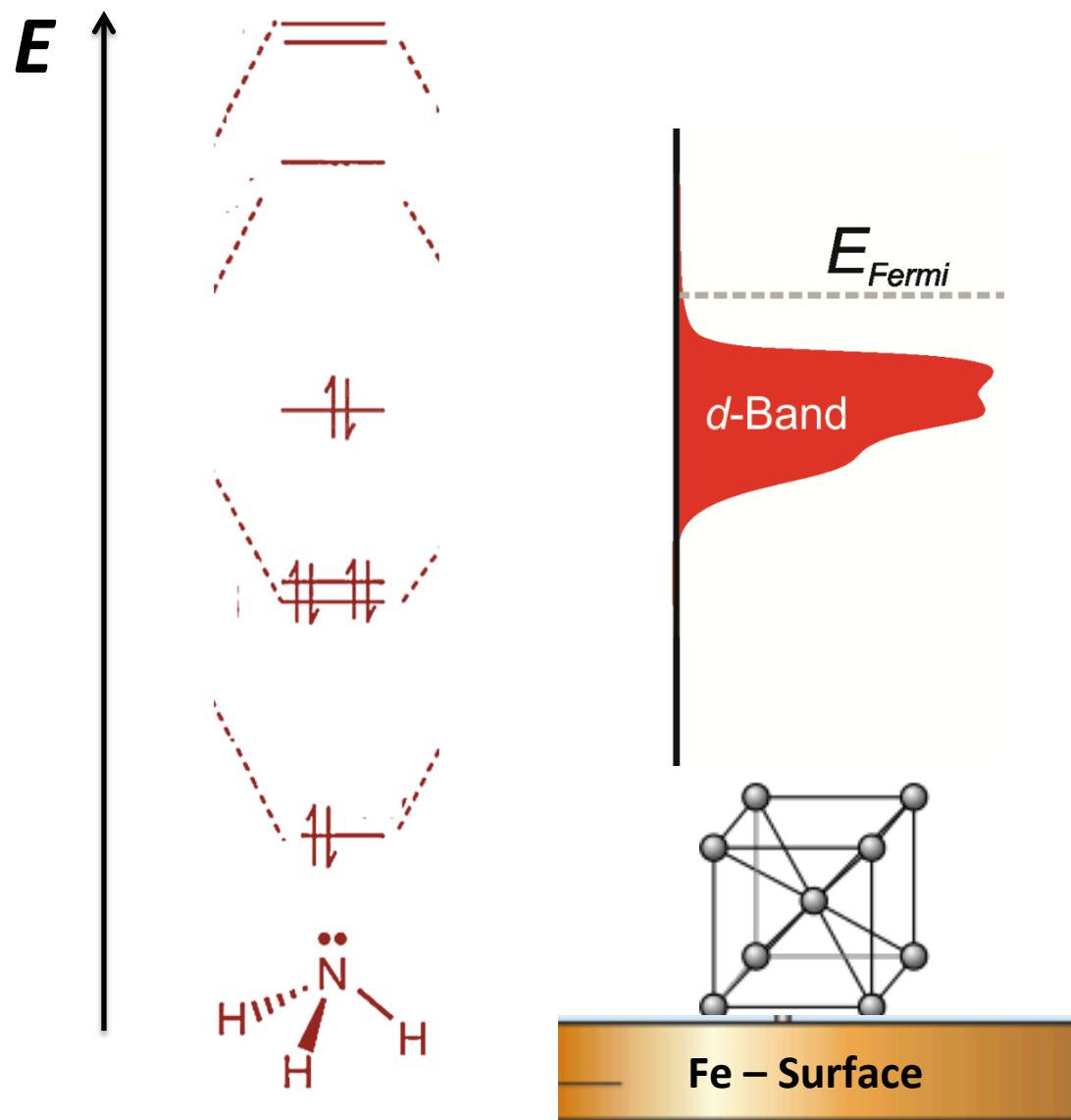
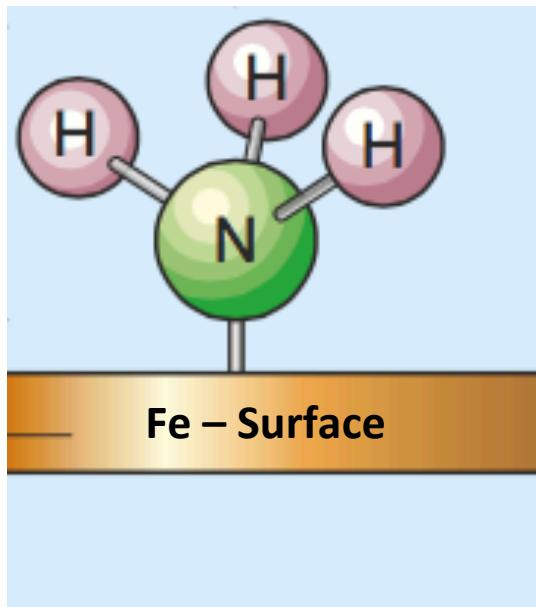




Chemical process of activating
 $\text{N}\equiv\text{N} \cdots \cdots \text{N} \cdots \cdots \text{N}$

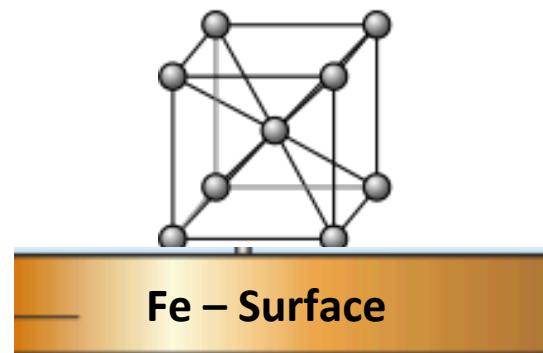
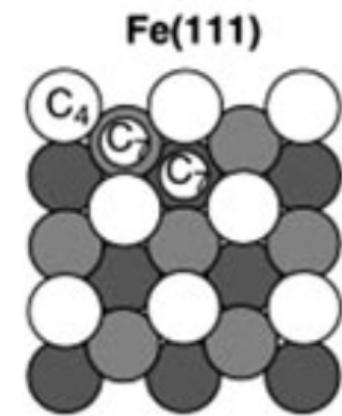
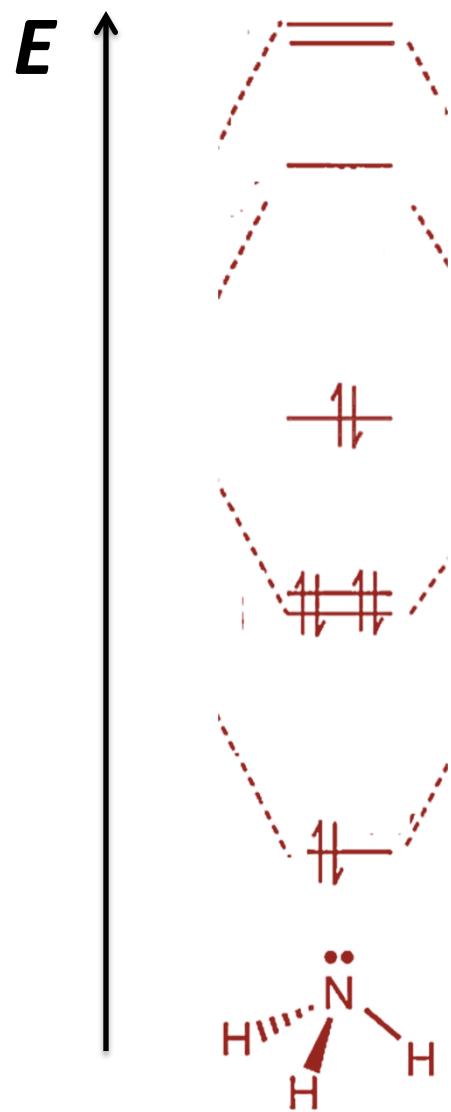
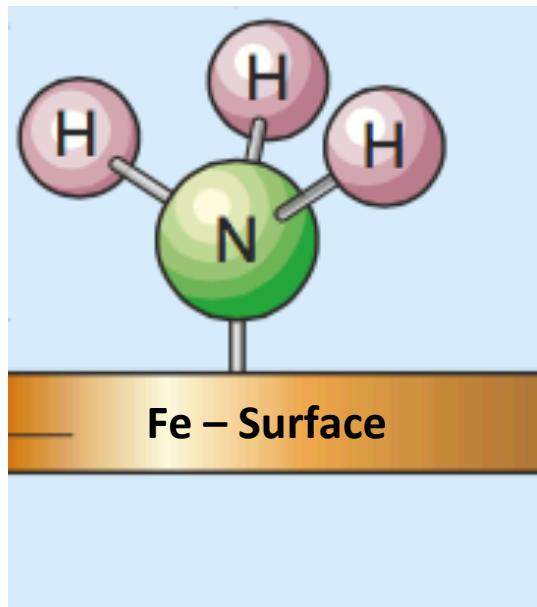


Chemical processes

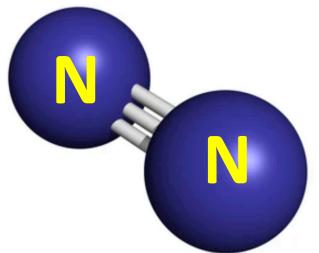


Schematic

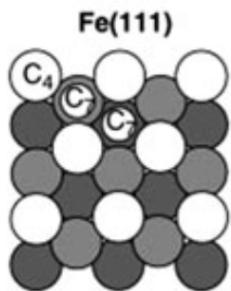
Chemical processes



Schematic



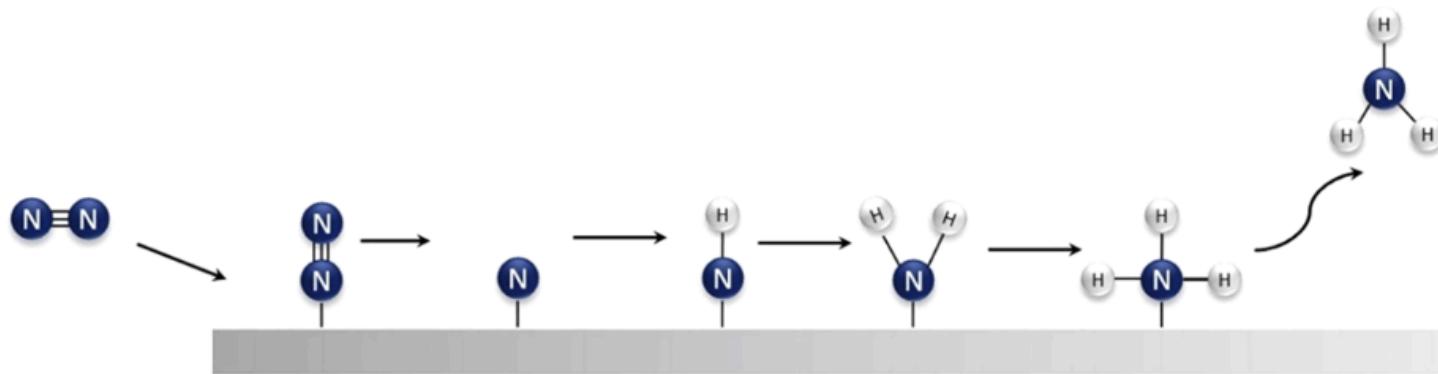
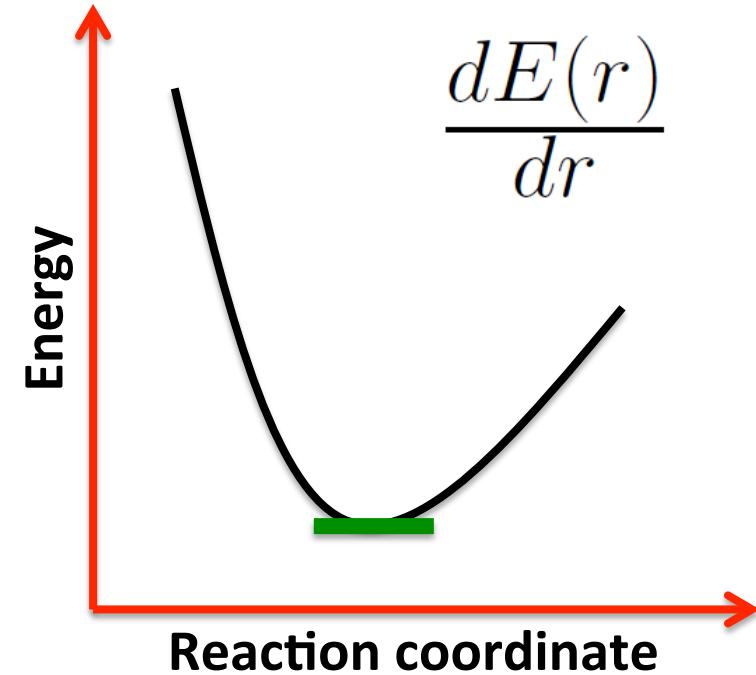
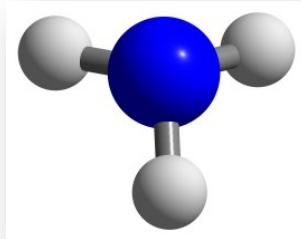
$$\psi(r) = E\psi(r)$$



$$\psi(r) = E\psi(r)$$

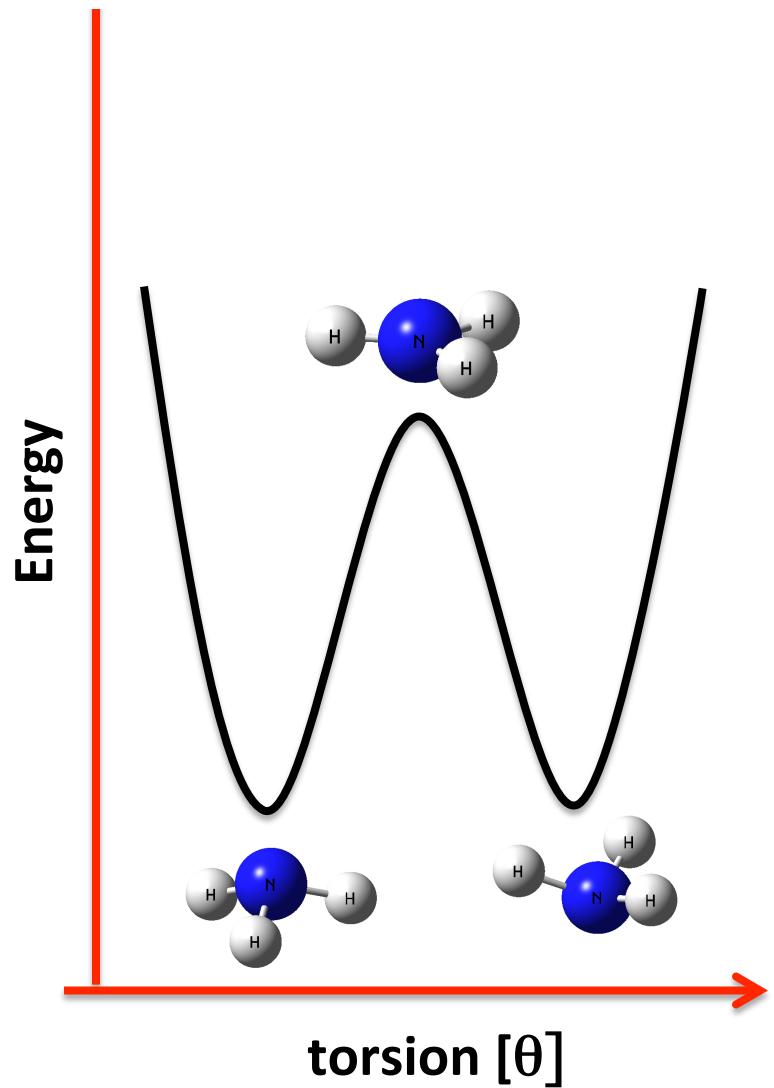
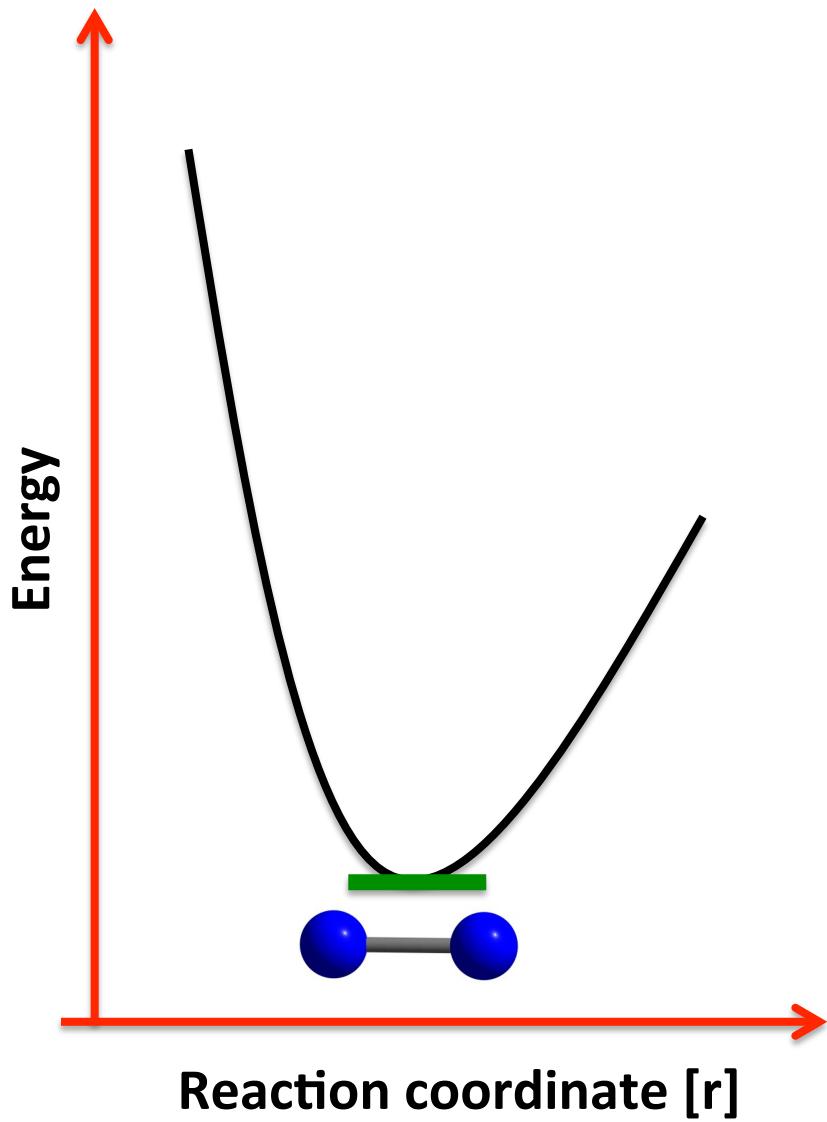
Energies & Forces

Is the structure/geometry in equilibrium?



$$\hat{H}\psi(r) = E\psi(r)$$

$$k_{\text{TST}} = \frac{k_B T}{b} (c^{\circ})^{\Delta v^\dagger} \exp\left(-\frac{\Delta G^{\circ\dagger}}{RT}\right)$$



Energies

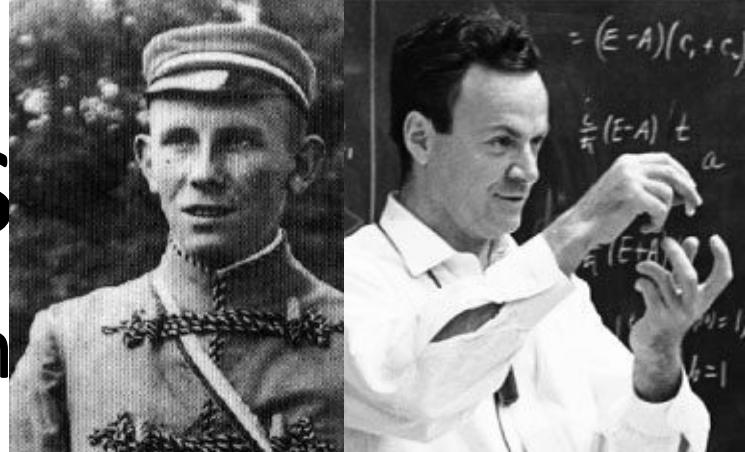
$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E \psi(r)$$

By applying some methods of approximations, we may obtain the expectation value for a given configuration

$$E = \frac{\int \psi^*(r) \hat{H} \psi(r) d\tau}{\int \psi^*(r) \psi(r) d\tau} = \langle \psi | \hat{H} | \psi \rangle$$

Forces

Hellmann-Feynman Theorem
Molecular Force Theorem:



AUGUST 15, 1939

PHYSICAL REVIEW

VOLUME 56

$$\frac{dE(r)}{dr}$$

Forces in Molecules

R. P. FEYNMAN

Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received June 22, 1939)

