Lecture # 0: The fun lecture - Why Science?

3 Aug 2011

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9908811010(mobile)

Prabhakar Bhimalapuram ph: x 1160 (off)

Teaching Assistants:

Course outline:

Topics	# Lectures
1. Introduction:	1
2. Scales in Nature; time, length and energy.	2
3. Mathematical modeling in sciences,	6
(i) geometry and linear algebra	
(ii) change and calculus	
(iii)chance and statistics	
(iv) vector formulation of a multi-variable problem.	
4. Forms in Nature: molecular structures,	6
crystal lattices,biological molecules,	
fractals and self organized structures,	
basic ideas of symmetry and group theory.	
5. Thermodynamics:	9
6. Classical fields and electromagnetism:	11
7. Special Theory of relativity:	3
8.Nuclear Physics:	3

Texts:

1. Berkeley Physics Course, vol. 1: Mechanics
by Charles Kittel, Walter D. Knight, Malvin A. Ruderman, A. Carl Helmholz and Burton J. Moyer

2. Lectures on Physics; vol. 1 and 2
by Richard P Feynman, Robert B Leighton and Matthew Sands

3. Physical Chemistry: Principles and Applications in Biological Sciences, Ignacio Tinoco, Jr., Kenneth Sauer and James C Wang

4. Physical Chemistry by P W Atkins

6. Berkeley Physics Course, vol. 2: Electricity and magnetism
by Edward M. Purcell

7. Concepts of Modern Physics by Arthur Beiser

8. Berkeley problems in mathematics
by Paulo Ney de Souza and Jorge-Nuno Silva

Grading Scheme and Marks Distribution

Regular Weekly Assignments	10%
Review of a research Paper on a relevant topic	10%
Two mid-semester examinations	15% each
Two quizzes	$2\frac{1}{2}$% each
Final examination	45%


COSMOLOGY
TRYING TO DESCRIBE THE SIZE OF THE BIG BANG

Most of us are fascinated by ideas like the BIG BANG

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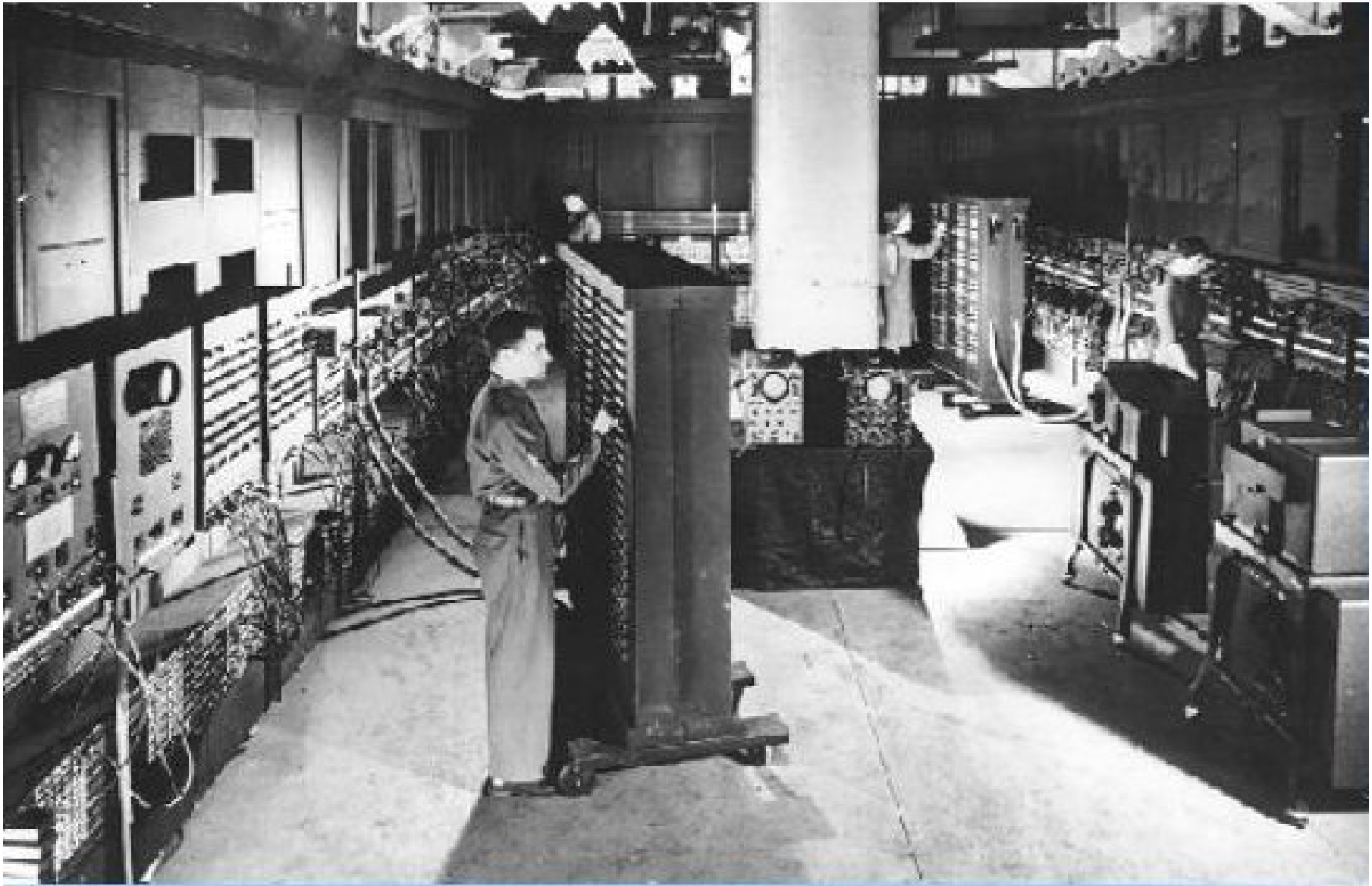
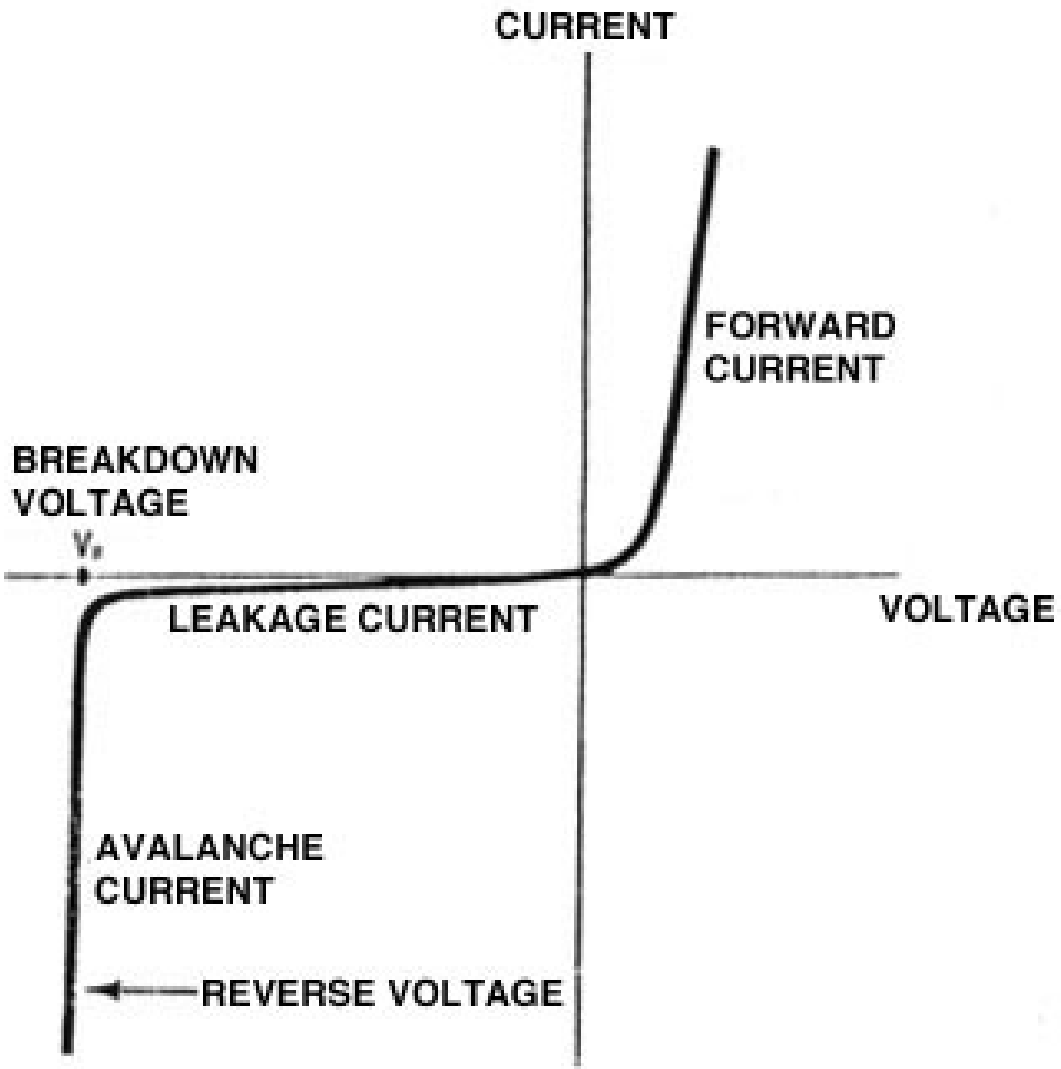
Most of science is quieter

All significant developments in IT have originated from compelling questions in science or as a part of scientific research.



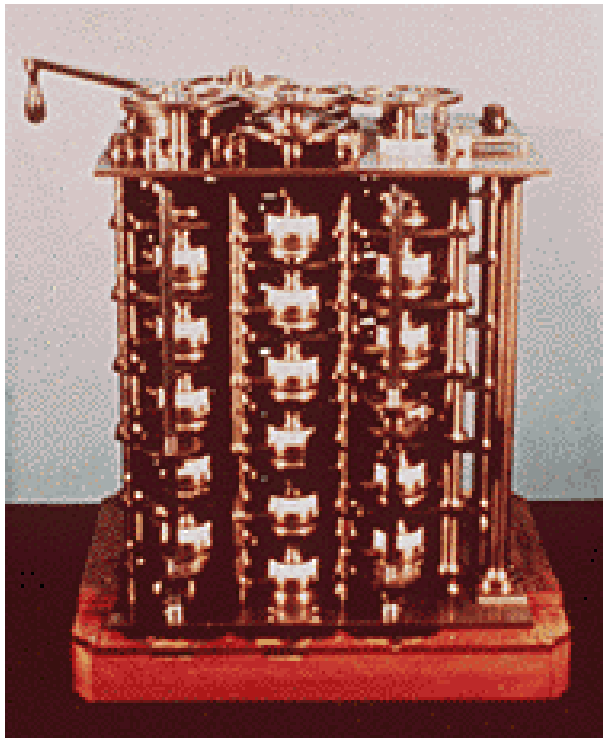
ENIAC - 1946

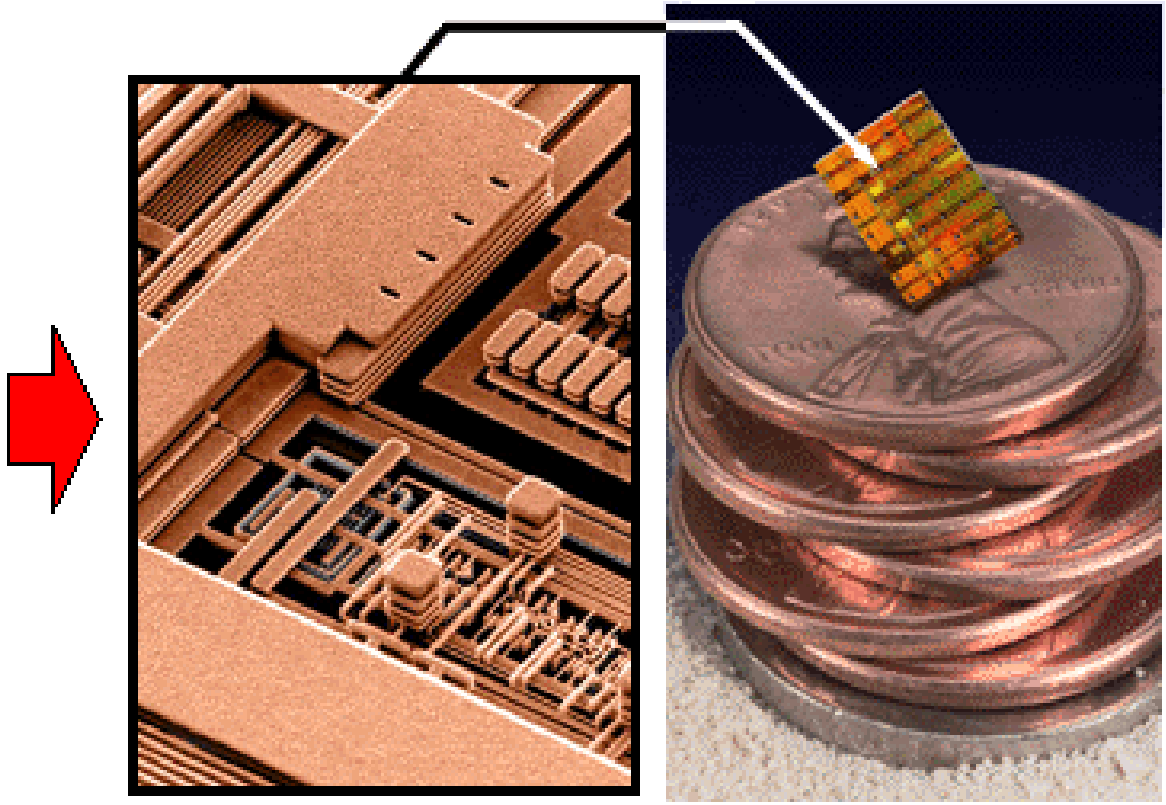
Past: The semiconductor technology: the magic curve



The digital logic

Macrotechnology to nanotechnology: from an early computing machine built from mechanical gears to a 2004 IBM chip with 0.25 micron features.





and further

Intel Technology Roadmap

Process Name	P1266	P1268	P1270	P1272	P1274
Lithography	45 nm	32 nm	22 nm	14 nm	10 nm
1st Production	2007	2009	2011	2013	2015

- As transistors became smaller more could be integrated into a single microchip, and so the computational power increased.
- this miniaturization process is now reaching a limit, a quantum threshold below which transistors will cease to function. Present state-of-the-art components possess features only a few tens of nanometres across

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- At the scale of tens of nanometres, their operation is disrupted by the emergence of quantum phenomena, such as electrons tunneling through the barriers between wires.

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Feynman offered two prizes each $1000
•to...who makes an electric motor
... [which] is only 1/64 inch cube
• to...who can take information
on the page of a book and put it
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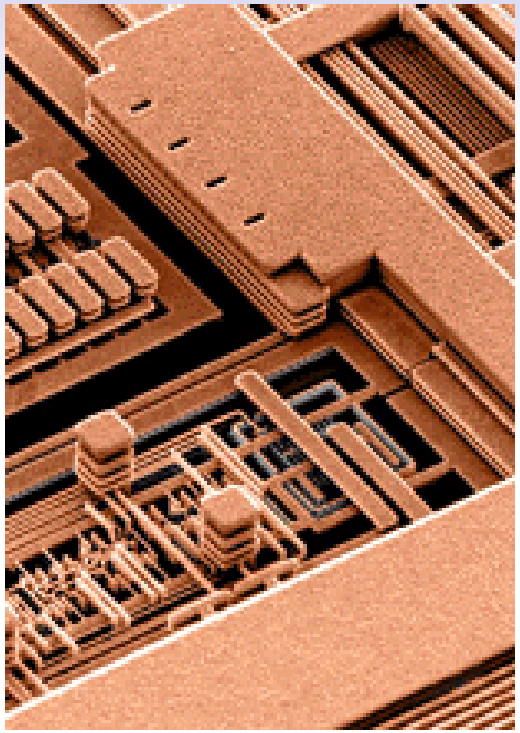
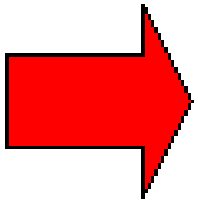
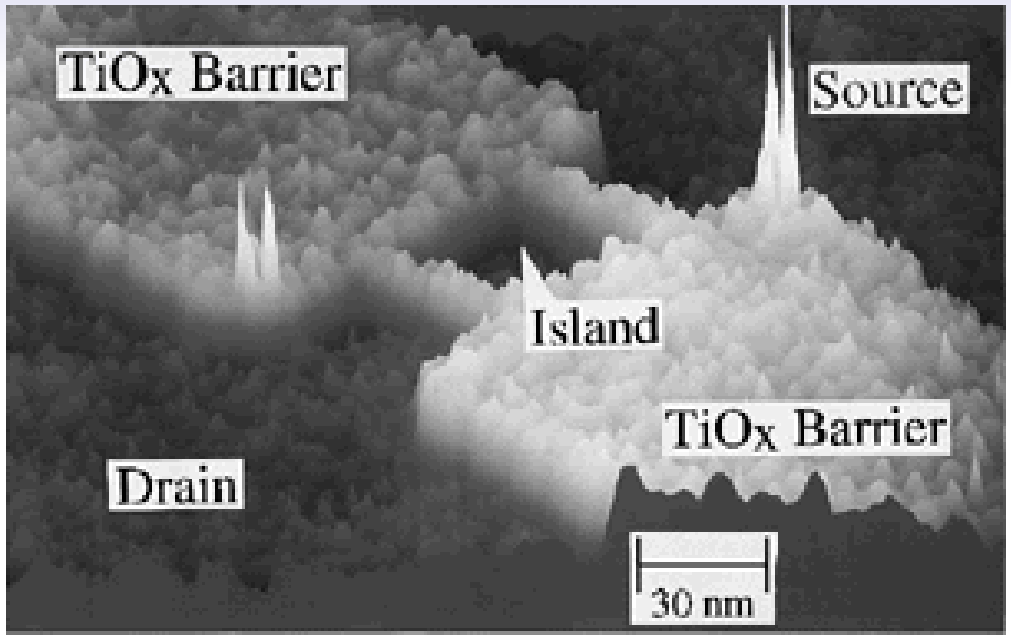
updated talk (1983): predicted that with today's technology we can easily...construct motors a fortieth of that size in each dimension, 64000 times smaller than... McLellans motor,...thousands of them at a time