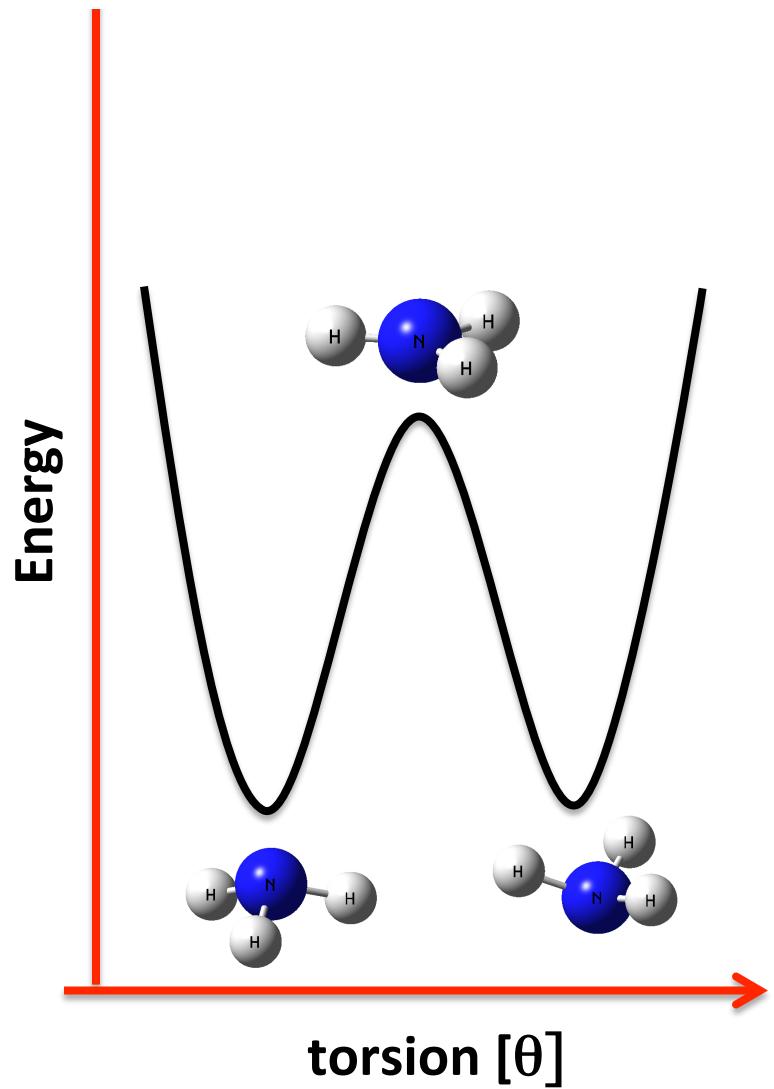
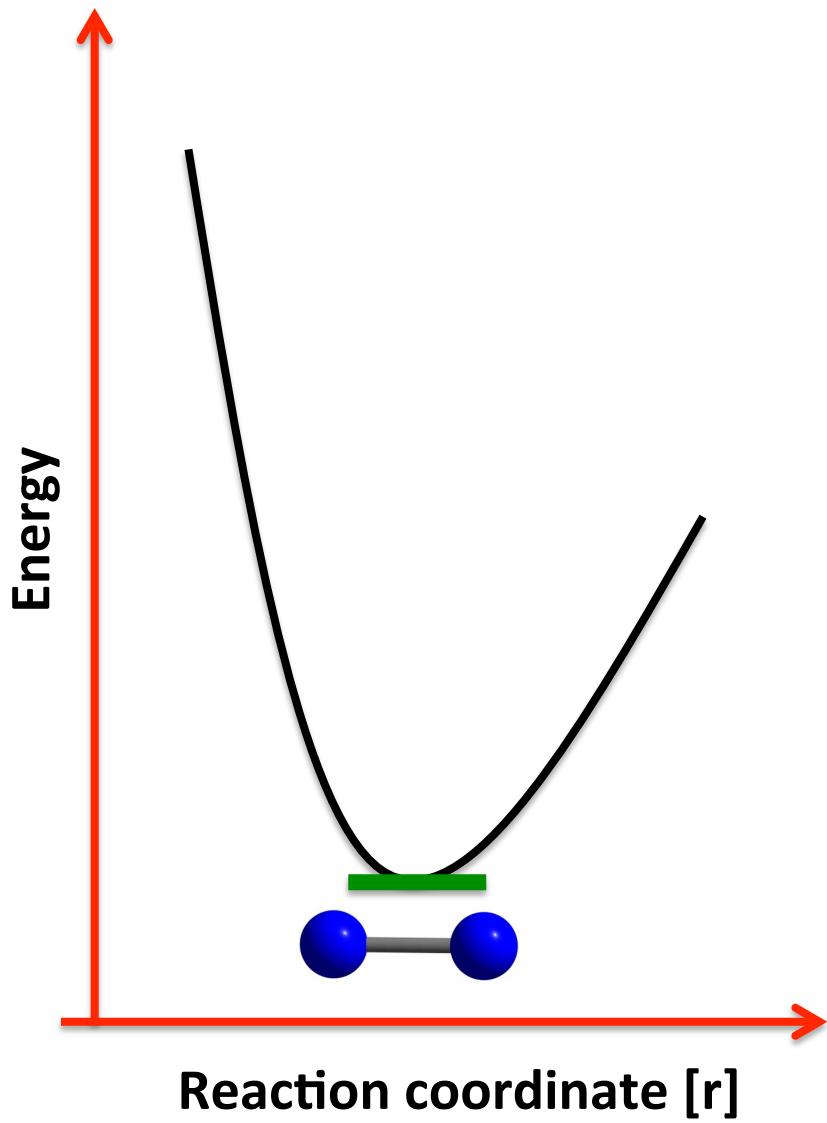
$$\frac{\partial E_\lambda}{\partial \lambda}$$

Formulas have been developed to calculate the forces in a molecular system directly, rather than indirectly through the agency of energy. This permits an independent calculation of the slope of the curves of energy *vs.* position of the nuclei, and may thus increase the accuracy, or decrease the labor involved in the calculation of these curves. The force on a nucleus in an atomic system is shown to be just the classical electrostatic force that would be exerted on this nucleus by other nuclei and by the electrons' charge distribution. Qualitative implications of this are discussed.

$$\frac{\partial E_\lambda}{\partial \lambda} = \langle \psi_\lambda | \frac{\partial \hat{H}}{\partial \lambda} | \psi_\lambda \rangle$$

$$\hat{H}\psi(r) = E\psi(r)$$

$$k_{\text{TST}} = \frac{k_B T}{b} (c^{\circ})^{\Delta v^\dagger} \exp\left(-\frac{\Delta G^{\circ\dagger}}{RT}\right)$$



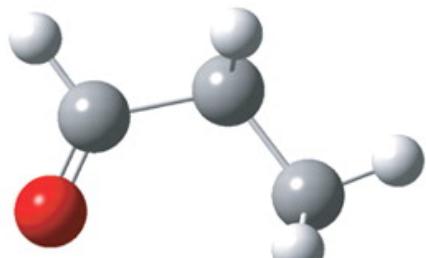
Formally the tools are Ready!

But how E?

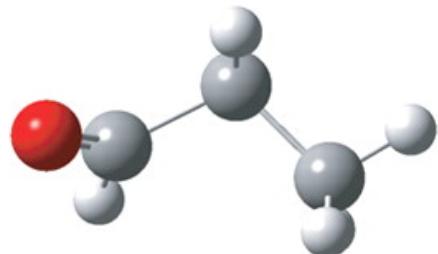
$$E = \frac{\int \psi^*(r) \hat{H} \psi(r) d\tau}{\int \psi^*(r) \psi(r) d\tau}$$

$$\frac{dE(r)}{dr}$$

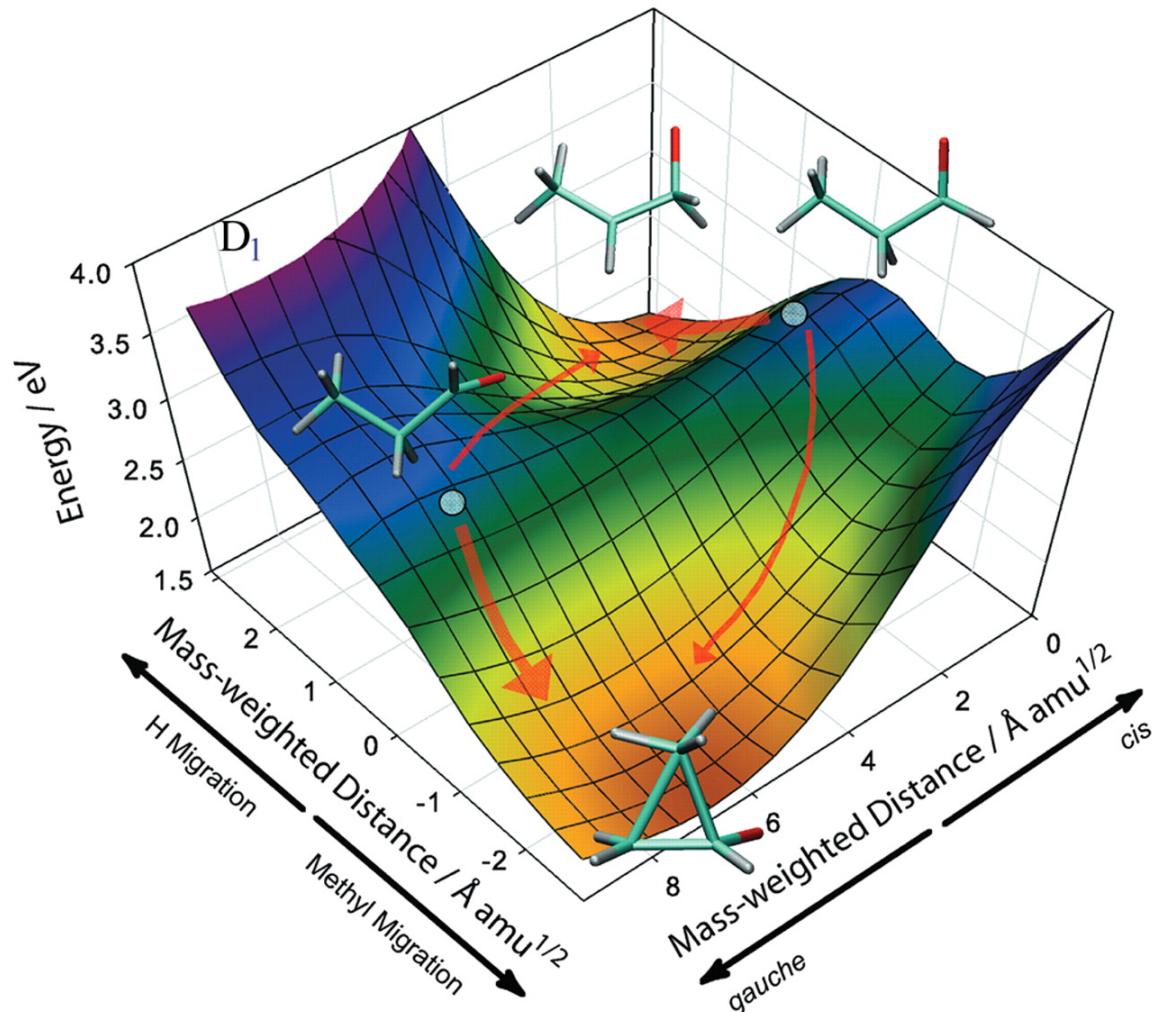
Conformationally Controlled Chemistry



cis- $\text{CH}_3\text{CH}_2\text{CHO}^+$



gauche- $\text{CH}_3\text{CH}_2\text{CHO}^+$



Molecular level understanding of chemical processes



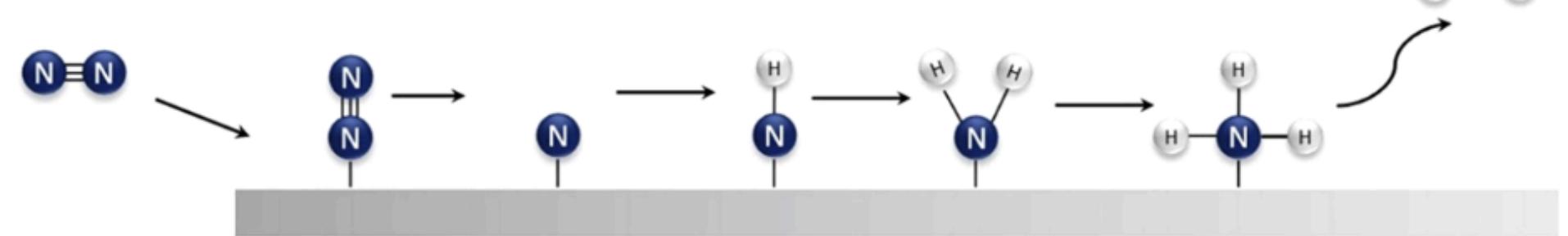
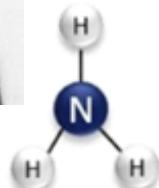
Kenichi Fukui



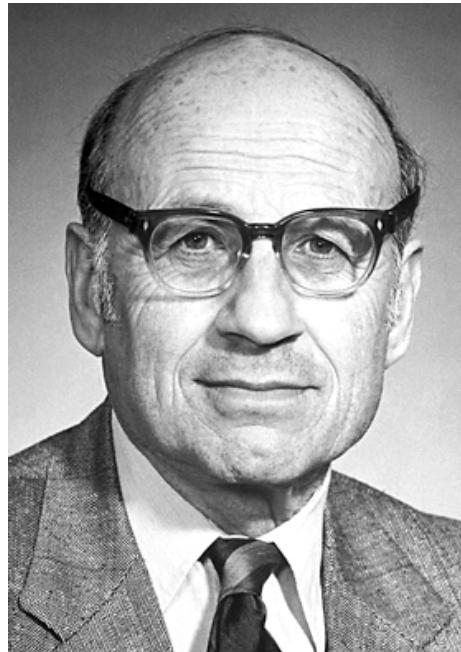
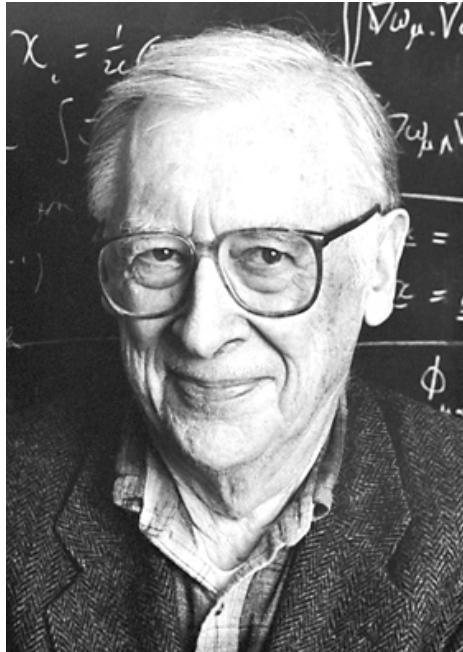
Roald Hoffmann



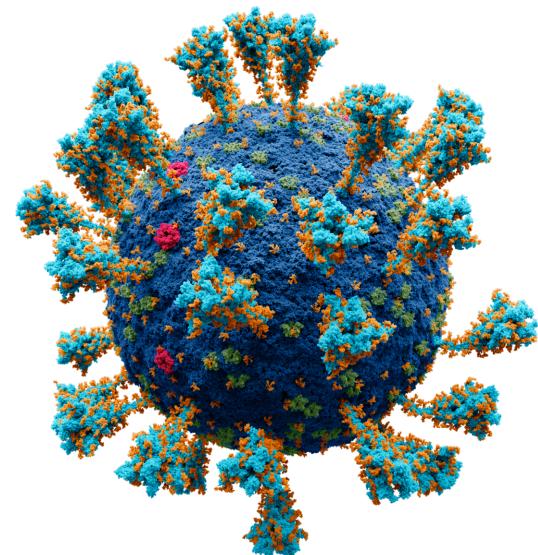
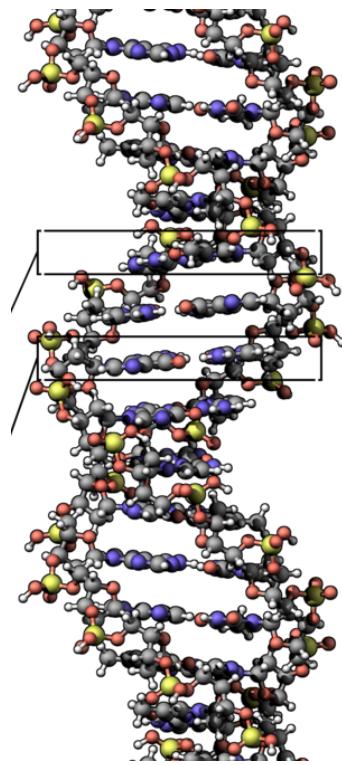
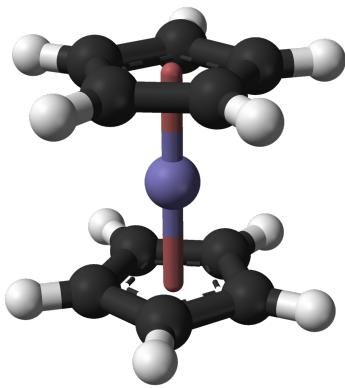
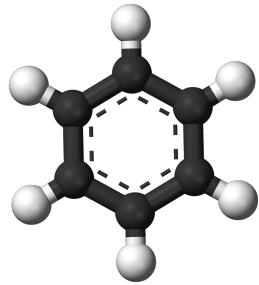
Michael Polanyi



The Nobel Prize in Chemistry 1998

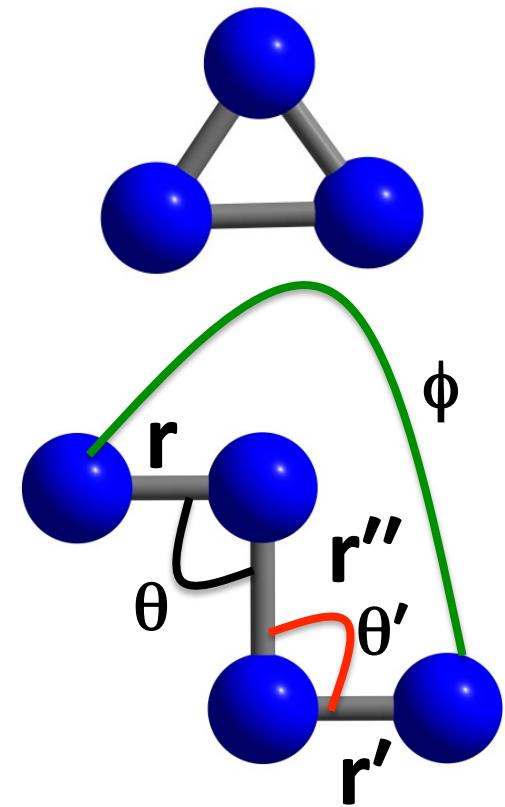
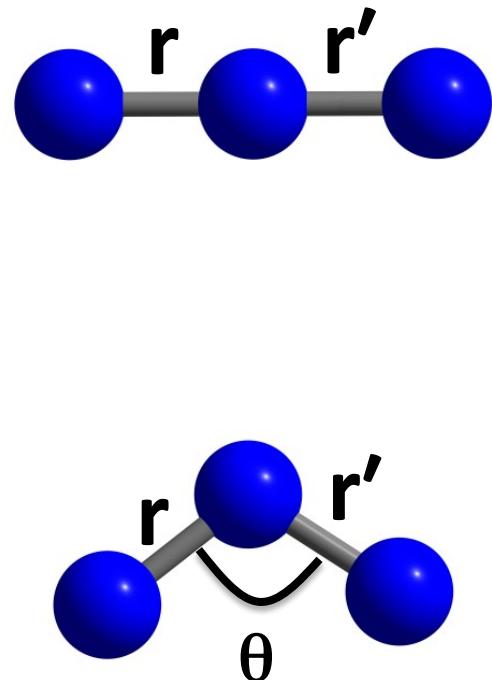
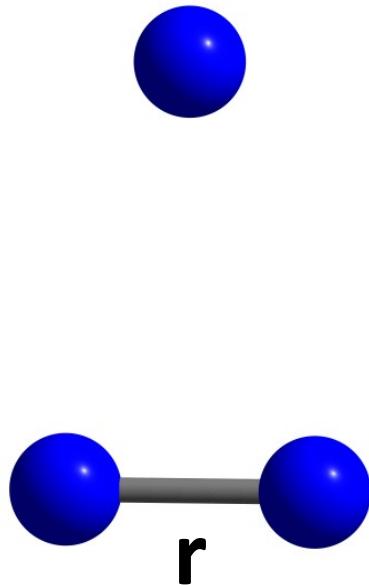


The Nobel Prize in Chemistry 1998 was awarded to John A. Pople (*left*) "for his development of computational methods in quantum chemistry" and Walter Kohn (*right*) "for his development of the density-functional theory (DFT)" .

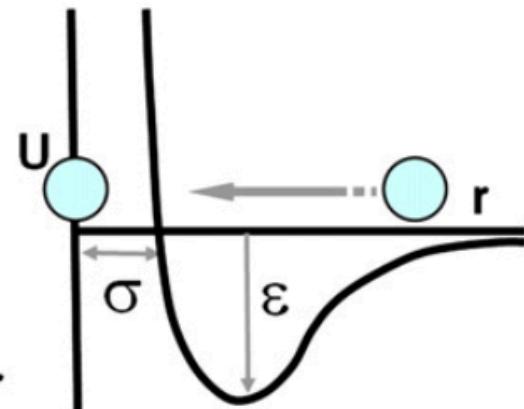


Configurations

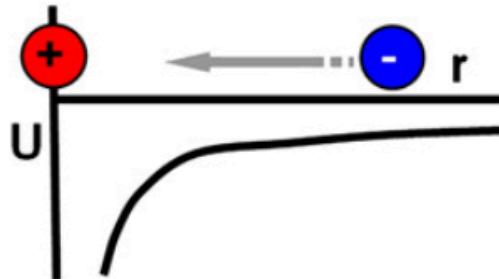
For a configuration! Of course!



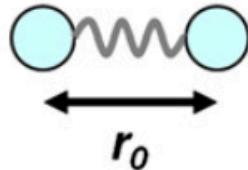
$$U = \sum_{i < j} \sum 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$



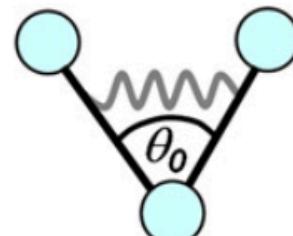
$$+ \sum_{i < j} \sum \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$



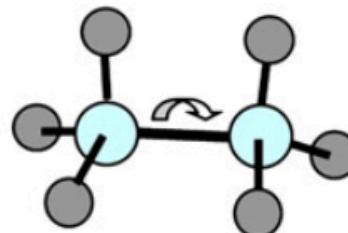
$$+ \sum_{bonds} \frac{1}{2} k_b (r - r_0)^2$$



$$+ \sum_{angles} \frac{1}{2} k_a (\theta - \theta_0)^2$$



$$+ \sum_{torsions} k_\phi [1 + \cos(n\phi - \delta)]$$



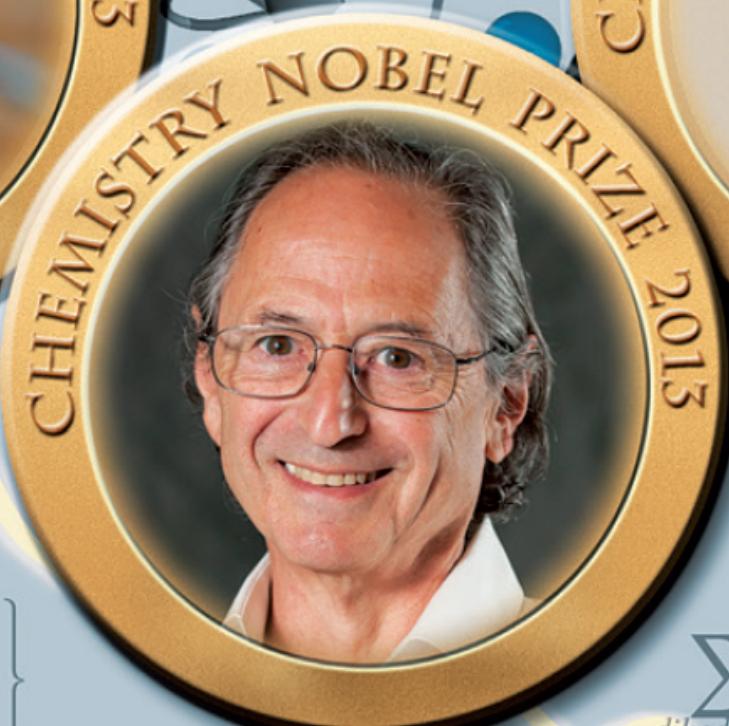
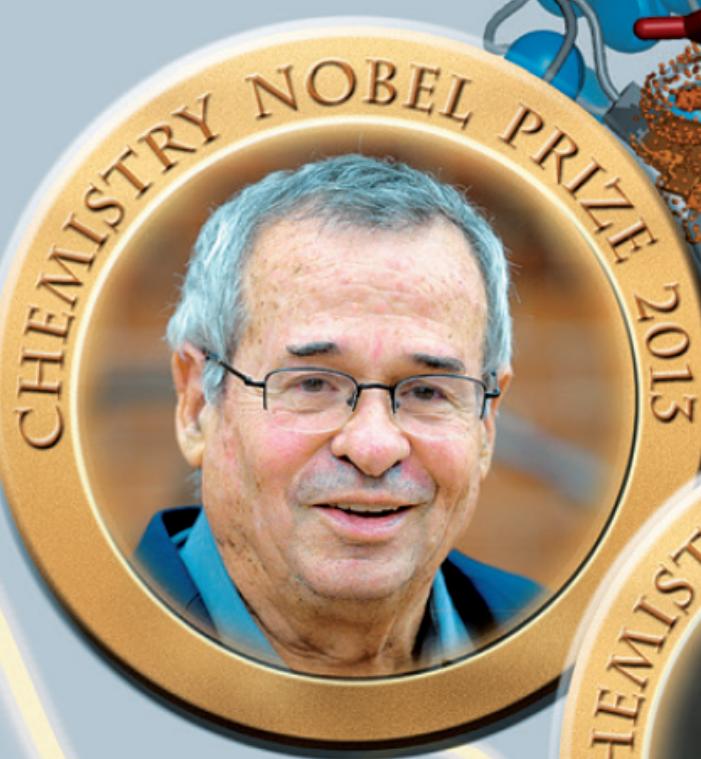
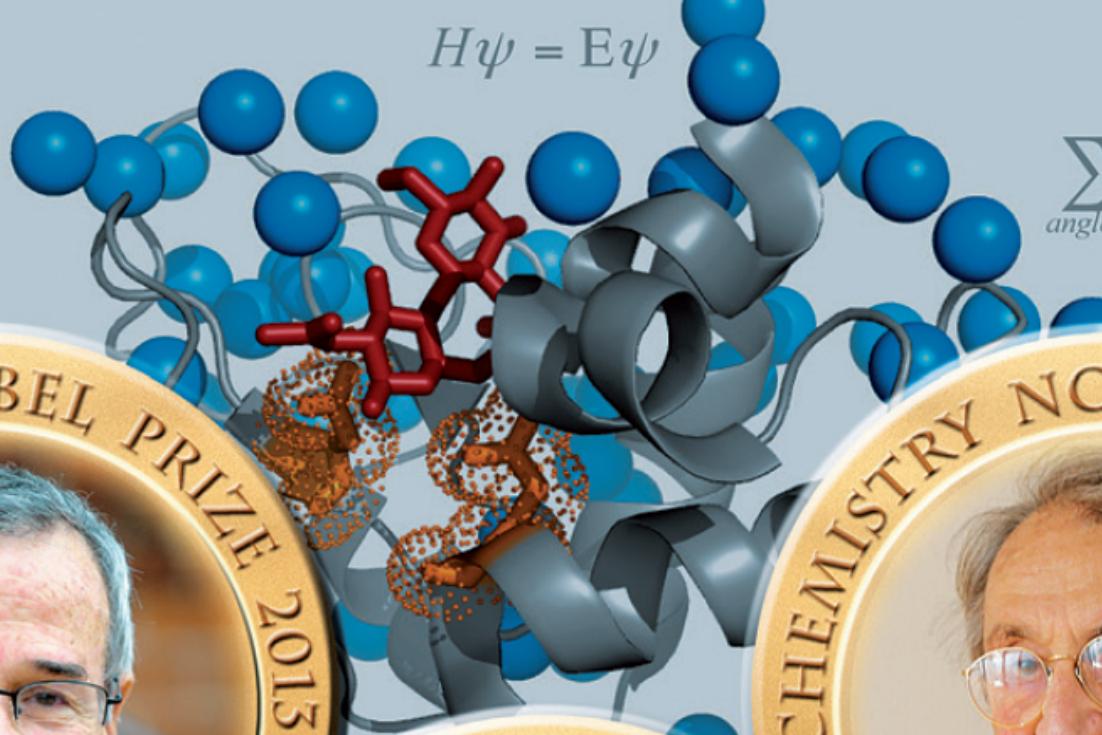
Just for notation and quick notes for reading.....
meaning of the terms for the previous equations...