Microtechnology $\Longrightarrow$ Nanotechnology.

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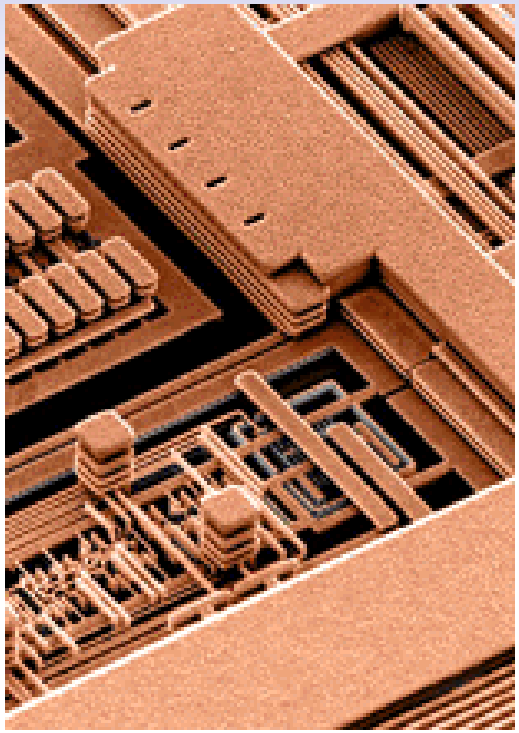

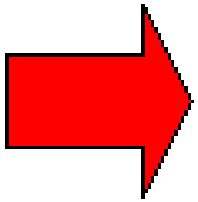

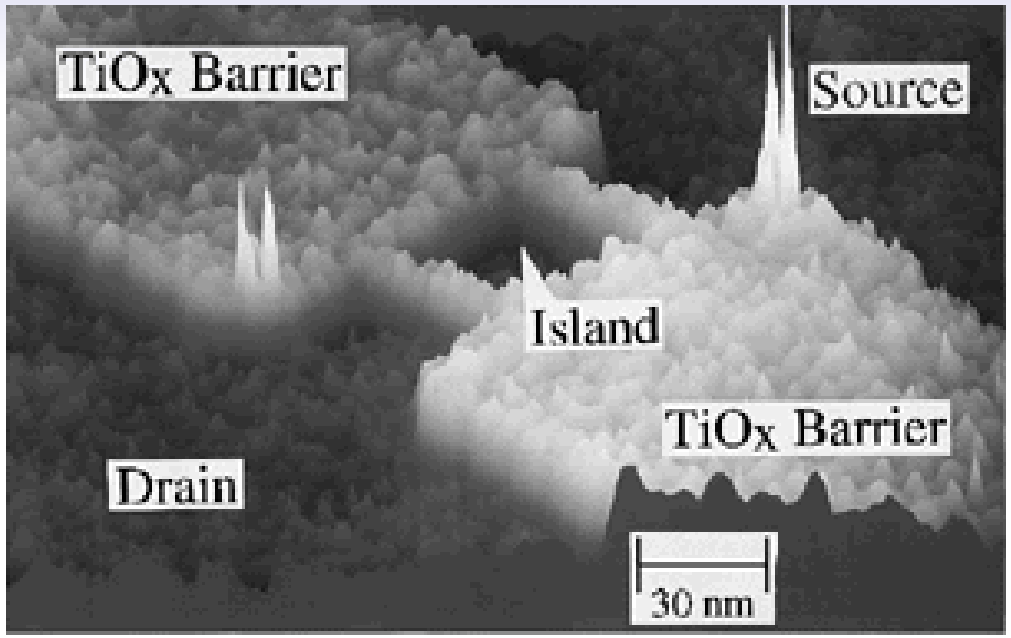

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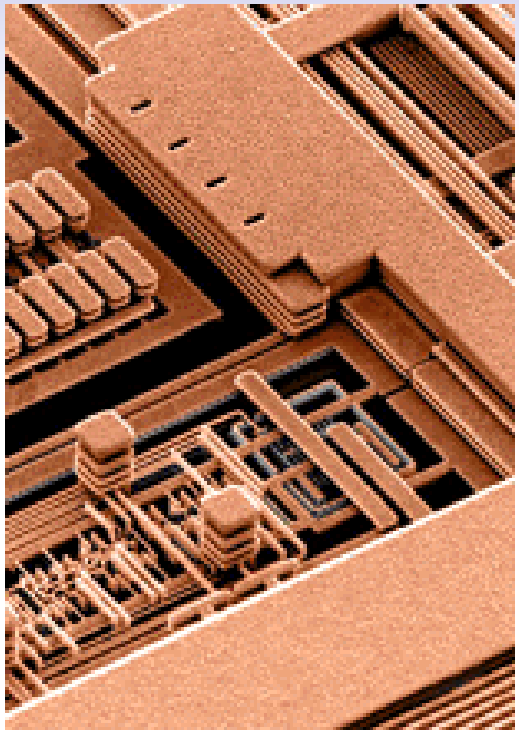
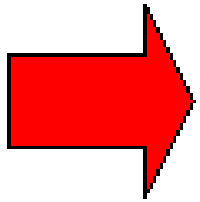
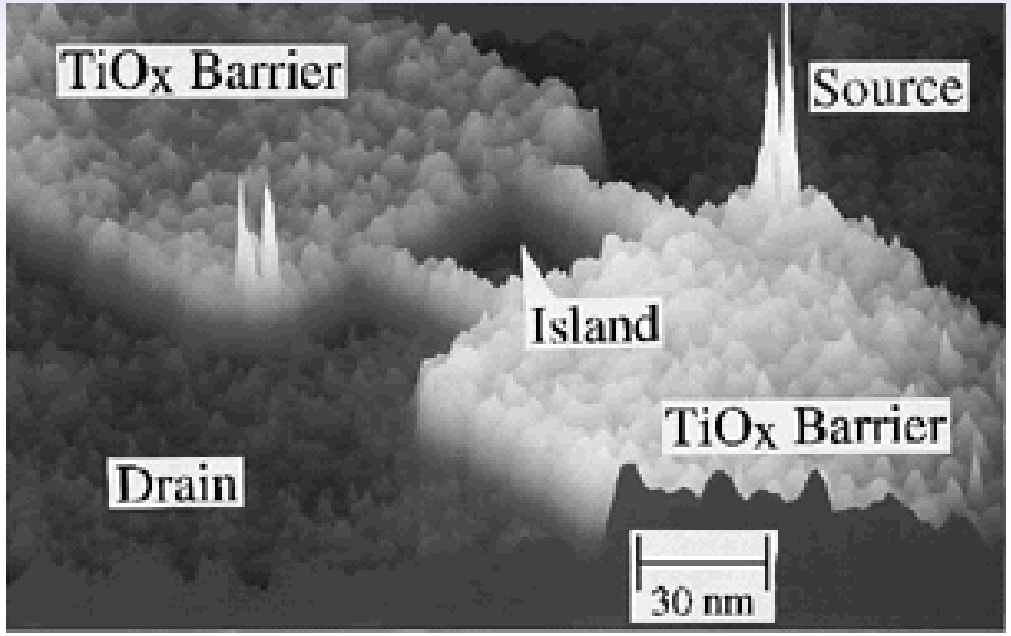
- Right: a single-electron transistor (SET) which was carved by the tip of a scanning tunneling microscope (STM).







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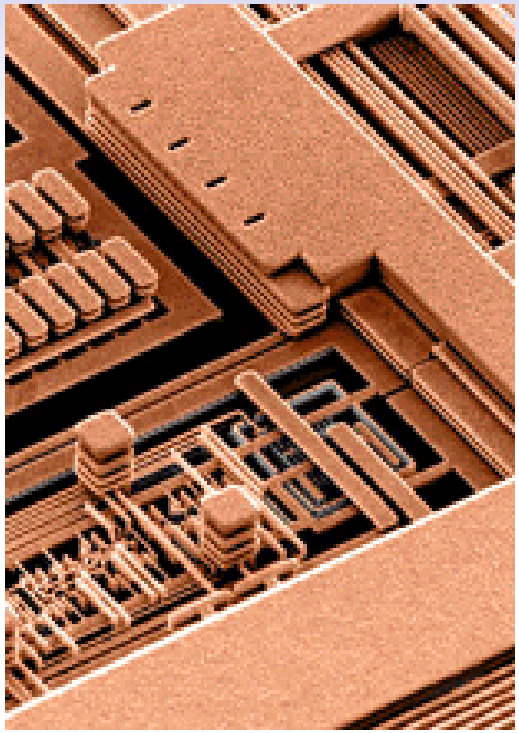
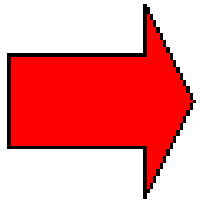