“Potential energy function for molecular interactions in the molecular mechanics approximation. The molecules are treated as consisting of balls (the atoms) connected by springs (the bonds). The first and second terms describes the van der Waals and Coulombic interactions respectively for atoms i and j .

The next set of terms describe the bond, bond angle and torsional energy of the molecules comprising the system. For the bonded terms (bonds, bond angles and torsions), the potential energy is relative to the atoms being in their equilibrium (preferred) state for which the energy is taken to be zero. The Lennard Jones parameters ϵ_{ij} and σ_{ij} , partial charges q_i and q_j , and the force constants k_b , k_a , and k_ϕ are all atom-specific parameters that are inputs to the simulation.”

$$H\psi = E\psi$$

$$-\frac{\partial U}{\partial r} = m \frac{d^2 r}{dt^2}$$

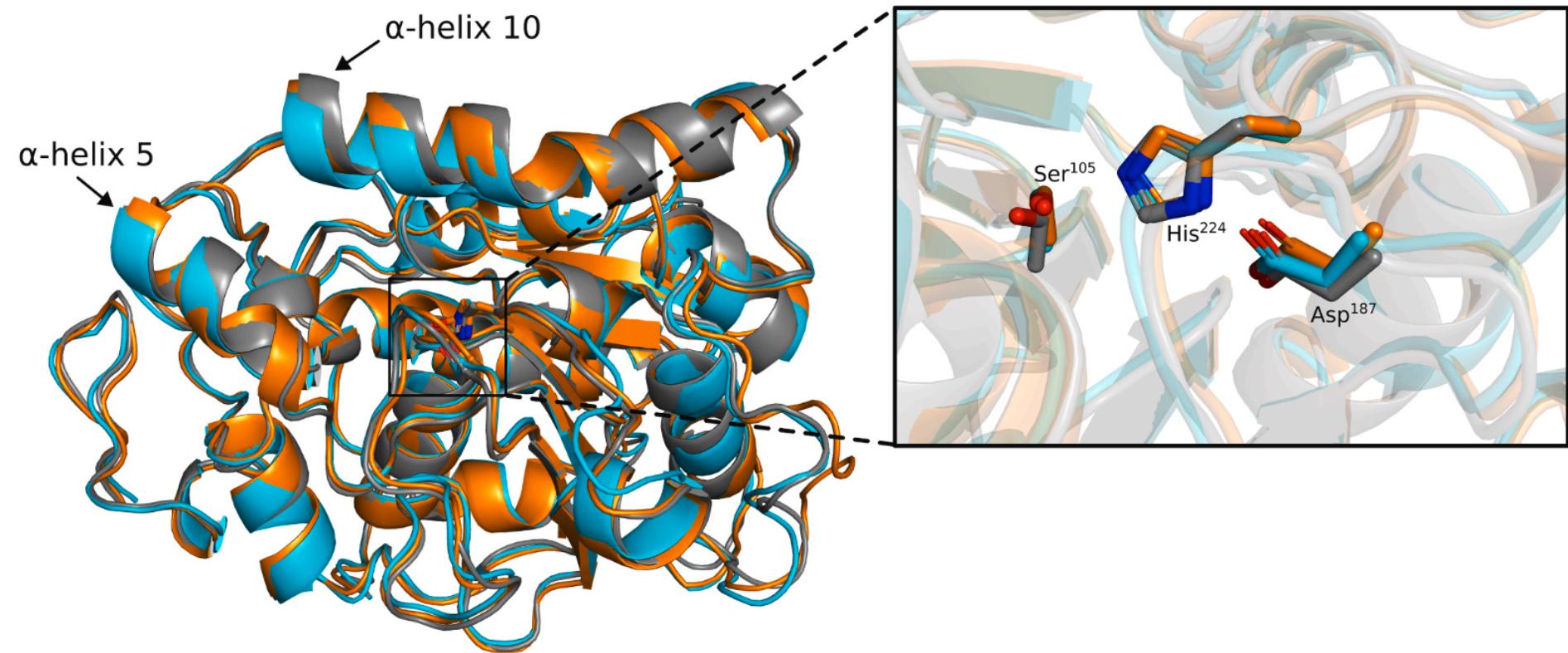


$$\sum \epsilon_{ij} \left(\frac{\sigma_{ij}}{r} \right)^{12}$$

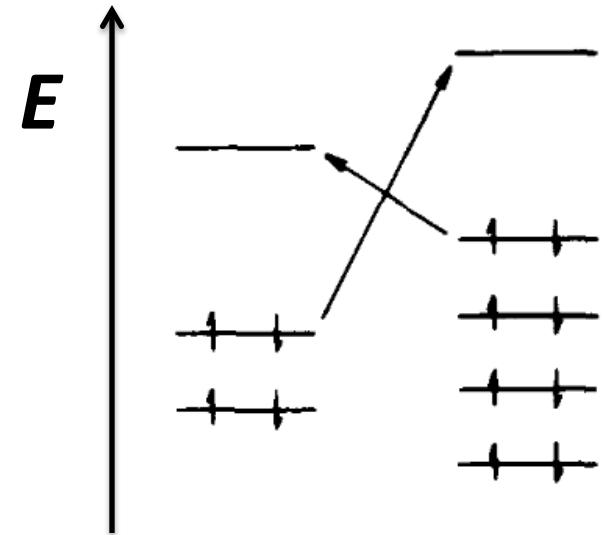
$$\sum \left\{ \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{r} \right)^6 \right] \right\}$$

$$\sum_{\text{bonds}} K_b (b - b_0)^2$$

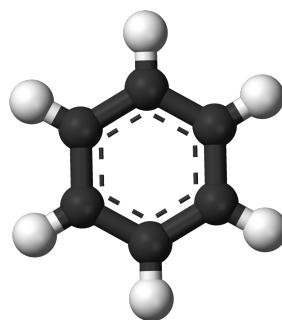
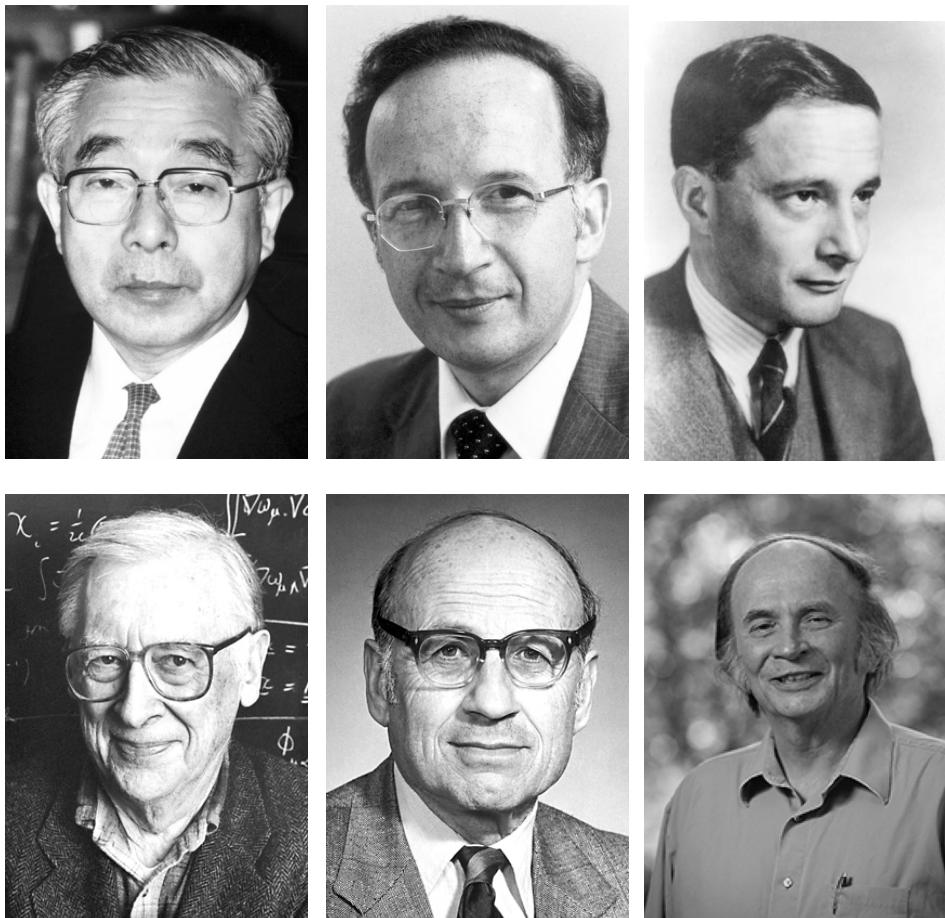
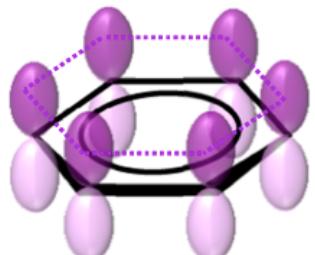
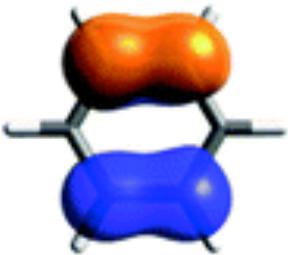
$$\sum_{\text{dihedrals}} K_\varphi [1 - \cos(n\varphi - \varphi_0)]$$

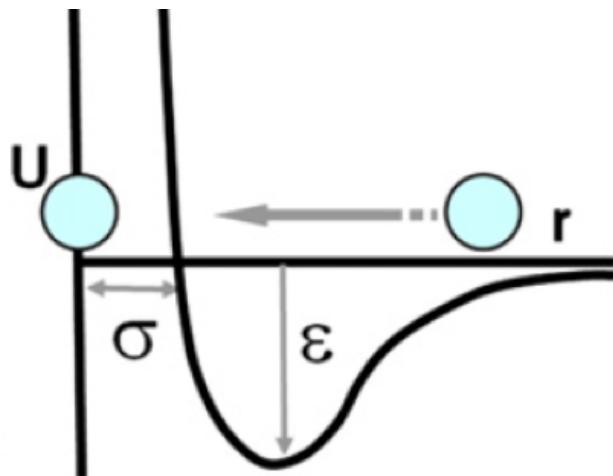




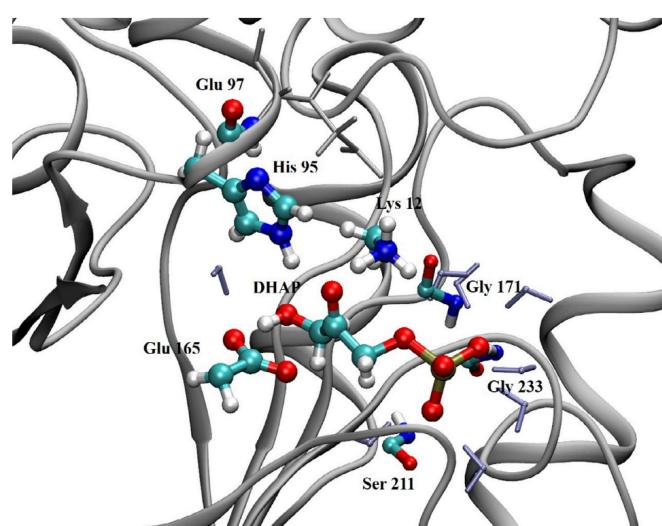
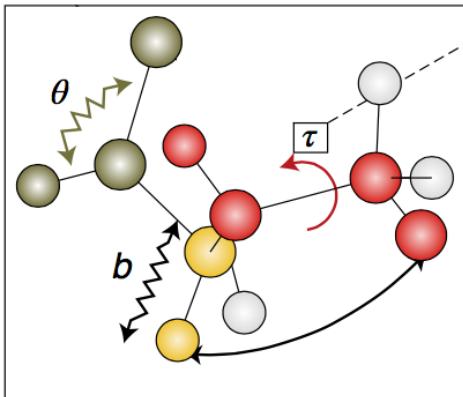


$$\hat{H}\psi(r) = E\psi(r)$$

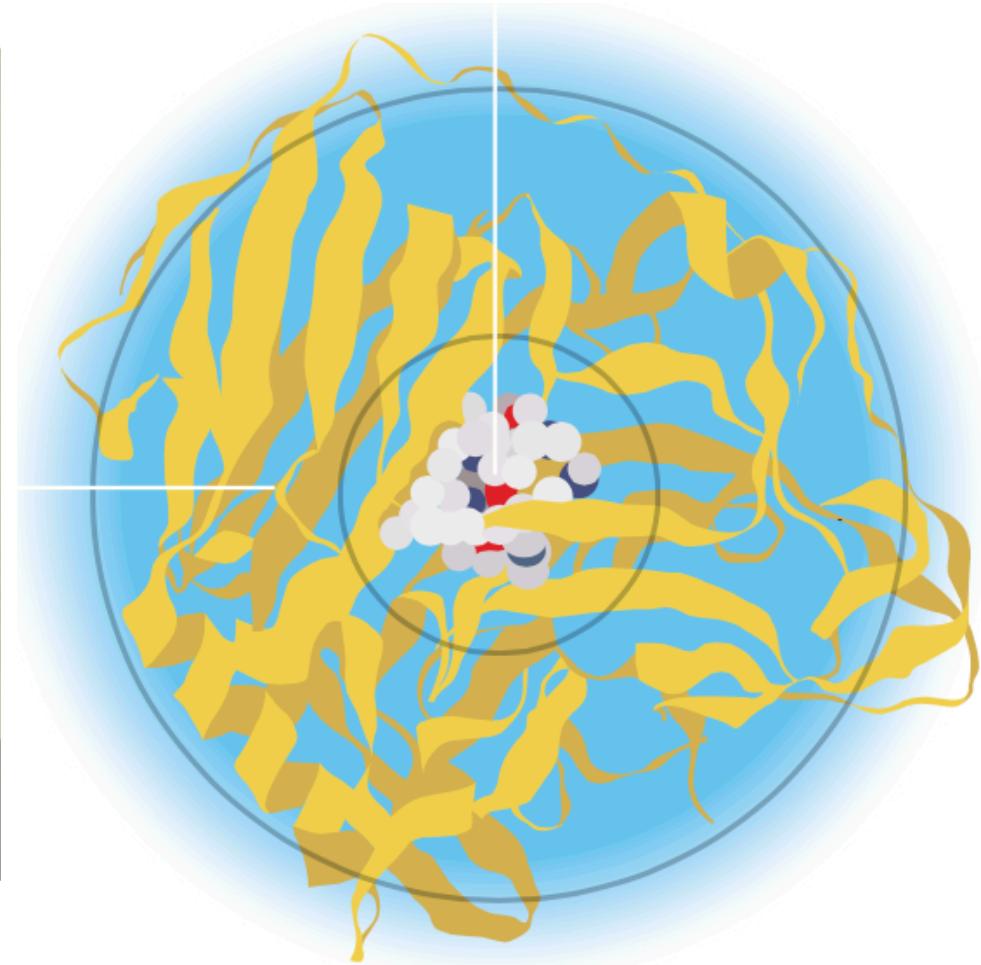




$$U = \sum_{i < j} \sum 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$

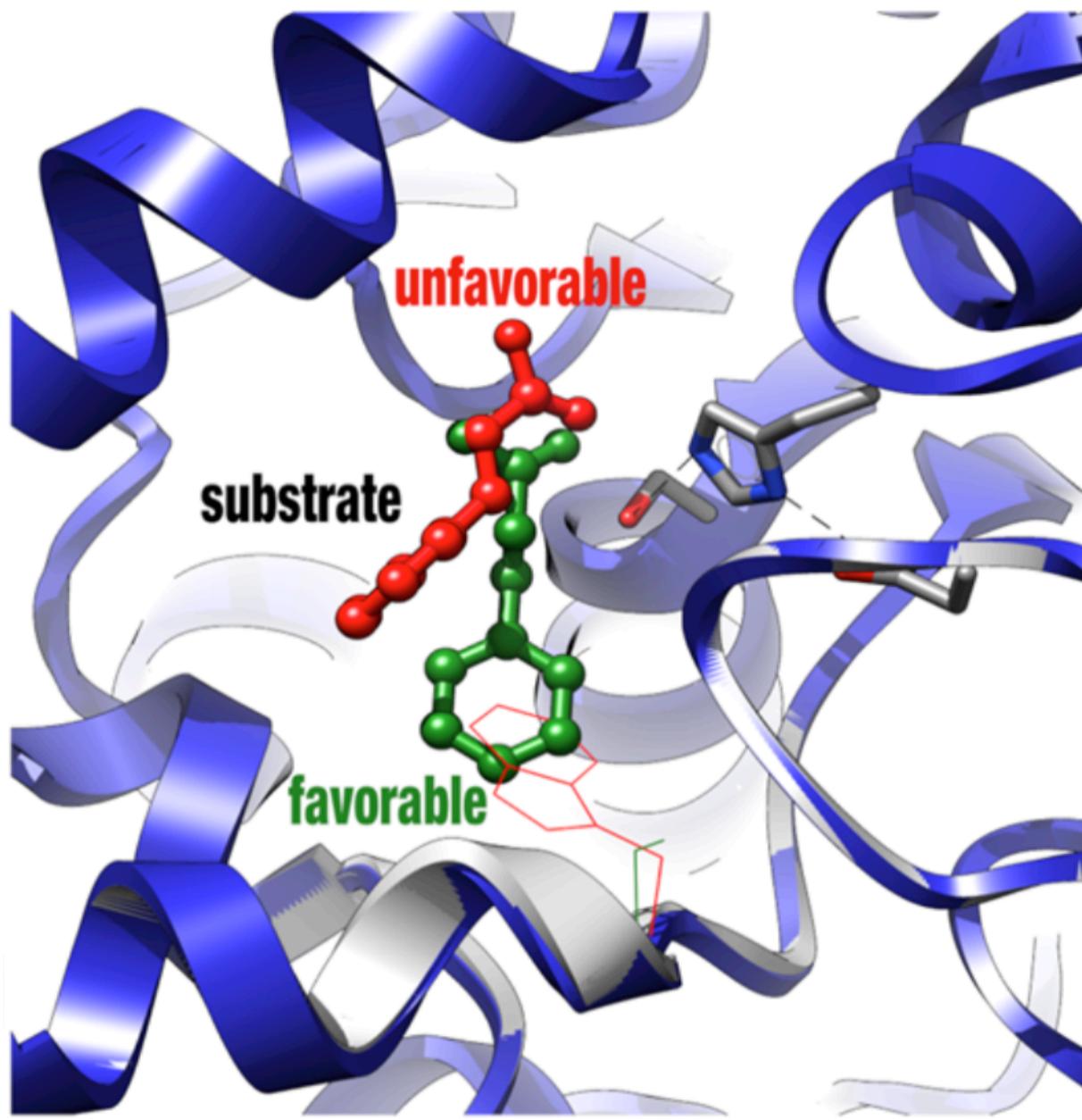


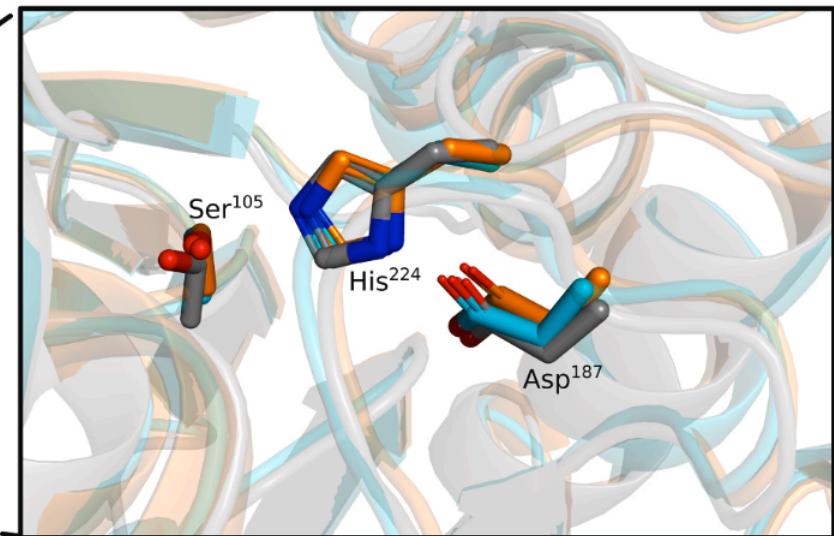
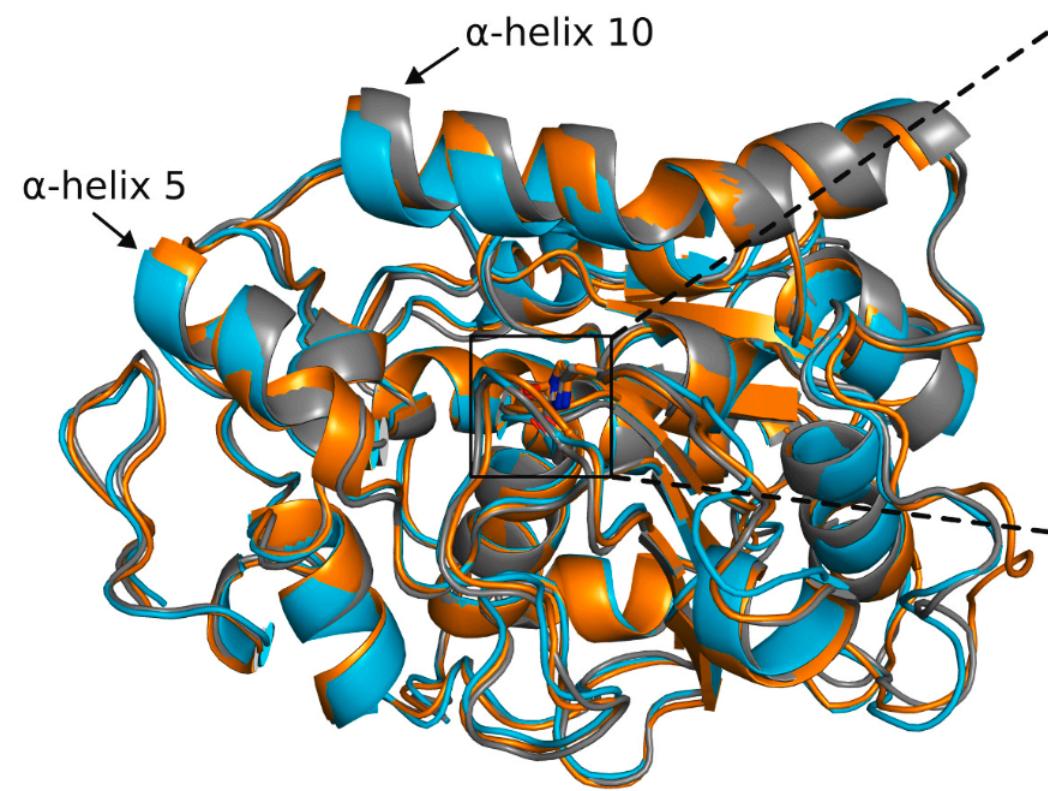
$$\hat{H}\psi(r) = E\psi(r)$$