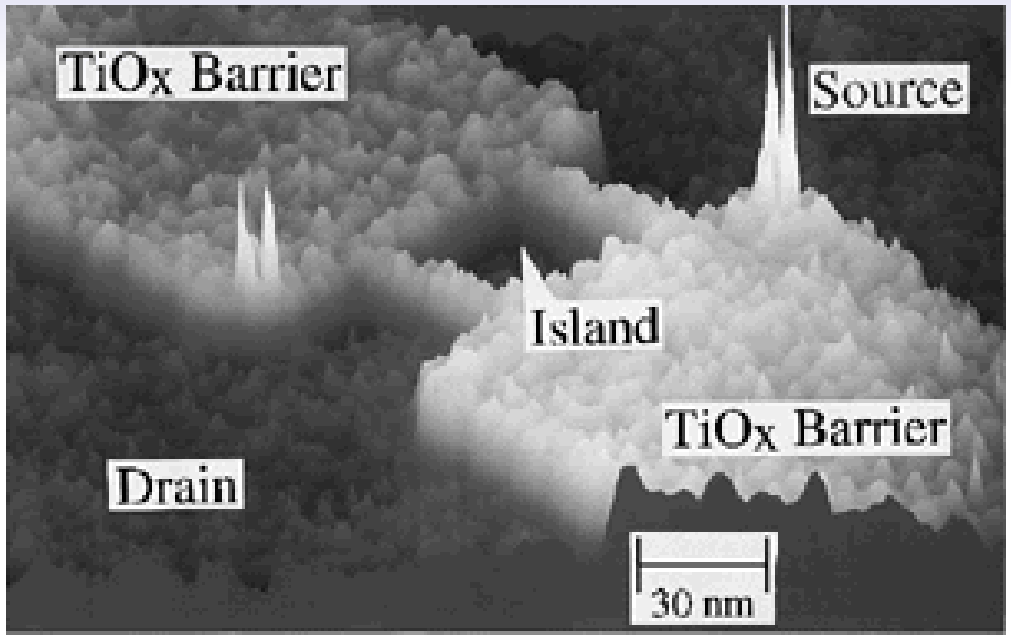
- Right: a single-electron transistor (SET) which was carved by the tip of a scanning tunneling microscope (STM).
- According to classical physics, there is no way that electrons can get from the 'source' to the 'drain', because of the two barrier walls either side of the 'island'. But the structure is so small that quantum effects occur, and electrons can tunnel through the barriers (but only one electron at a time can do this!).