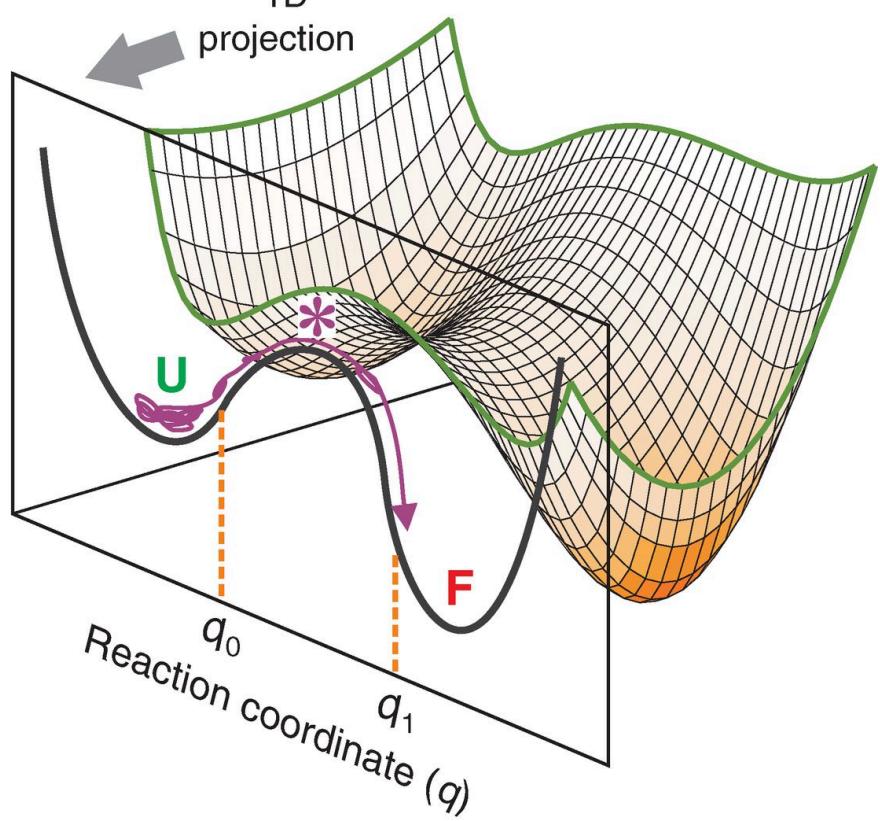
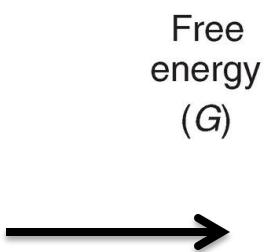
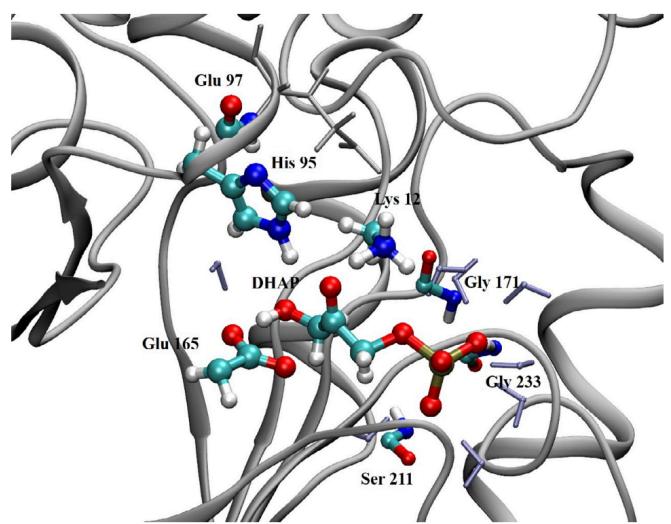
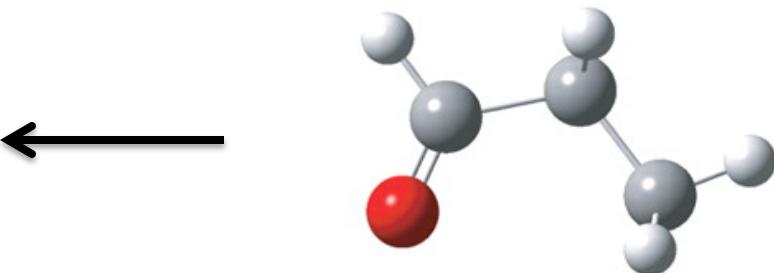
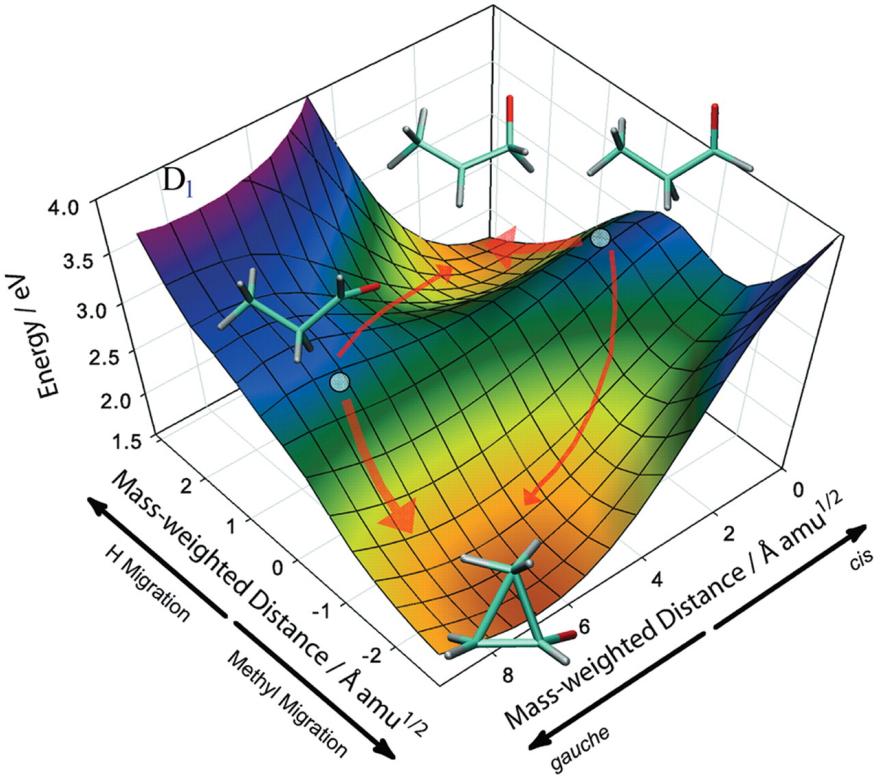


$$-\frac{dU}{dr} = m \frac{d^2r}{dt^2}$$

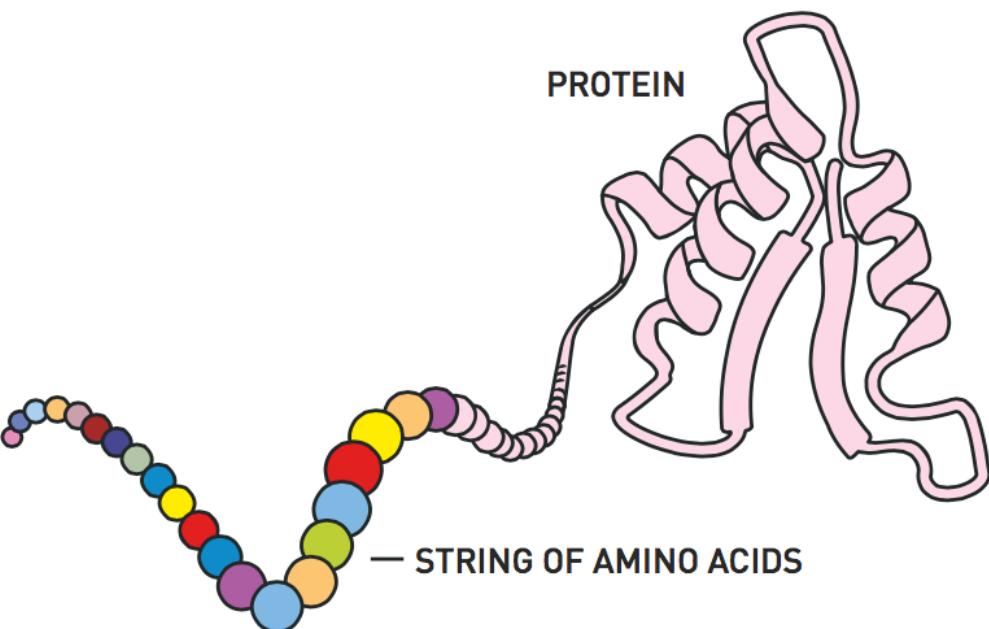
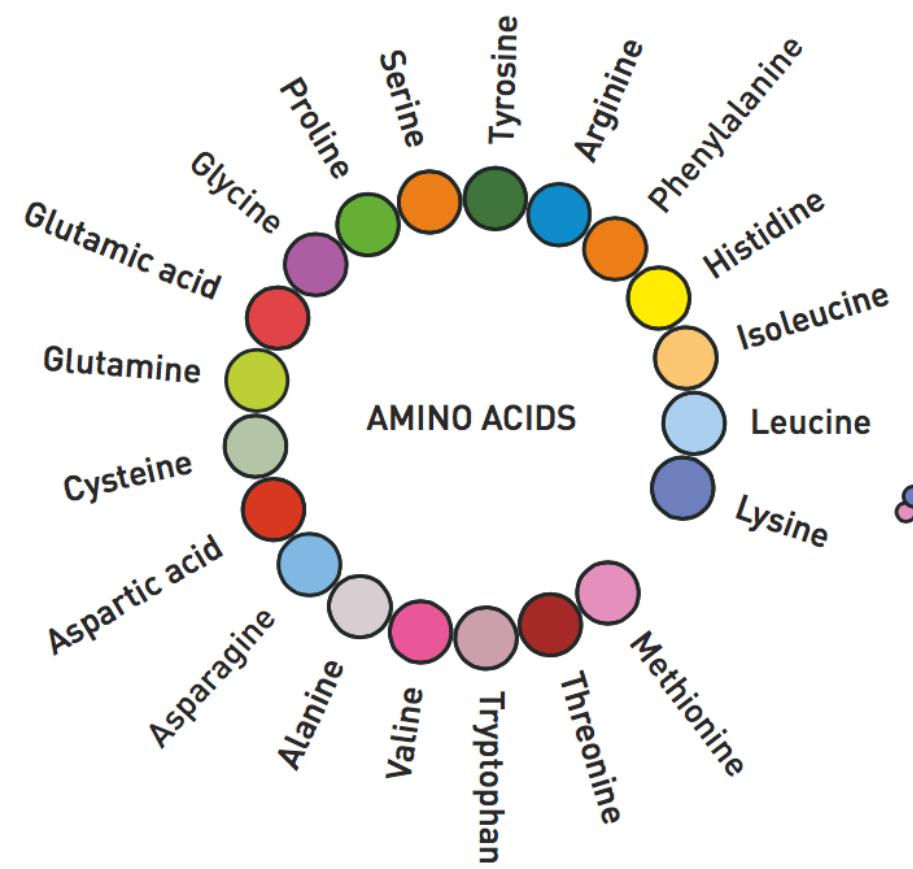
Modeling favorable and unfavorable interactions



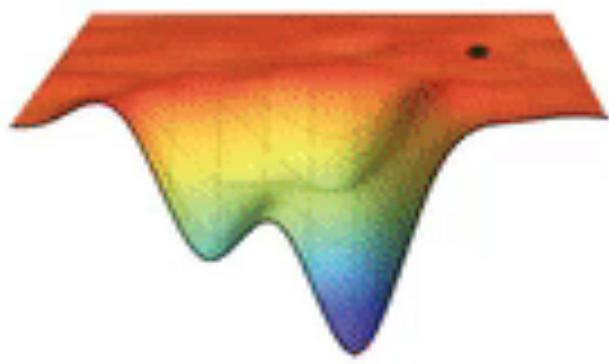
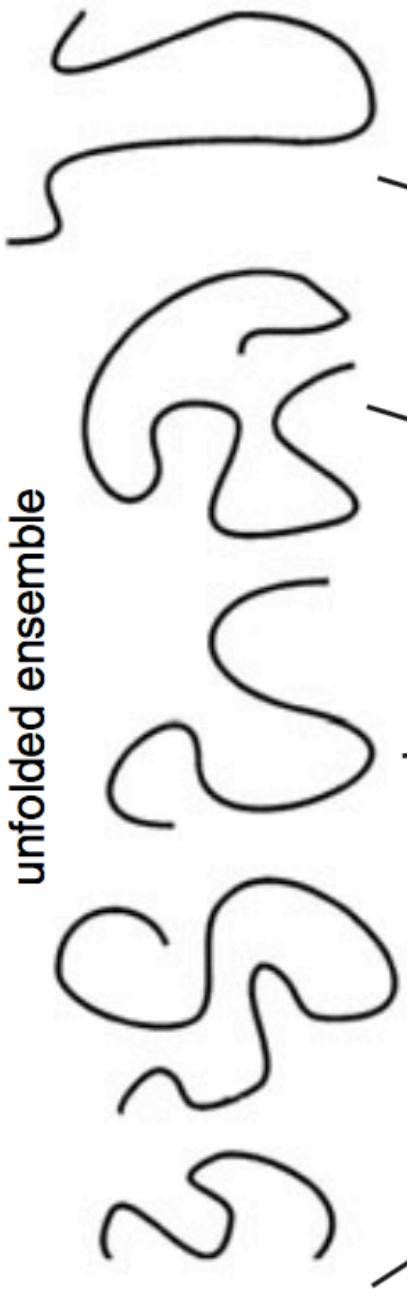








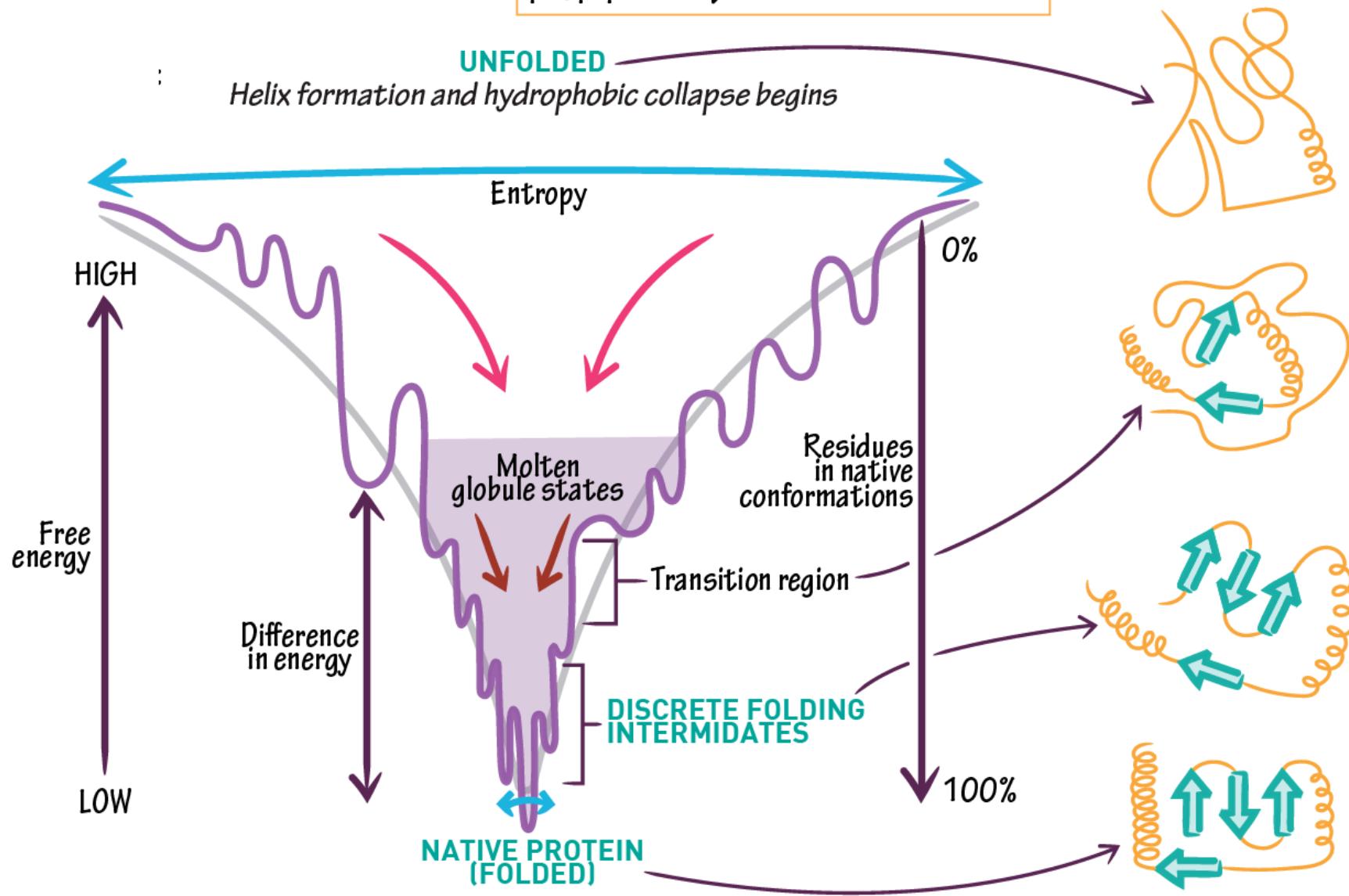
unfolded ensemble



- ✓ Protein folding is “all or none”: proteins fold via cooperative transition

Levinthal’s Paradox

Proteins take as little as a microsecond to completely fold, despite the astronomical number of possible conformations for each polypeptide sequence.



Levinthal's paradox

ROBERT ZWANZIG, ATTILA SZABO, AND BIMAN BAGCHI*

Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, Building 2, National Institutes of Health, Bethesda, MD 20892

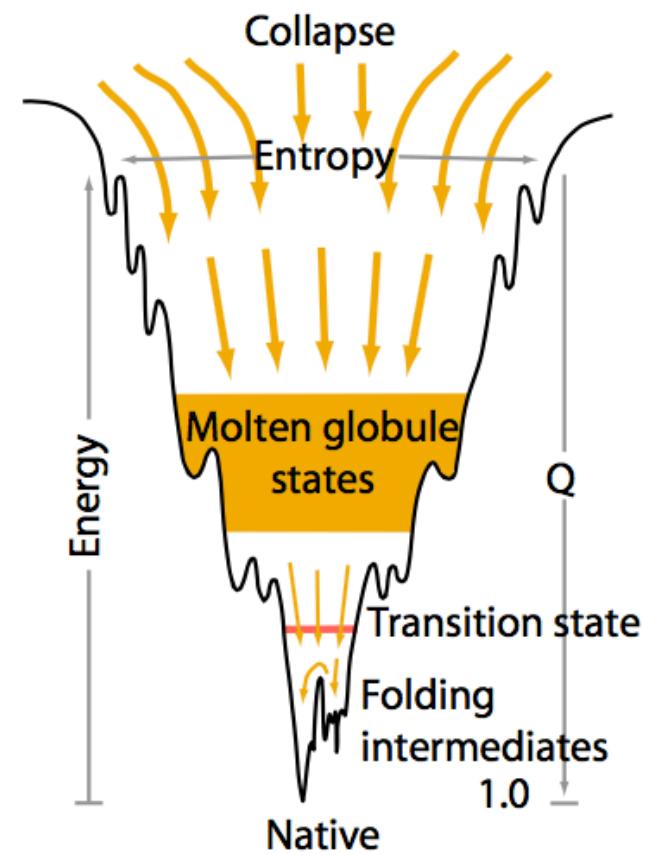
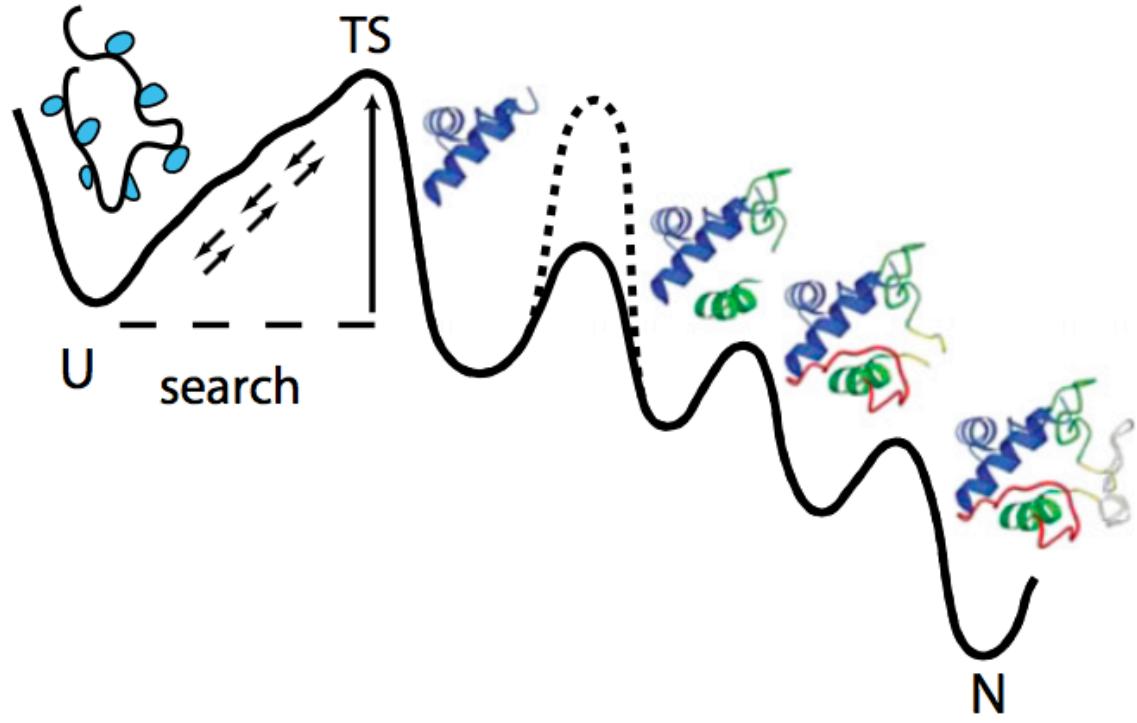
Contributed by Robert Zwanzig, October 7, 1991