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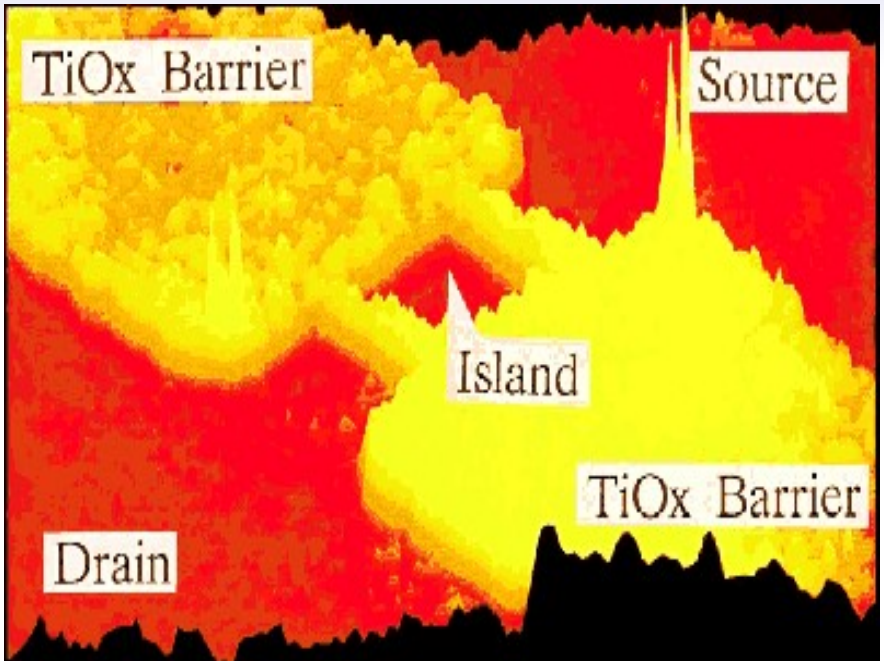
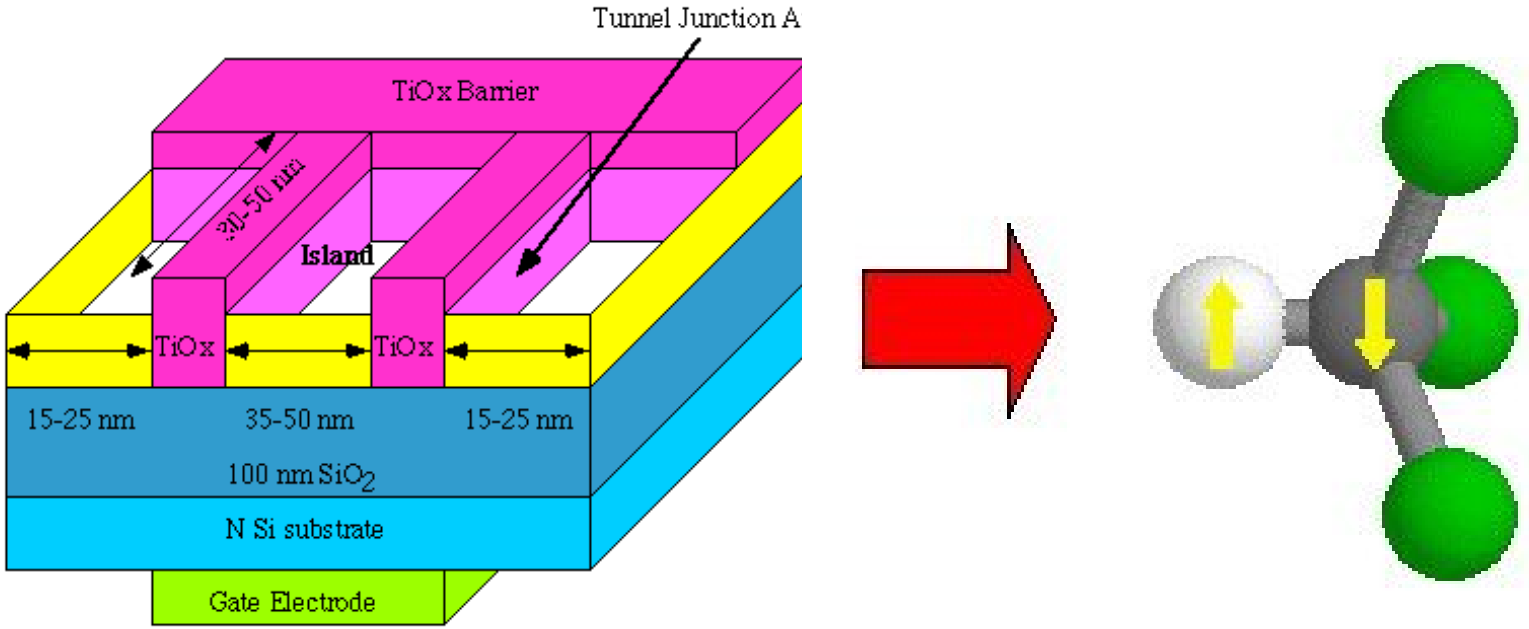
- **SET wouldn't work without quantum mechanics.**



- The first generation of nanocomputers have components that behave according to quantum mechanics, but the algorithms that they run do not involve quantum mechanics.
- There is another, more exciting possibility - quantum mechanics might be used in an entirely new kind of algorithm that would be fundamentally more powerful than any classical scheme. A computer that runs such an algorithm is a true 'quantum computer'.



From an SET (on the left) to the ultimate computer element: a molecule
Although both these structures use quantum mechanics, only the one on the right could be employed in a true 'quantum computer'. The 1H and 13C nuclei in isotopically labeled chloroform behave like small magnets, and interact with an external magnetic field. Nuclear spins can store and process information in "quantum superpositions".

Quantum Computers

A synthesis of classical information theory, computer science and quantum physics

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A bit - 0 or 1

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the state of an atom/molecule as a physical bit

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superposition $\leftrightarrow$ a quantum mechanical phenomenon:

$$|x\rangle = \alpha|0\rangle + \beta|1\rangle;\ \alpha^2 + \beta^2 = 1$$

Consider 3 physical bits.

classical register $\Rightarrow$ can store at a given moment of time only one out of eight different numbers,

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If we keep adding qubits to the register we increase its storage capacity exponentially i.e. three qubits can store 8 different numbers at once, four qubits can store 16 different numbers at once, and so on; in general L qubits can store 2^L numbers at once.

NOT

$$\begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}$$

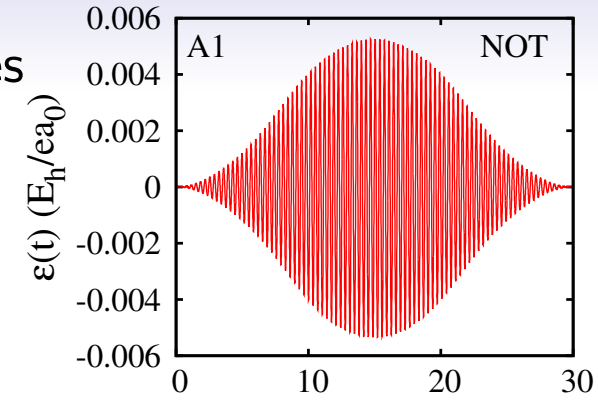
$$\Downarrow$$

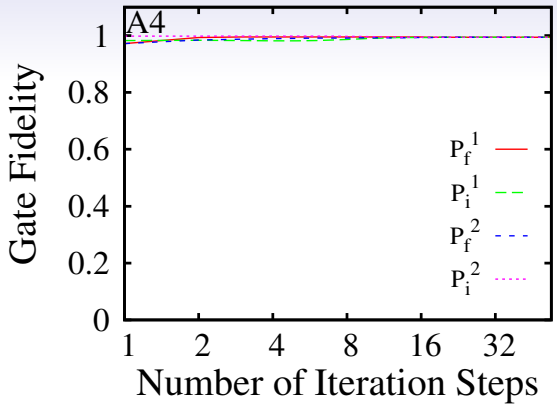
$$\begin{pmatrix} |1\rangle \\ |0\rangle \end{pmatrix}.$$

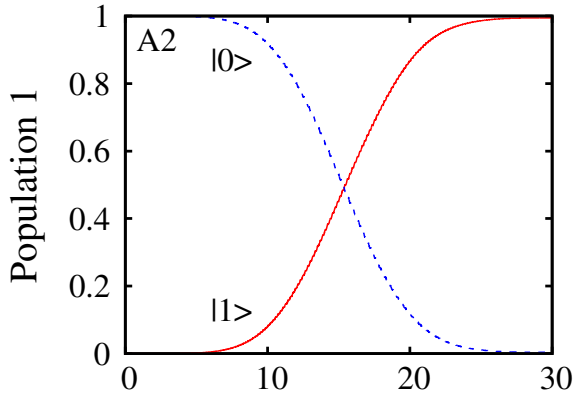
Single qubit quantum gates

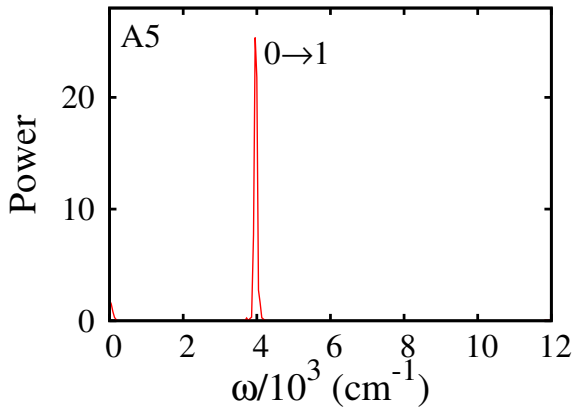
NOT

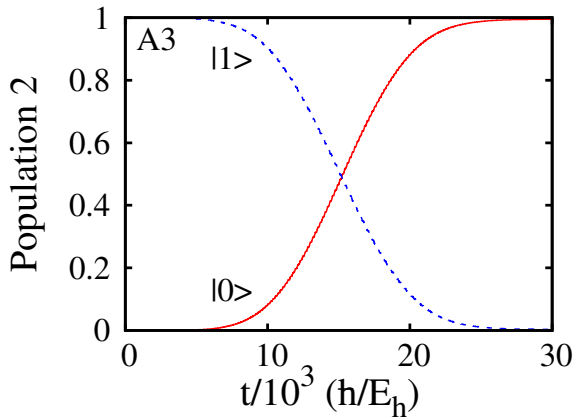
$$\begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix} \Downarrow \begin{pmatrix} |1\rangle \\ |0\rangle \end{pmatrix}.$$