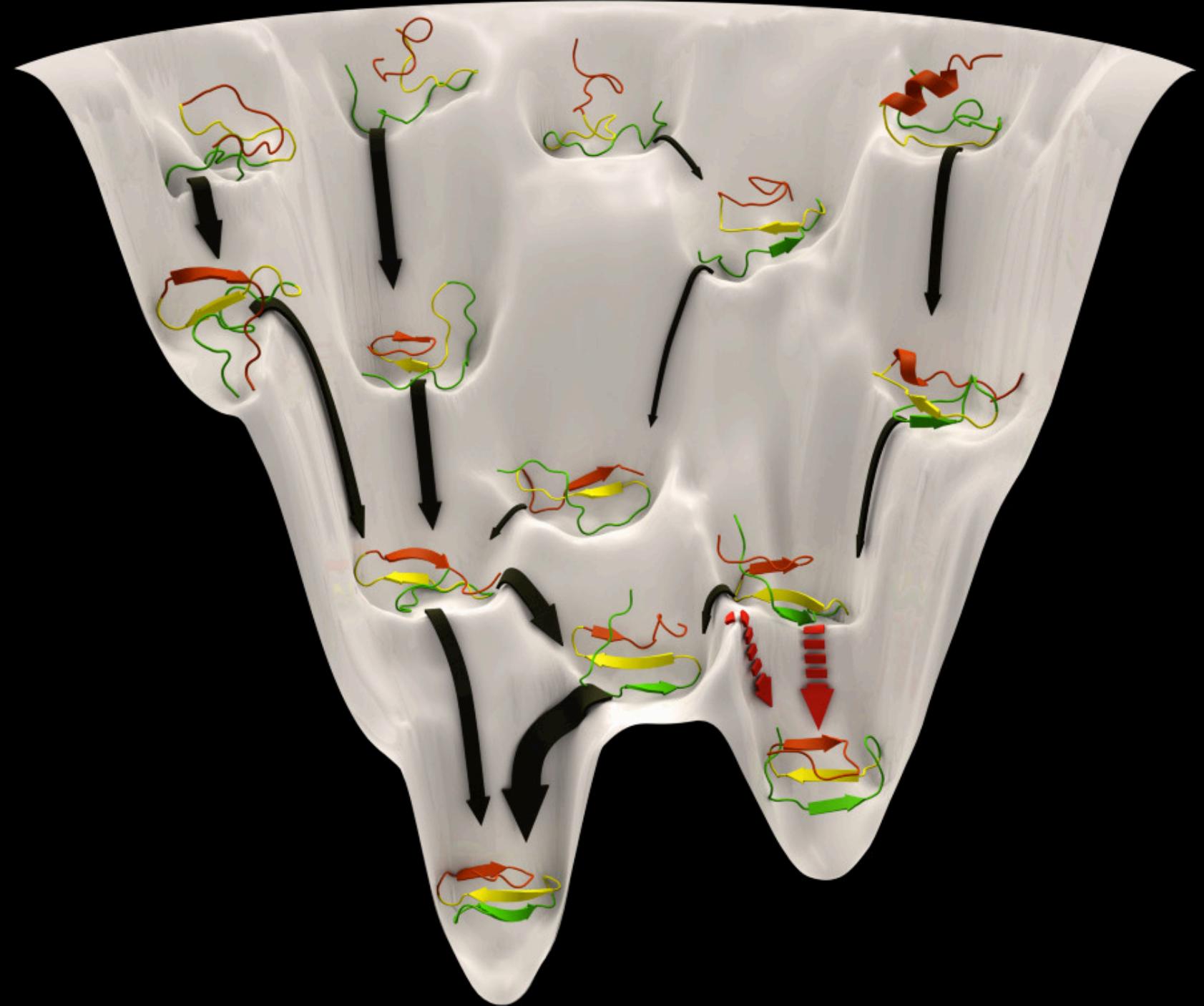
ABSTRACT Levinthal's paradox is that finding the native folded state of a protein by a random search among all possible configurations can take an enormously long time. Yet proteins can fold in seconds or less. Mathematical analysis of a simple model shows that a small and physically reasonable energy bias against locally unfavorable configurations, of the order of a few kT , can reduce Levinthal's time to a biologically significant size.

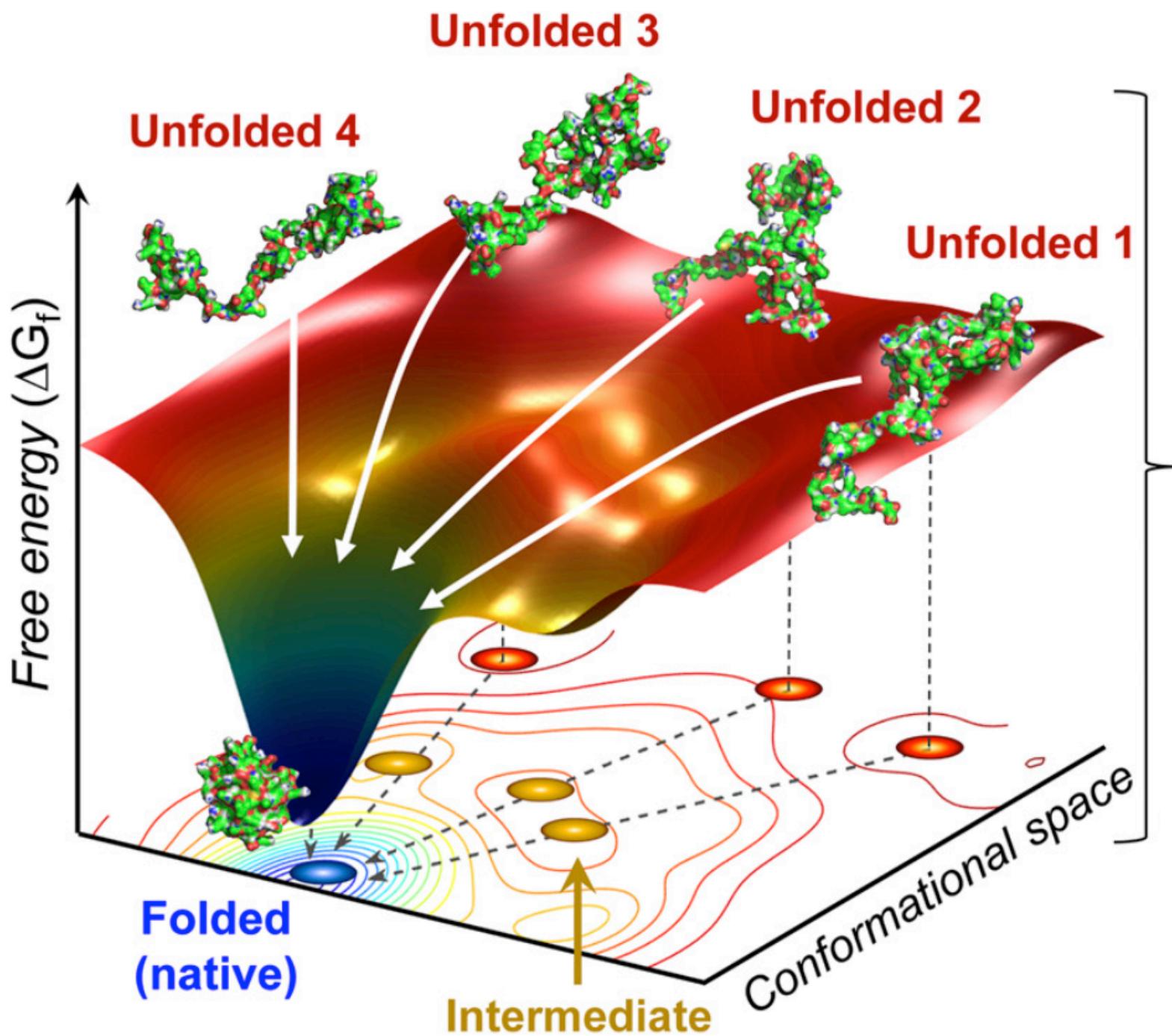
time to the fully correct state can be very much shorter. In fact, this time can become biologically significant.

Model and Results

Since the goal is not to understand the folding of any particular protein, but only to present an elementary resolution of Levinthal's paradox, precise details of the protein structure will be ignored. Consequently, the model to be

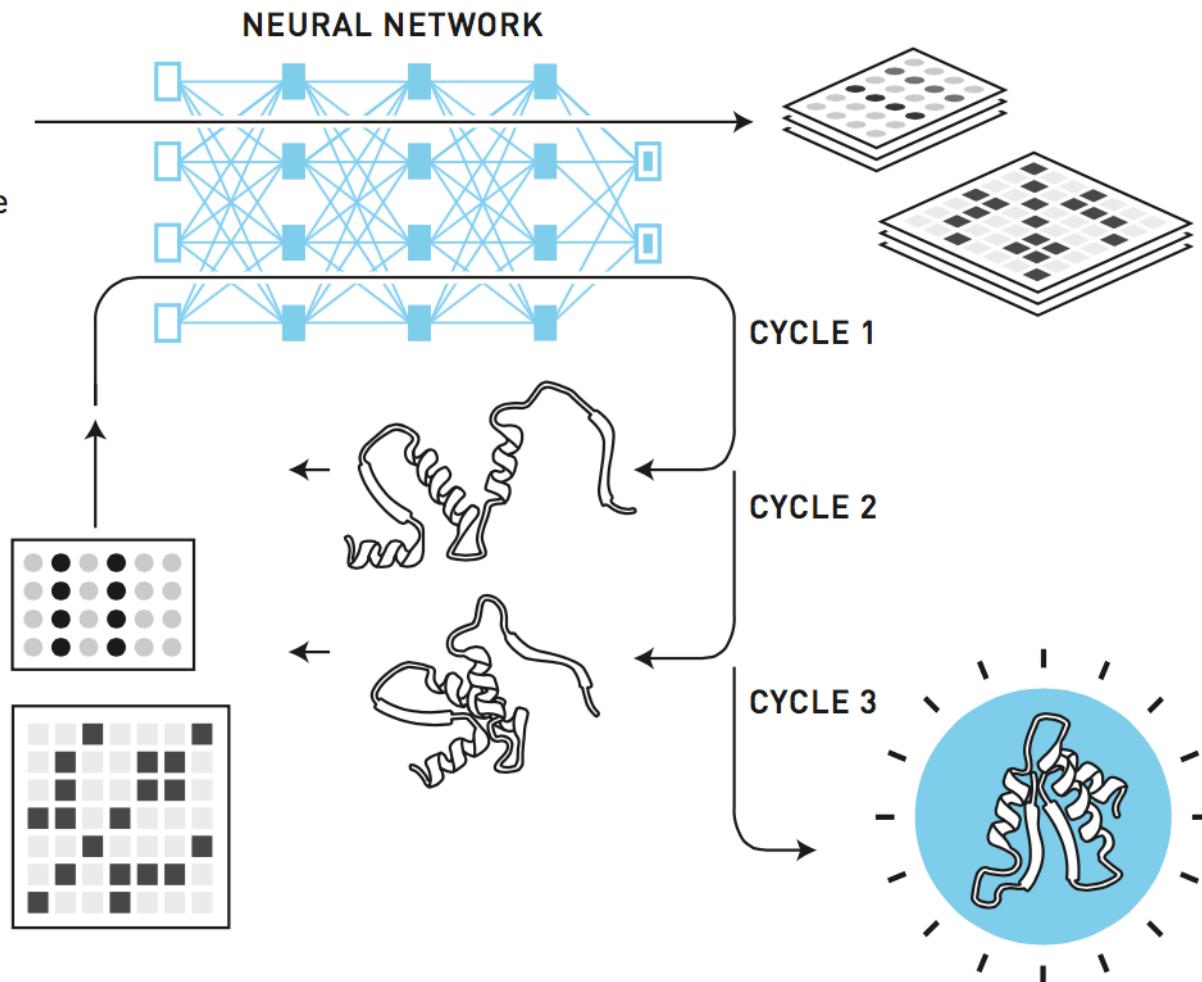






3. AI ANALYSIS

Using an iterative process, AlphaFold2 refines the sequence analysis and distance map. The AI model uses neural networks called transformers, which have a great capacity to identify important elements to focus on. Data about other protein structures – if they were found in step 1 – is also utilised.



4. HYPOTHETICAL STRUCTURE

AlphaFold2 puts together a puzzle of all the amino acids and tests pathways to produce a hypothetical protein structure. This is re-run through step 3. After three cycles, AlphaFold2 arrives at a particular structure. The AI model calculates the probability that different parts of this structure correspond to reality.

Protein Structure Predictions – Materials Structure Prediction

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Article

Structural Phase Transitions in Perovskite BaCeO_3 with Data Mining and First-Principles Theoretical Calculations

Farha Naaz, Manendra S. Chauhan, Kedar Yadav, Surender Singh, Ashok Kumar,
and Dasari L. V. K. Prasad*



Cite This: *J. Phys. Chem. C* 2024, 128, 4766–4778



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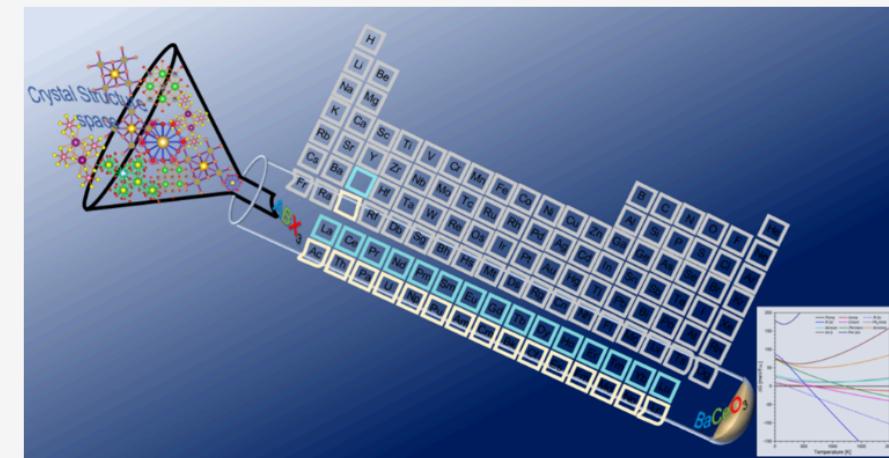
ACCESS |

Metrics & More

Article Recommendations

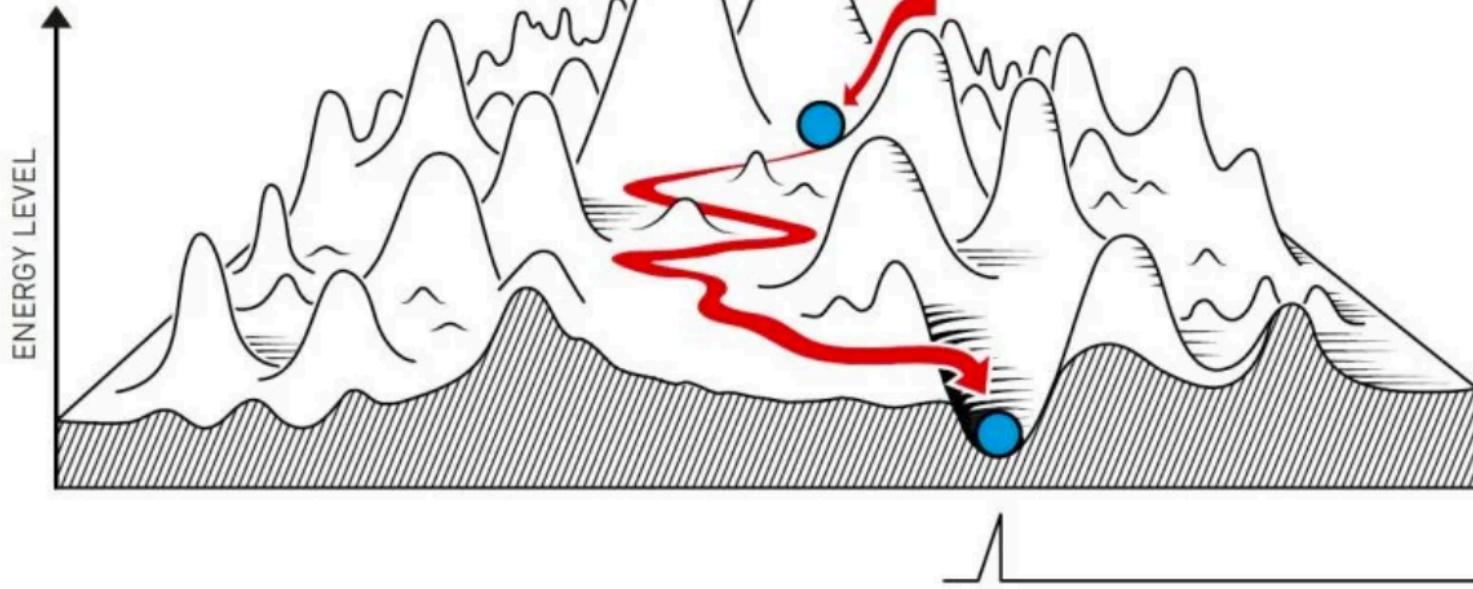
Supporting Information

ABSTRACT: Several neutron diffraction, Raman spectroscopy, and thermoanalytical experiments conducted over decades have revealed that perovskite-structured BaCeO_3 goes through a series of temperature-induced structural phase transitions. However, it has been frequently observed that the number of phases and the sequence in which they appear as a function of temperature differ between experiments. Insofar as neutron diffraction experiments are concerned, in the temperature range of 4.2 to 1273 K, four structures are crystallographically well characterized with three transitions, orthorhombic $Pnma$ \rightarrow orthorhombic $Imma$ [563 K] \rightarrow rhombohedral $R\bar{3}c$ [673 K] \rightarrow cubic $Pm\bar{3}m$ [1173 K], which lately have been reciprocally realized in the studies of polarized Raman spectroscopy. In contrast, thermoanalytical methods such as dilatometry showed multiple singularities corresponding to at least three more structural phase transitions at around 830, 900, and 1030 K, in addition to those recorded by neutron studies. In account of these conflicting experimental findings, we computed a free-energy landscape for BaCeO_3 and performed a detailed thermodynamic analysis to predict the equilibrium phase diagram.



Memories are stored in a landscape

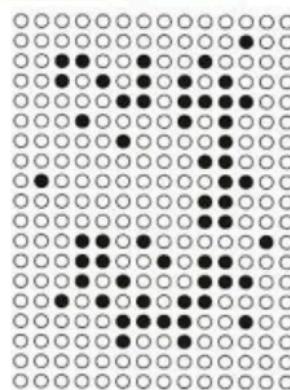
John Hopfield's associative memory stores information in a manner similar to shaping a landscape. When the network is trained, it creates a valley in a virtual energy landscape for every saved pattern.



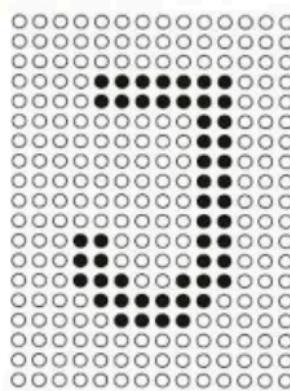
- 1 When the trained network is fed with a distorted or incomplete pattern, it can be likened to dropping a ball down a slope in this landscape.

- 2 The ball rolls until it reaches a place where it is surrounded by uphills. In the same way, the network makes its way towards lower energy and finds the closest saved pattern.

INPUT PATTERN



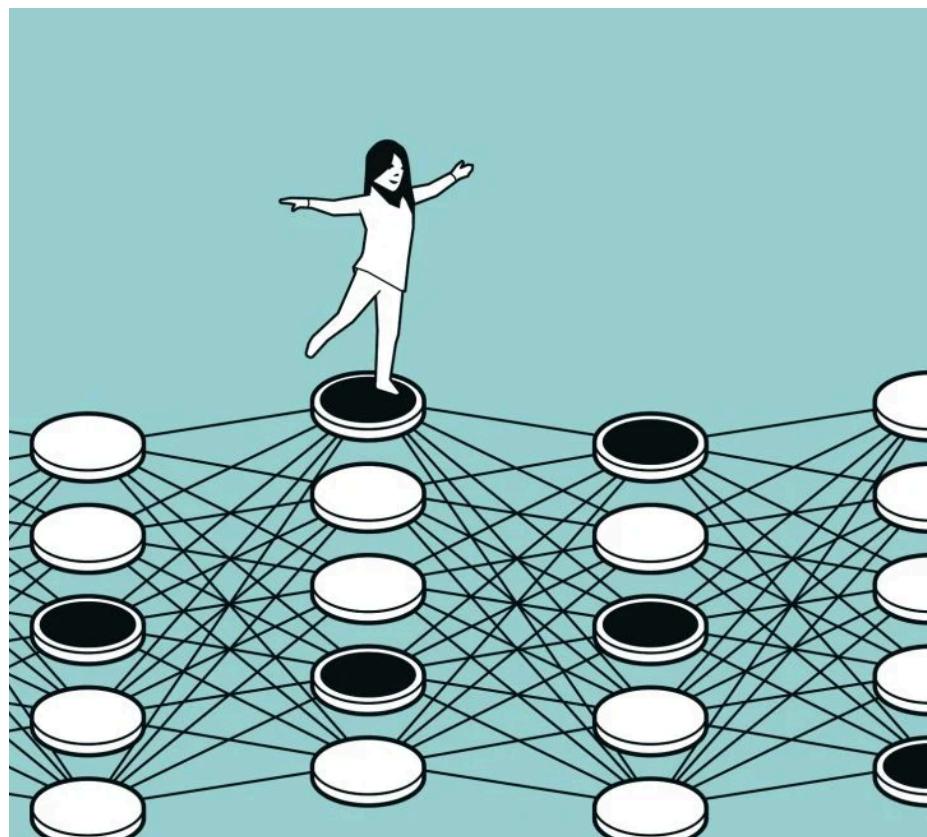
SAVED PATTERN



$$\hat{H}\psi(r) = E\psi(r)$$



$$h_i = \sum_{j \neq i} w_{ij} s_j$$



$$-\frac{dU}{dr} = m \frac{d^2r}{dt^2}$$

$$E = -\sum_{i < j} w_{ij} s_i s_j - \sum_i \theta_i s_i$$

The Nobel Prize in Chemistry

2024

For the computational protein design and
structure prediction



Ill. Niklas Elmehed © Nobel Prize Outreach
David Baker
Prize share: 1/2



Ill. Niklas Elmehed © Nobel Prize Outreach
Demis Hassabis
Prize share: 1/4



Ill. Niklas Elmehed © Nobel Prize Outreach
John M. Jumper
Prize share: 1/4

THE GOOD, THE BAD AND THE UGLY

AlphaFold's predictions of a folded protein's structure come with confidence estimates. Superimposing each model on the experimentally determined structure (if available) shows the accuracy of the prediction.

Protein Data Bank
(PDB) structure

AlphaFold structure, with confidence
estimates for each section.



Very
high



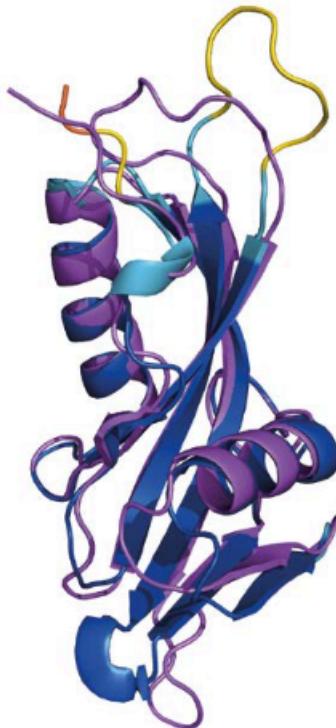
High



Low

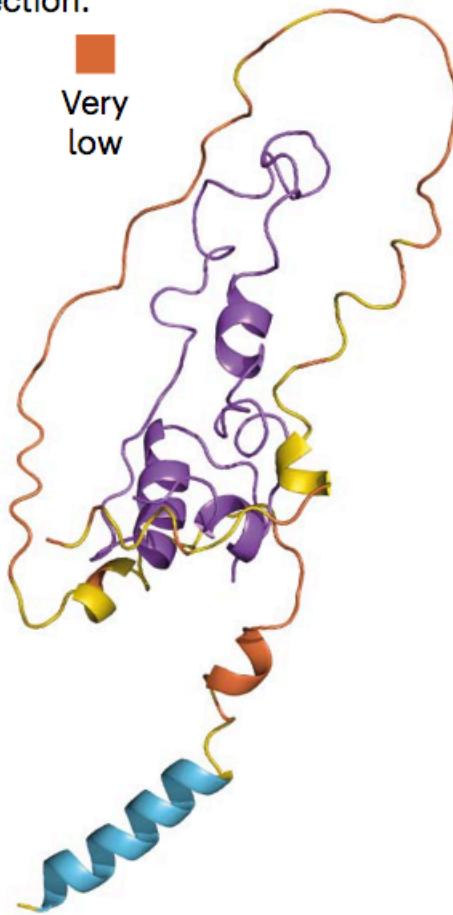


Very
low



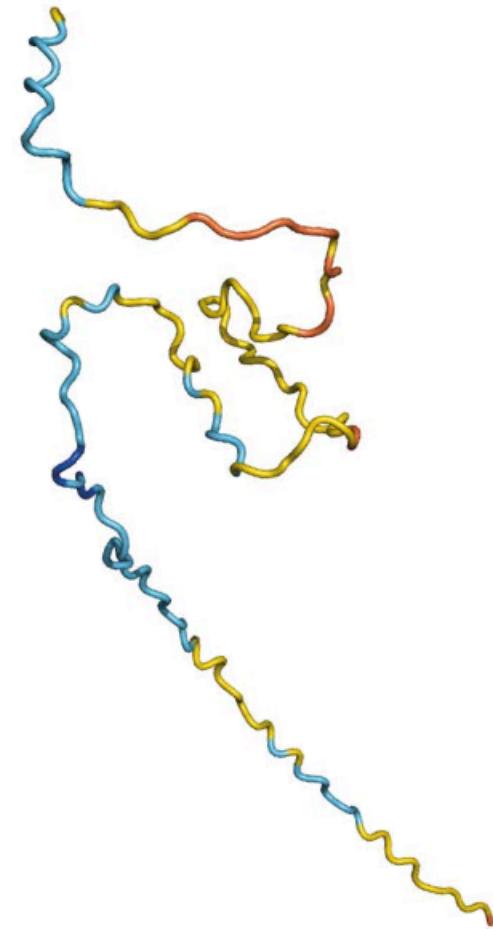
Good

AlphaFold model of phosphohistidine phosphatase overlaps closely with PDB structure.



Bad

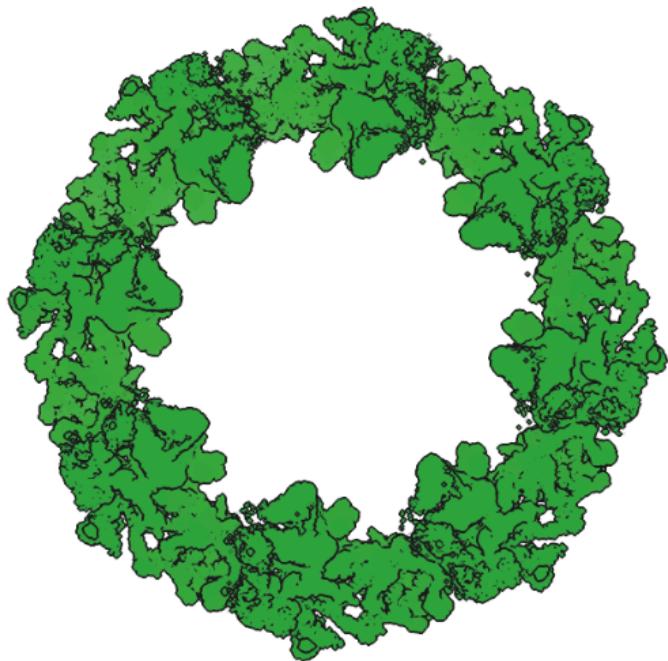
AlphaFold model of human insulin bears no relation to the PDB structure.



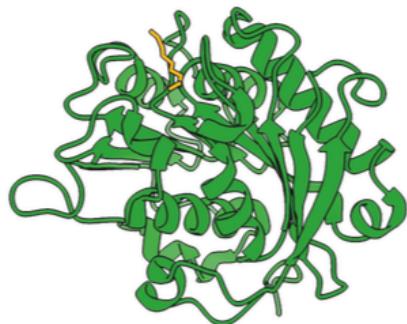
Ugly

AlphaFold has little confidence across much of its prediction for this human ubiquitin-protein ligase. There is no PDB structure to compare it with.

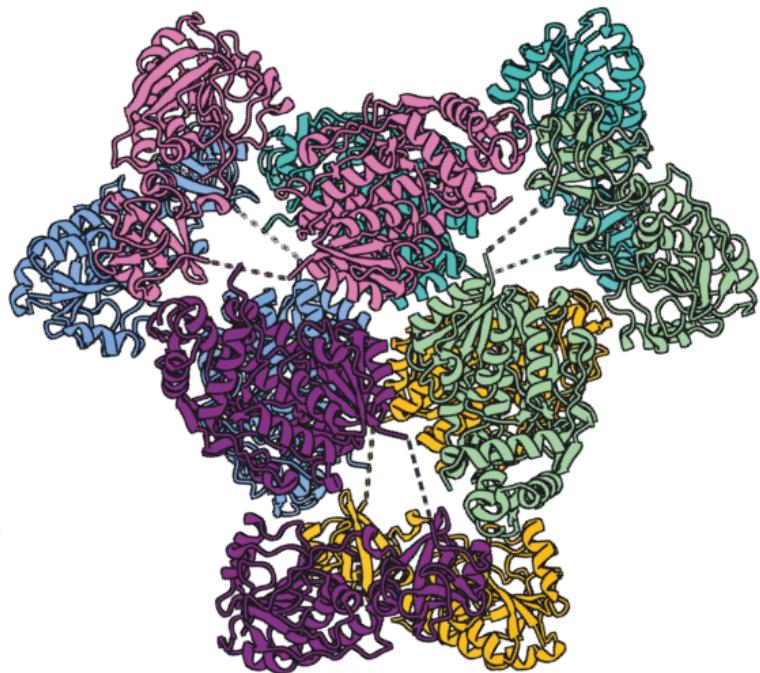
Figure 5. Protein structures determined using AlphaFold2.



2022: Part of a huge molecular structure in the human body. More than a thousand proteins form a pore through the membrane surrounding the cell nucleus.



2022: Natural enzymes that can decompose plastic. The aim is to design proteins that can be used to recycle plastic.

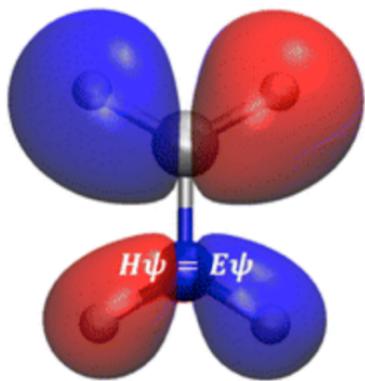


2023: A bacterial enzyme that causes antibiotic resistance. The structure is important for discovering ways of preventing antibiotic resistance.



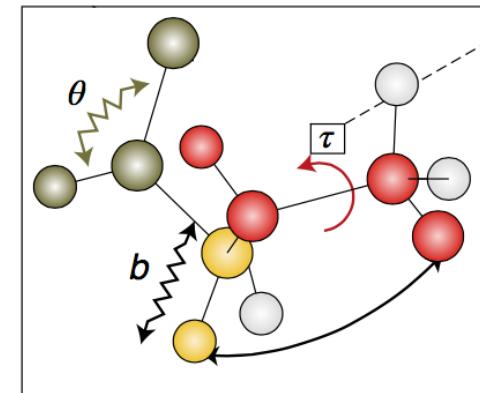
Chemical processes through
electronic structure

$$\hat{H}\psi(r) = E\psi(r)$$



Chemical processes through
force fields

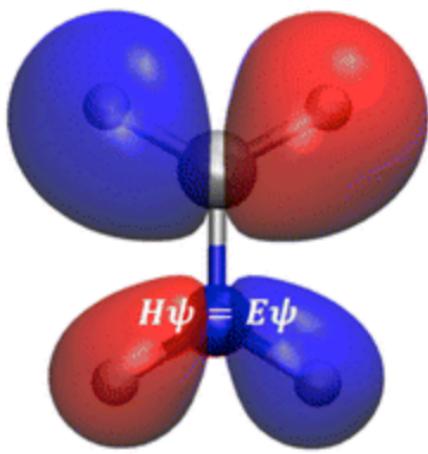
$$U = \sum_{i < j} \sum 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$



fs-ps ~100 atoms

electronic-structure models

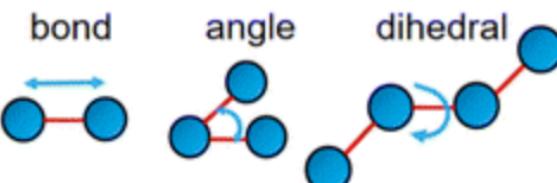
Schrödinger equation



excitation energies
conical intersection
reaction pathways

10 μs ~10⁴ atoms

atomic-structure models



$$E_{bond} = K_l(l - l_0)^2$$

$$E_{angle} = K_\theta(\theta - \theta_0)^2$$

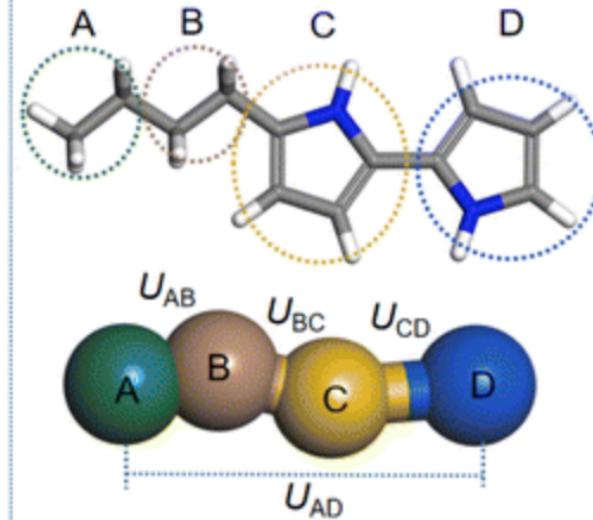
$$E_{dihedral} = \sum_{n=0}^N K_n [1 + \cos(n\phi - \delta_n)]$$

$$U(r_{ij}) = 4 \times \varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$

molecular conformation
transport properties
binding site control

1 ms ~1M atoms

coarse-grained models



$U_{total} = U_{AB} + U_{BC} + U_{CD} + U_{AD}$

protein folding
ion transport in membrane
macroscopic deformation

Amount of Physical Detail →



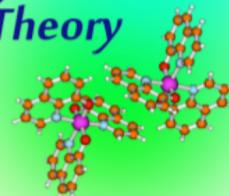
$$H\Psi=E\Psi$$

100 fs, 30 atoms:
photochemistry

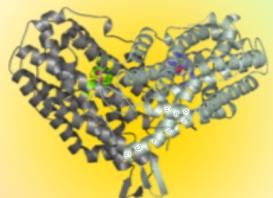


Correlated methods
(MP2, CCSD, CI)

Density Functional Theory

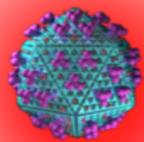


Hartree-Fock



Atomistic MM

1 μ s–1 ms, 100k atoms:
protein dynamics,
drug binding

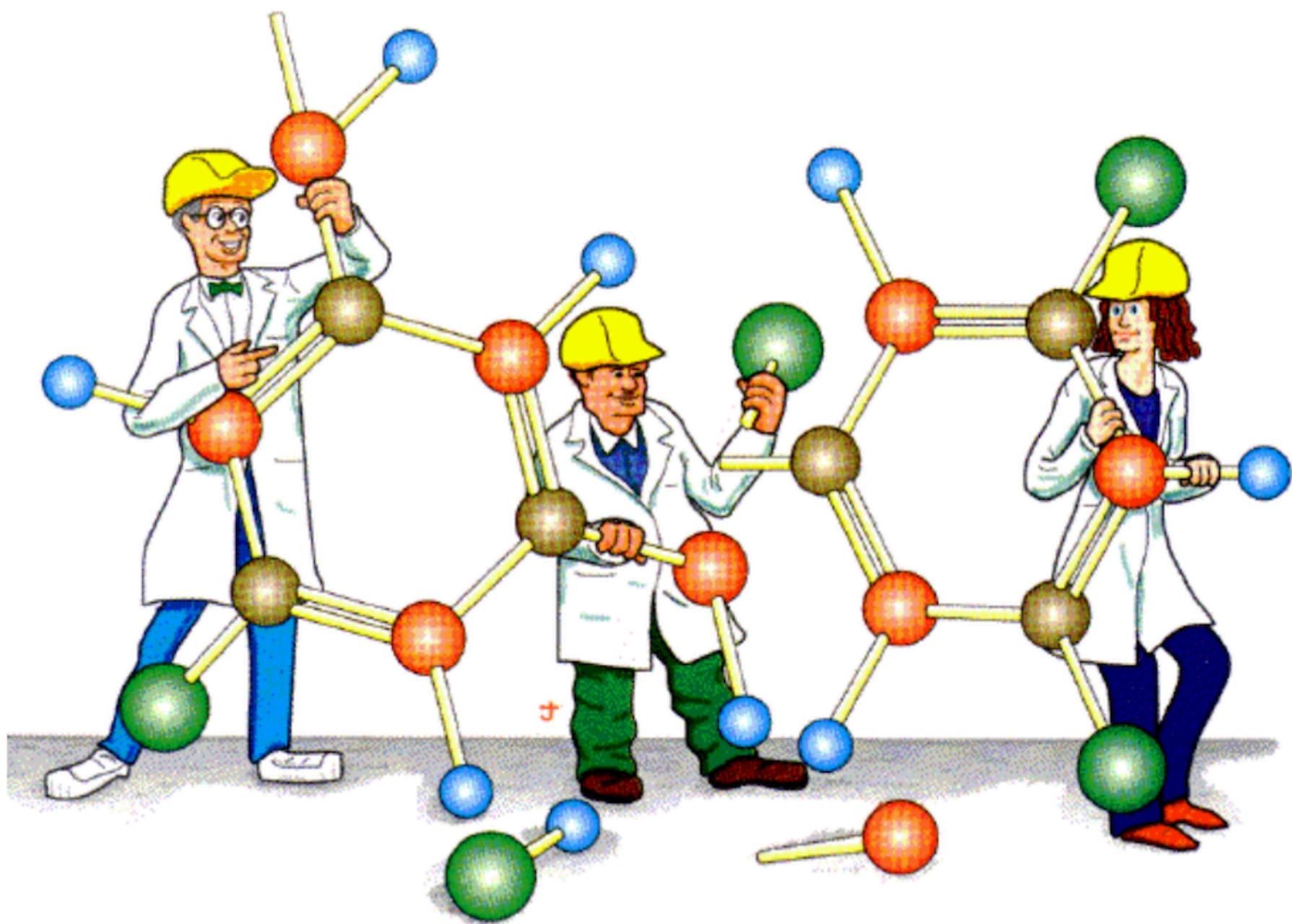


Coarse-grained simulations

Continuum mechanics

Cost of Calculation →





**Returning to the problem of
chemical processes**

Molecular level understanding of chemical processes



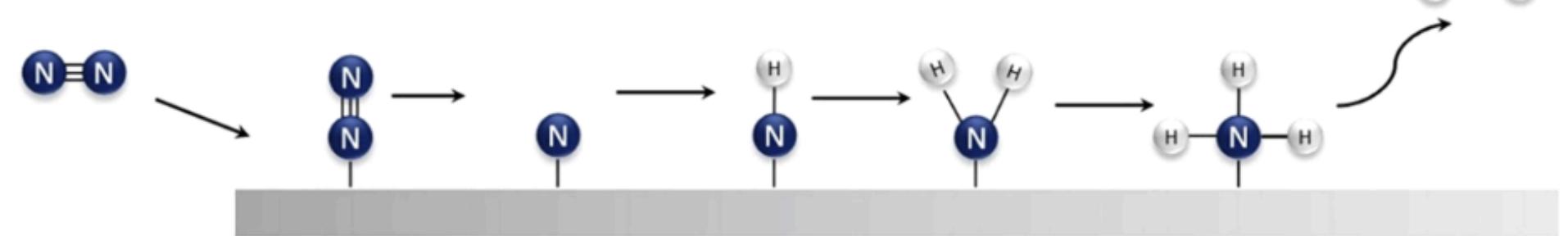
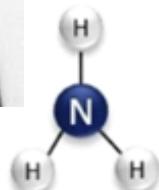
Kenichi Fukui

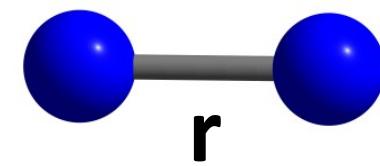
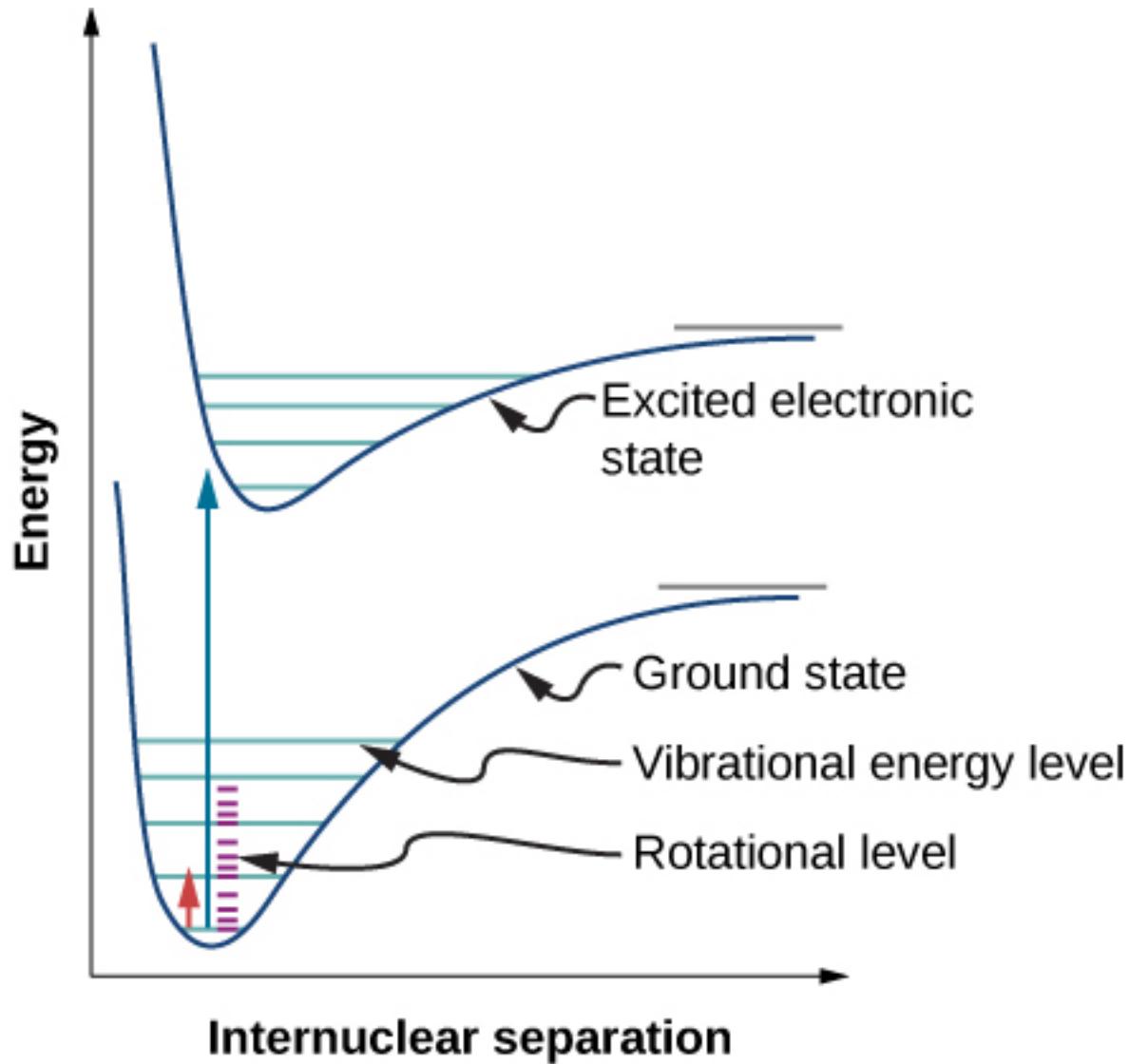


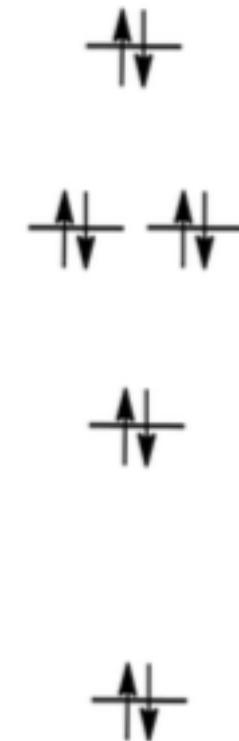
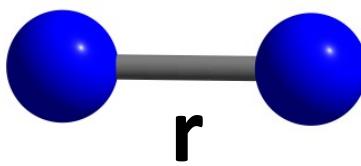
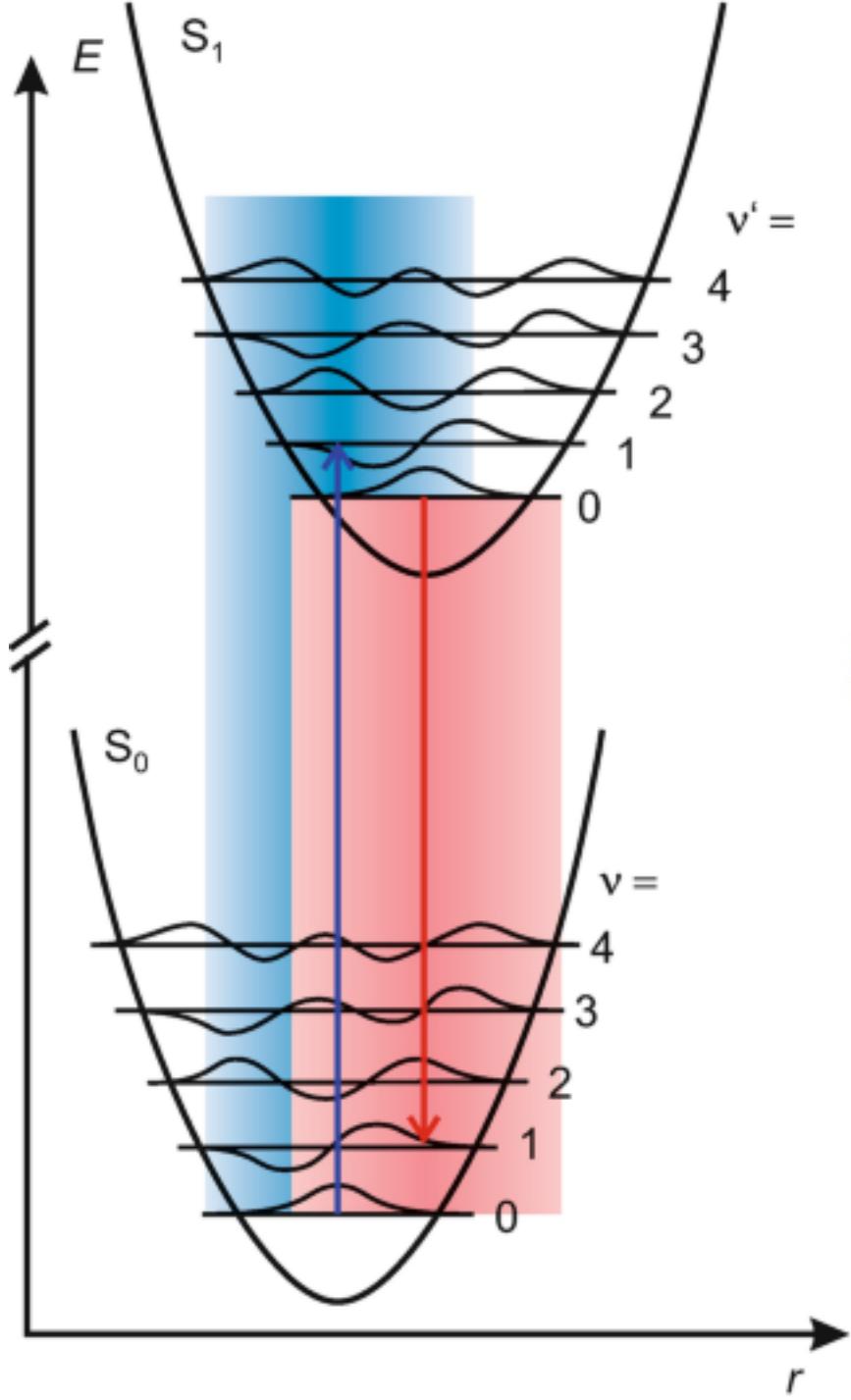
Roald Hoffmann

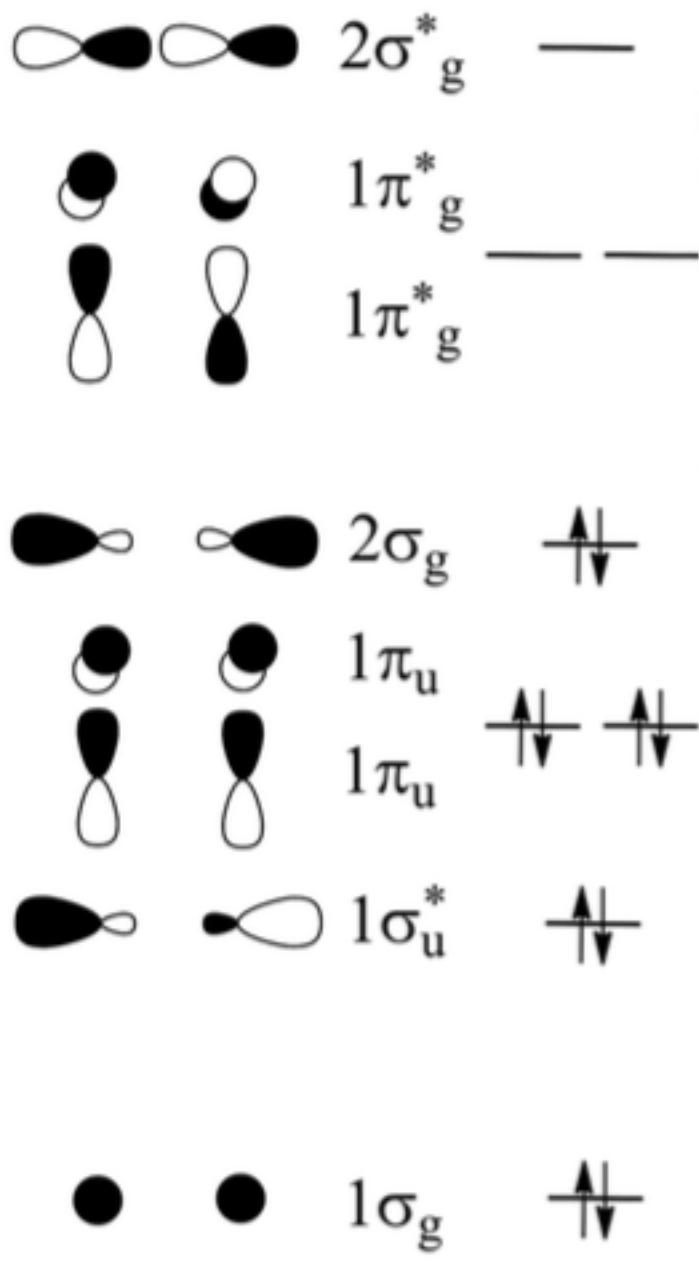
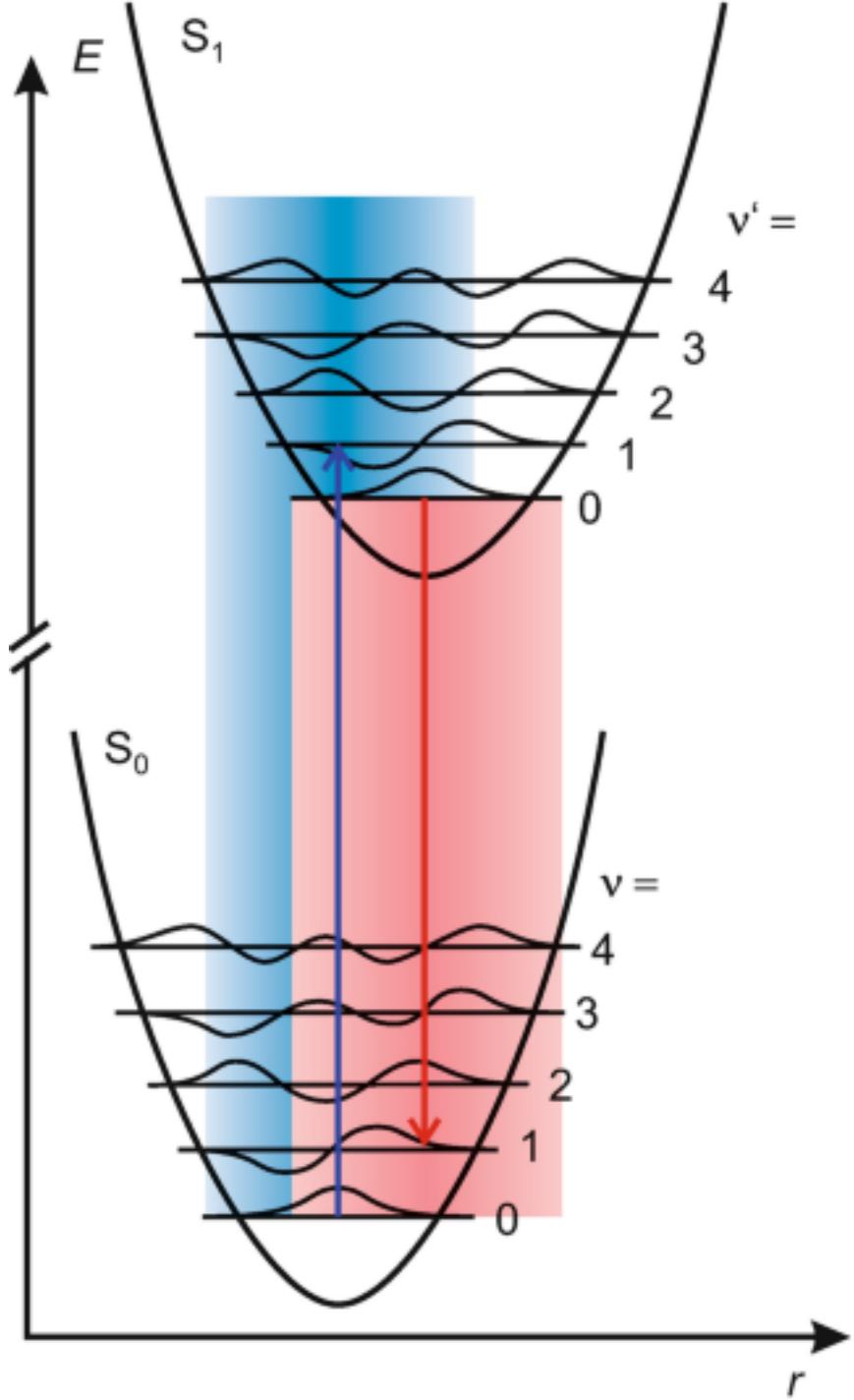


Michael Polanyi

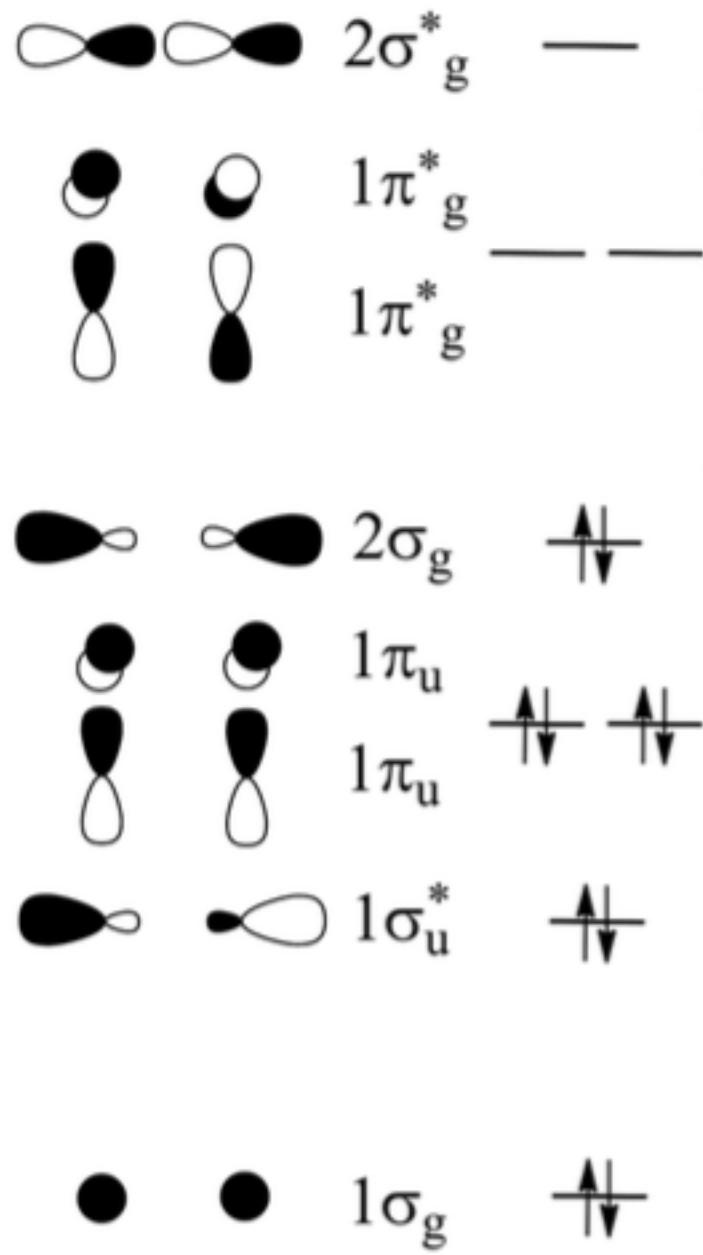
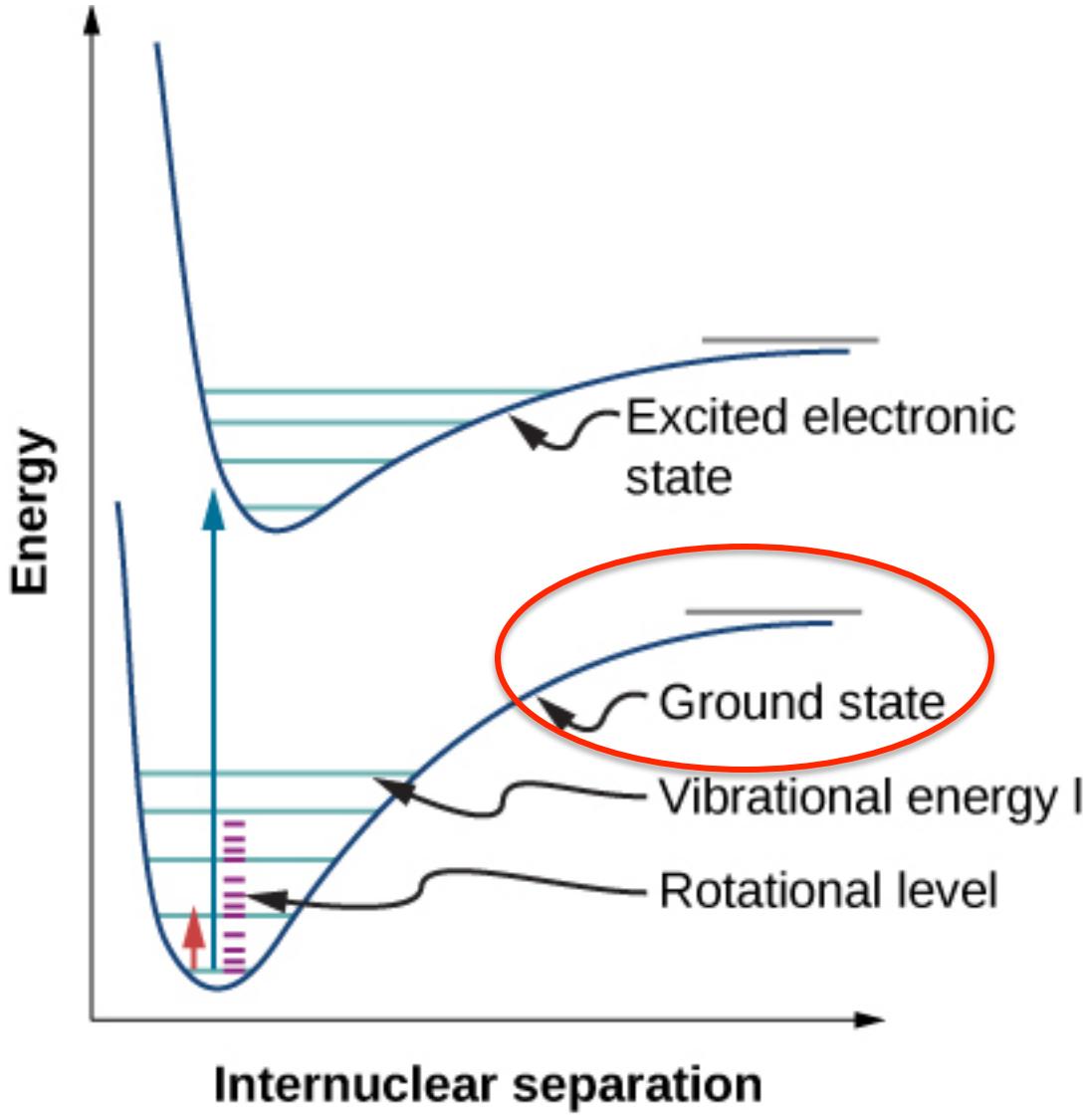


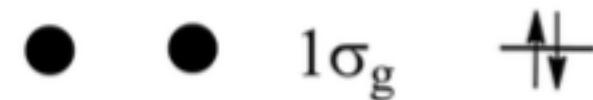
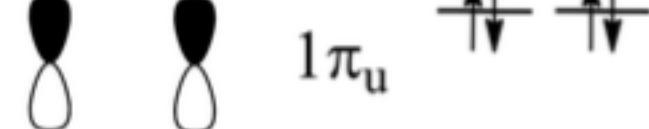
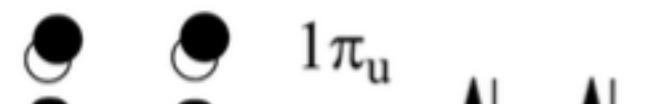
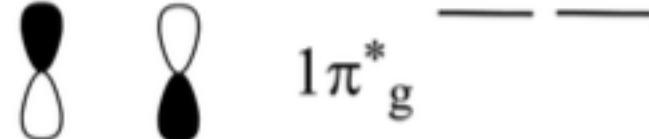
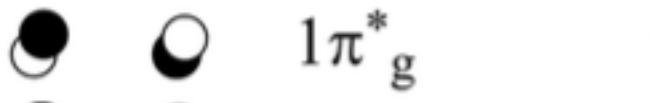




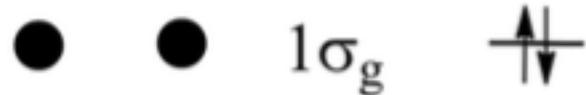
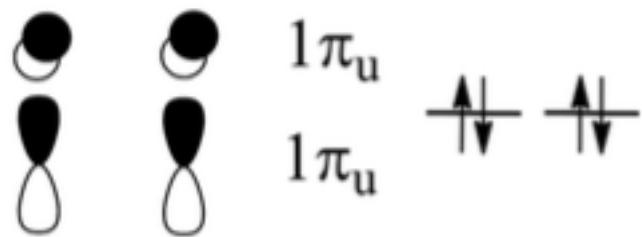
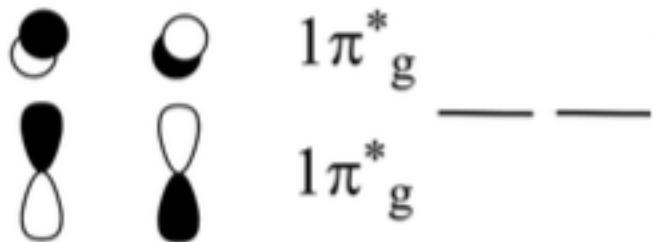


All in the Ground State





How one would get
these states?



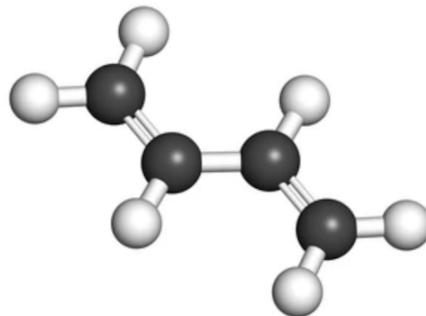
$$\hat{H}\psi(r) = E\psi(r)$$

How one would get these states?

$$\psi(r) = \sum_{\mu=1}^K C_{\mu i} \tilde{\chi}_{\mu}$$

Chemical Reactivity.....

$$\psi(r) = \sum_{\mu=1}^K C_{\mu i} \tilde{\chi}_{\mu}$$



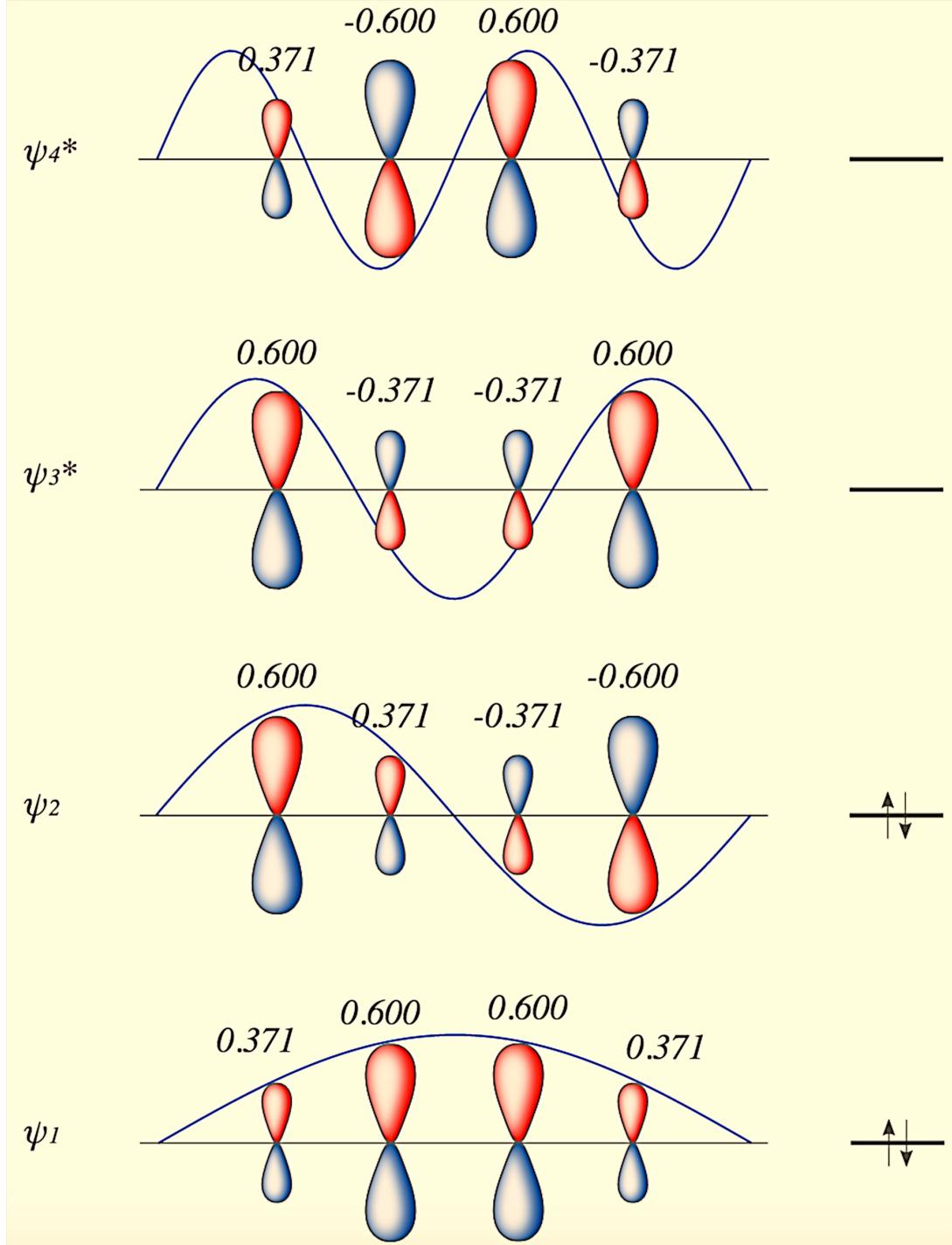
$$\psi_1 = 0.372\phi_1 + 0.602\phi_2 + 0.602\phi_3 + 0.372\phi_4$$

$$\psi_2 = 0.602\phi_1 + 0.372\phi_2 - 0.372\phi_3 - 0.602\phi_4$$

$$\psi_3 = 0.602\phi_1 - 0.372\phi_2 - 0.372\phi_3 + 0.602\phi_4$$

$$\psi_4 = 0.372\phi_1 - 0.602\phi_2 + 0.602\phi_3 - 0.372\phi_4$$

$$\psi(r) = \sum_{\mu=1}^K C_{\mu i} \tilde{\chi}_{\mu}$$

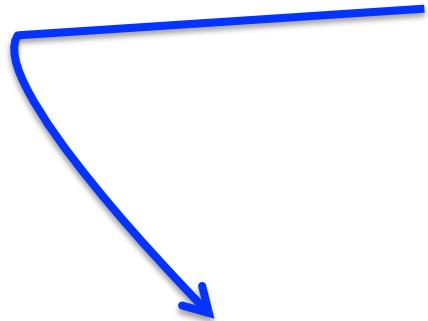


Molecular Orbital Theory

Linear Combination of Atomic Orbitals

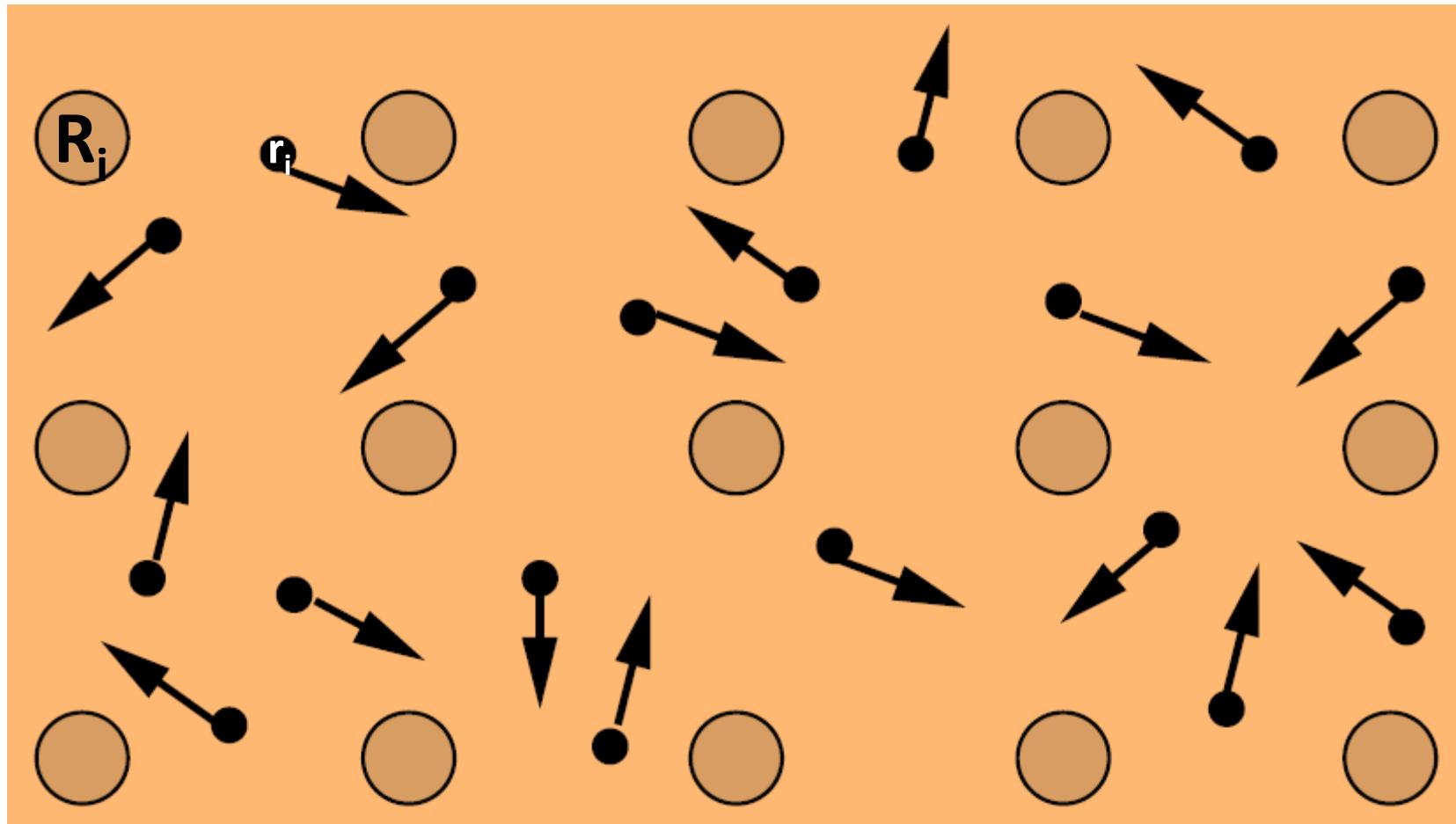
Superposition of Atomic Orbitals

$$\psi(r) = \sum_{\mu=1}^K C_{\mu i} \tilde{\chi}_{\mu}$$



Determination and
Interpretation of Molecular
Wave Functions

Interacting particles



Clamped-Nuclei

$$\hat{H} = -\frac{1}{2} \cancel{\sum_{\alpha} \nabla_{\alpha}^2} - \frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{\alpha \neq \beta} \cancel{\frac{Z_{\alpha} Z_{\beta} e^2}{R_{\alpha} - R_{\beta}}} -$$
$$\frac{1}{2} \sum_{\alpha, i} \frac{Z_{\alpha} e^2}{r_i - R_{\alpha}} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_i - r_j}$$

$$\hat{H}_{el} = -\frac{1}{2} \sum_i \nabla_i^2 - \frac{1}{2} \sum_{\alpha, i} \frac{Z_{\alpha} e^2}{r_i - R_{\alpha}} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_i - r_j}$$

Clamped-Nuclei

$$\hat{H}_{el} = -\frac{1}{2}\sum_i \nabla_i^2 - \frac{1}{2}\sum_{\alpha,i} \frac{Z_\alpha e^2}{r_i - R_\alpha} + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{r_i - r_j}$$

$$\hat{H}_{el} = \hat{T}_{el}(r) + \hat{V}_{eN}(r, R) + \hat{V}_{rr}$$

$$\hat{H}_{el}\psi(r, R) = E_{el}\psi(r, R)$$

Born-Oppenheimer Approximation

Independent Particle Model

Let's say we have two (1, 2) particles

$$\hat{H}(1, 2) = h(1) + h(2) + \cancel{g(1, 2)}$$

$$h(1) = -\frac{1}{2}\nabla^2(1) + V(1)$$

$$h(2) = -\frac{1}{2}\nabla^2(2) + V(2)$$

Independent Particle Model

$$\hat{H}(1, 2) = h(1) + h(2) + \cancel{g(1, 2)}$$

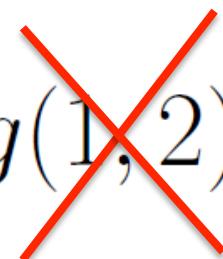
$$\hat{H}_0(1, 2) = h(1) + h(2)$$

$$\psi_{mn}(1, 2) = \psi(r_1, r_2) = \phi_m(r_1)\phi_n(r_2)$$

$$h(1)\phi_m = \epsilon_m\phi(r_1) ; \quad h(2)\phi_n = \epsilon_n\phi(r_2)$$

Independent Particle Model

$$\hat{H}(1, 2) = h(1) + h(2) + g(1, 2)$$



$$\hat{H}_0(1, 2) = h(1) + h(2)$$

$$\psi_{mn}(1, 2) = \psi(r_1, r_2) = \phi_m(r_1)\phi_n(r_2)$$

$$h \phi(r) = \epsilon \phi(r) \quad ; \quad E = \epsilon_m + \epsilon_n$$

One electron Schrödinger equation

Independent Particle Model

$$\hat{H}_0(1, 2) = h(1) + h(2)$$

$$\psi_{mn}(r_1, r_2) = \phi_m(r_1)\phi_n(r_2)$$

$$E = \epsilon_m + \epsilon_n$$

$$\hat{H}_\pi = \sum_i^{n_\pi} H^{eff}(i)$$

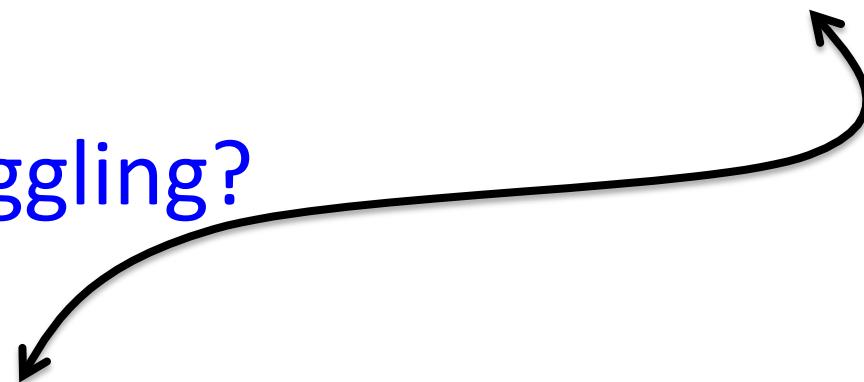
$$\psi_\pi = \prod_i^{n_\pi} \phi(i)$$

$$E_\pi = \sum_i^{n_\pi} \epsilon(i)$$

Independent Particle Model

$$\hat{H}(1, 2) = h(1) + h(2) + g(1, 2)$$

What about this jiggling?



$$g(1, 2) = \frac{e^2}{r_i - r_j} = \frac{1}{r_{12}}$$

One Step Further

$$\hat{H}(1, 2) = h(1) + h(2) + g(1, 2)$$

$$\langle E \rangle = \langle \psi_{11} | h(1) + h(2) + g(1, 2) | \psi_{11} \rangle$$

$$\langle E \rangle = 2 \langle \phi_1 | h | \phi_1 \rangle + \langle \phi_1 \phi_1 | g | \phi_1 \phi_1 \rangle$$



one electron
integral



two electron
integral

One Step Further

$$\langle E \rangle = 2 \langle \phi_1 | h | \phi_1 \rangle + \langle \phi_1 \phi_1 | g | \phi_1 \phi_1 \rangle$$

$$\langle \phi_1 | h | \phi_1 \rangle = \int \phi_1^* h \phi_1 dr_1$$

$$\langle \phi_1 \phi_1 | g | \phi_1 \phi_1 \rangle = \text{J}_{11} \xrightarrow{\text{Coulomb Integral}} \int \phi_1^*(r_1) \phi_1^*(r_2) \frac{1}{r_{12}} \phi_1(r_1) \phi_1(r_2) dr_1 dr_2$$

Fixing Wavefunction

$$\hat{H} = \sum_i h(i) + \frac{1}{2} \sum_{i,j} g(i, j)$$

$$\psi_{gd} = \prod_i \phi(i)$$

$$\psi_0 = \phi_0(1) \times \phi_0(2) \times \dots \times \phi_0(n)$$

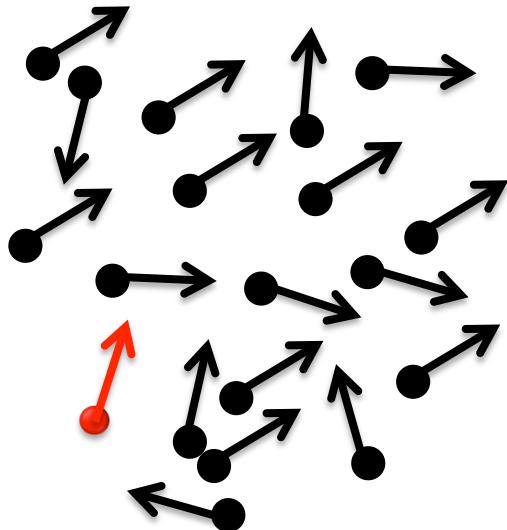
$$\hat{H}\psi_0(r, R) = E_0\psi_0(r, R)$$

Fixing Wavefunction

$$\psi_0 = \phi_0(1) \times \phi_0(2) \times \dots \times \phi_0(n)$$

$\phi_1(1) \rightarrow$ due to the average field of

$$\phi_0(2), \phi_0(3), \phi_0(4), \dots, \phi_0(n)$$



$\phi_0(1)$ in the average field
of other electrons

$$\phi_0(1) = Ne^{-\zeta r}$$

[ζ = Slater's effective nuclear charge]

Group ► 1 2

3 4 5 6 7 8 9 10 11 12

13 14 15 16 17 18

Period ▼

Noble
gases2
He

| | | | |
|----------------------|---------|---------|------------------------|
| <i>Nonmetals</i> | 1 | 1 | H |
| <i>Metals</i> | 2 | 3 | 4 |
| | Li | Be | |
| | 11 | 12 | |
| | Na | Mg | |
| | 19 | 20 | |
| | K | Ca | |
| | 37 | 38 | |
| | Rb | Sr | |
| | 55 | 56 | |
| | Cs | Ba | La to Yb |
| | 87 | 88 | Ac to No |
| s-block (plus He) | f-block | d-block | p-block (excluding He) |

$$\phi_0(1) = Ne^{-\zeta r}$$

Some elements near
the dashed staircase are
sometimes called *metalloids*

| | | | | | |
|-----|-----|-----|-----|-----|-----|
| 5 | 6 | 7 | 8 | 9 | 10 |
| B | C | N | O | F | Ne |
| 13 | 14 | 15 | 16 | 17 | 18 |
| Al | Si | P | S | Cl | Ar |
| 31 | 32 | 33 | 34 | 35 | 36 |
| Ga | Ge | As | Se | Br | Kr |
| 49 | 50 | 51 | 52 | 53 | 54 |
| In | Sn | Sb | Te | I | Xe |
| 81 | 82 | 83 | 84 | 85 | 86 |
| Tl | Pb | Bi | Po | At | Rn |
| 113 | 114 | 115 | 116 | 117 | 118 |
| Nh | Fl | Mc | Lv | Ts | Og |

| | | | | | | | | | | | | | | |
|--------------------|----|----|----|----|----|----|----|----|----|----|----|-----|-----|-----|
| <i>Lanthanides</i> | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 |
| | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb |
| <i>Actinides</i> | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 |
| | Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | No |

Fixing Wavefunction

$$\psi_0 = \phi_0(1) \times \phi_0(2) \times \dots \times \phi_0(n)$$

$$\phi_1(1) \leftarrow \phi_0(2), \phi_0(3), \phi_0(4), \dots, \phi_0(n)$$

$$\phi_0(1) \rightarrow \phi_1(1)$$

$$\phi_1(2) \leftarrow \underline{\phi_1(1)}, \phi_0(3), \phi_0(4), \dots, \phi_0(n)$$

$$\phi_0(2) \rightarrow \phi_1(2)$$

Fixing Wavefunction

$$\psi_0 = \phi_0(1) \times \phi_0(2) \times \dots \times \phi_0(n)$$

$$\phi_0(1) \rightarrow \phi_1(1)$$

$$\phi_0(2) \rightarrow \phi_1(2)$$

$$\phi_0(n) \xrightarrow{\vdots} \phi_1(n)$$

$$\psi_1 = \phi_1(1) \times \phi_1(2) \times \dots \times \phi_1(n)$$

$$\hat{H}\psi_1(r, R) = E_1\psi_1(r, R)$$

Fixing Wavefunction

$$\psi_0 = \phi_0(1) \times \phi_0(2) \times \dots \times \phi_0(n)$$

$$\hat{H}\psi_0(r, R) = E_0\psi_0(r, R)$$

↓

$$\psi_1 = \phi_1(1) \times \phi_1(2) \times \dots \times \phi_1(n)$$

$$\hat{H}\psi_1(r, R) = E_1\psi_1(r, R)$$

↓

$$\psi_k = \phi_k(1) \times \phi_k(2) \times \dots \times \phi_k(n)$$

$$\hat{H}\psi_k(r, R) = E_k\psi_k(r, R)$$

Convergence achieved

One More Step Further

“Wavefunction is antisymmetric
under the exchange of spins”
electrons are fermions!

$$J_{ij} = \langle \phi_i \phi_j | g(1, 2) | \phi_i \phi_j \rangle$$

$$J_{ij} = \int \phi_i^*(r_1) \phi_j^*(r_2) \frac{1}{r_{12}} \phi_i(r_1) \phi_j(r_2) dr_1 dr_2$$

$$K_{ij} = \langle \phi_i \phi_j | g(1, 2) | \phi_j \phi_i \rangle$$

$$K_{ij} = \int \phi_i^*(r_1) \phi_j^*(r_2) \frac{1}{r_{12}} \phi_j(r_1) \phi_i(r_2) dr_1 dr_2$$

One More Step Further

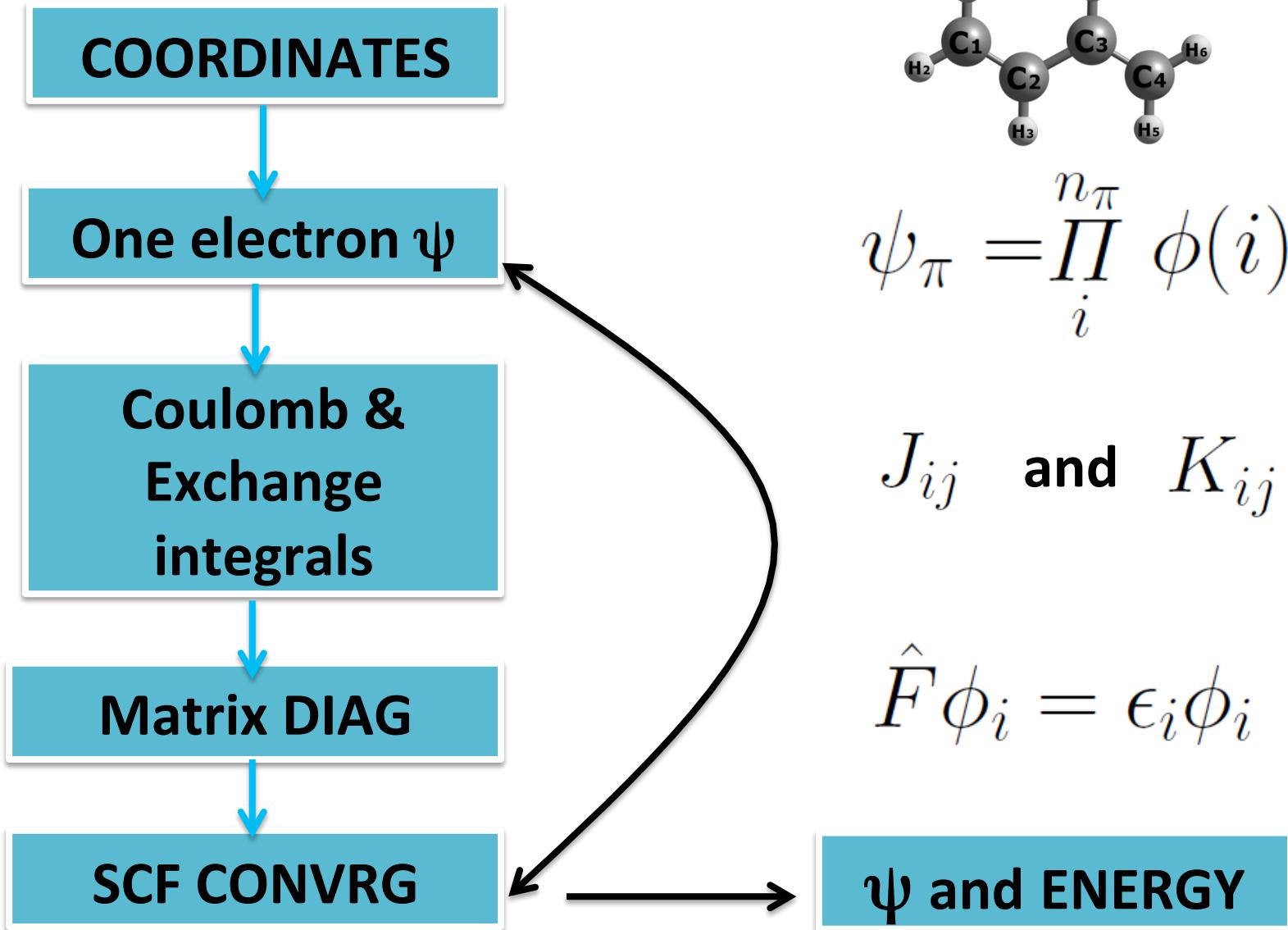
$$\hat{H} = \sum_i h(i) + \frac{1}{2} \sum_{i,j} g(i, j)$$

$$J_{ij} = \int \phi_i^*(r_1) \phi_j^*(r_2) \frac{1}{r_{12}} \phi_i(r_1) \phi_j(r_2) dr_1 dr_2$$

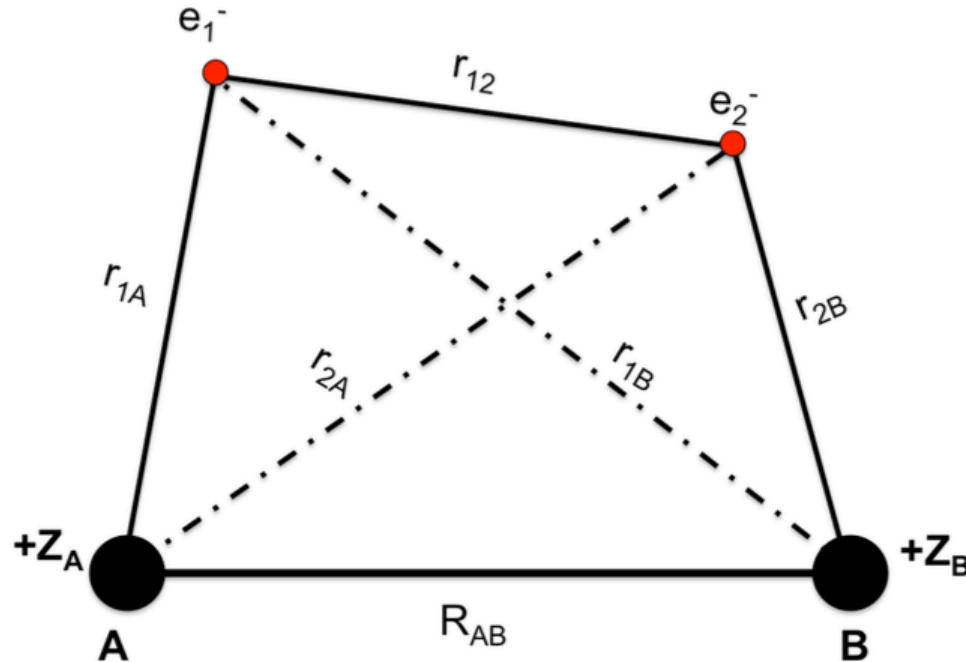
$$K_{ij} = \int \phi_i^*(r_1) \phi_j^*(r_2) \frac{1}{r_{12}} \phi_j(r_1) \phi_i(r_2) dr_1 dr_2$$

$$\langle E \rangle = 2 \sum_i \langle \phi_i | h | \phi_i \rangle + 2 \sum_{j,i} J_{i,j} - \sum_{j,i} K_{i,j}$$

SCF Procedure



Let's Solve.....



$$\hat{H}_{el}\psi(r, R) = E_{el}\psi(r, R)$$

$$\hat{H}_{el} = -\frac{1}{2}\sum_i \nabla_i^2 - \frac{1}{2}\sum_{\alpha,i} \frac{Z_\alpha e^2}{r_i - R_\alpha} + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{r_i - r_j}$$