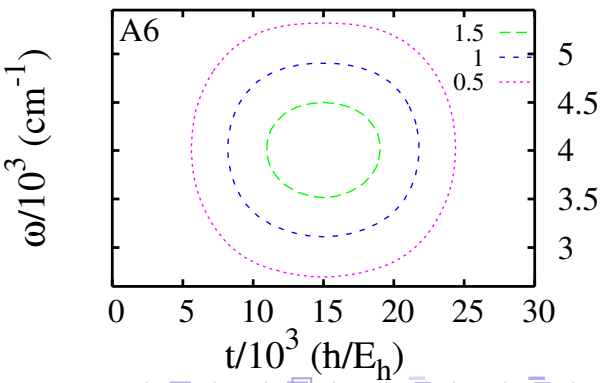












HADAMARD

$$\begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}$$

$$\Downarrow$$

$$\begin{pmatrix} \frac{|0\rangle+|1\rangle}{\sqrt{2}} \\ \frac{|0\rangle-|1\rangle}{\sqrt{2}} \end{pmatrix}.$$

Single qubit quantum gates

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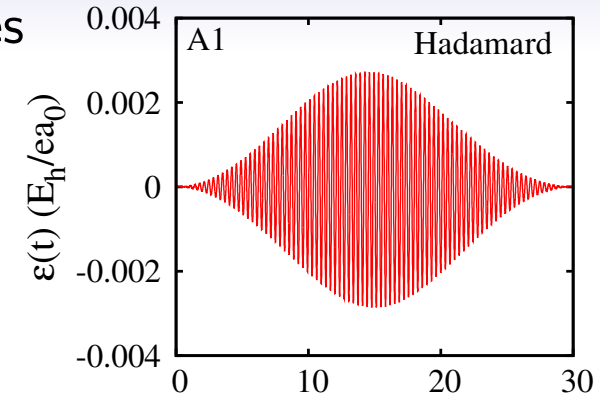
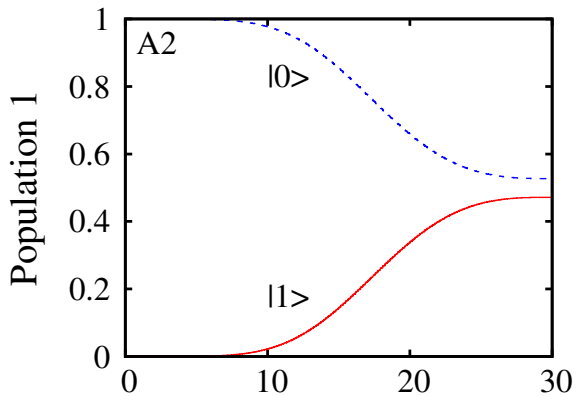
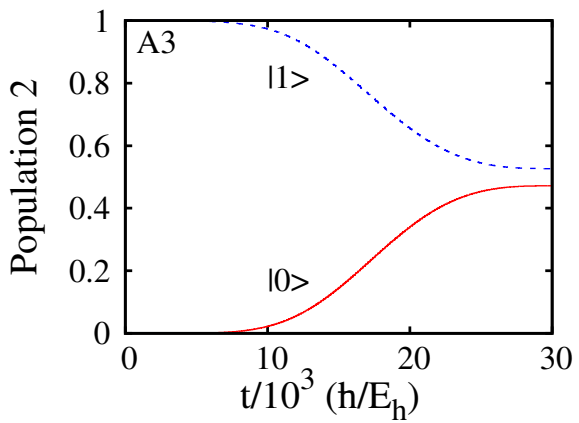
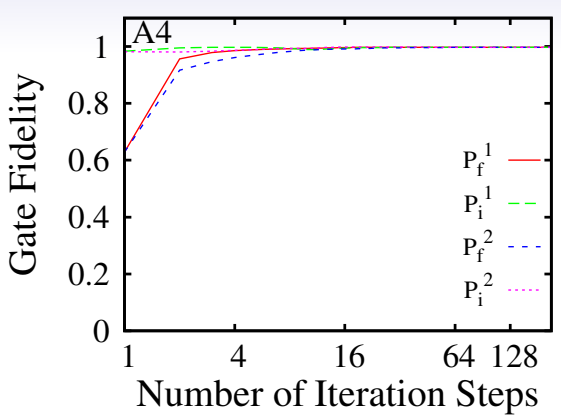
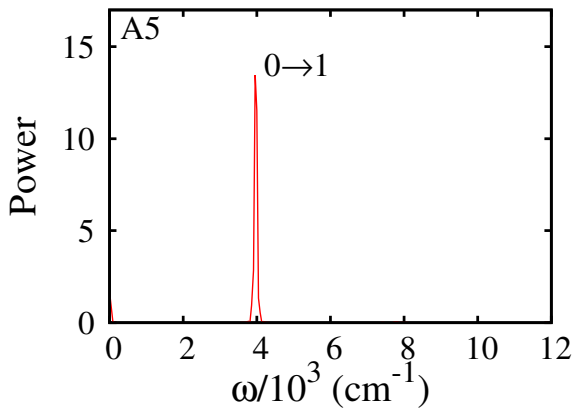
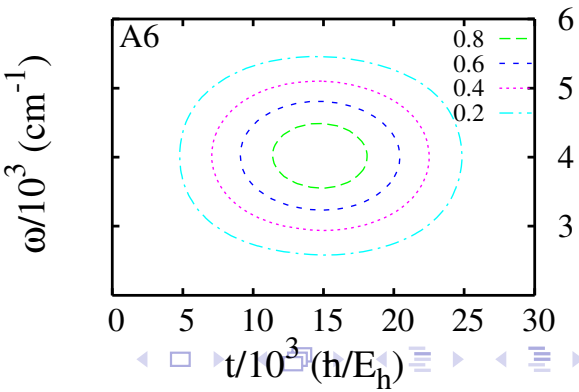


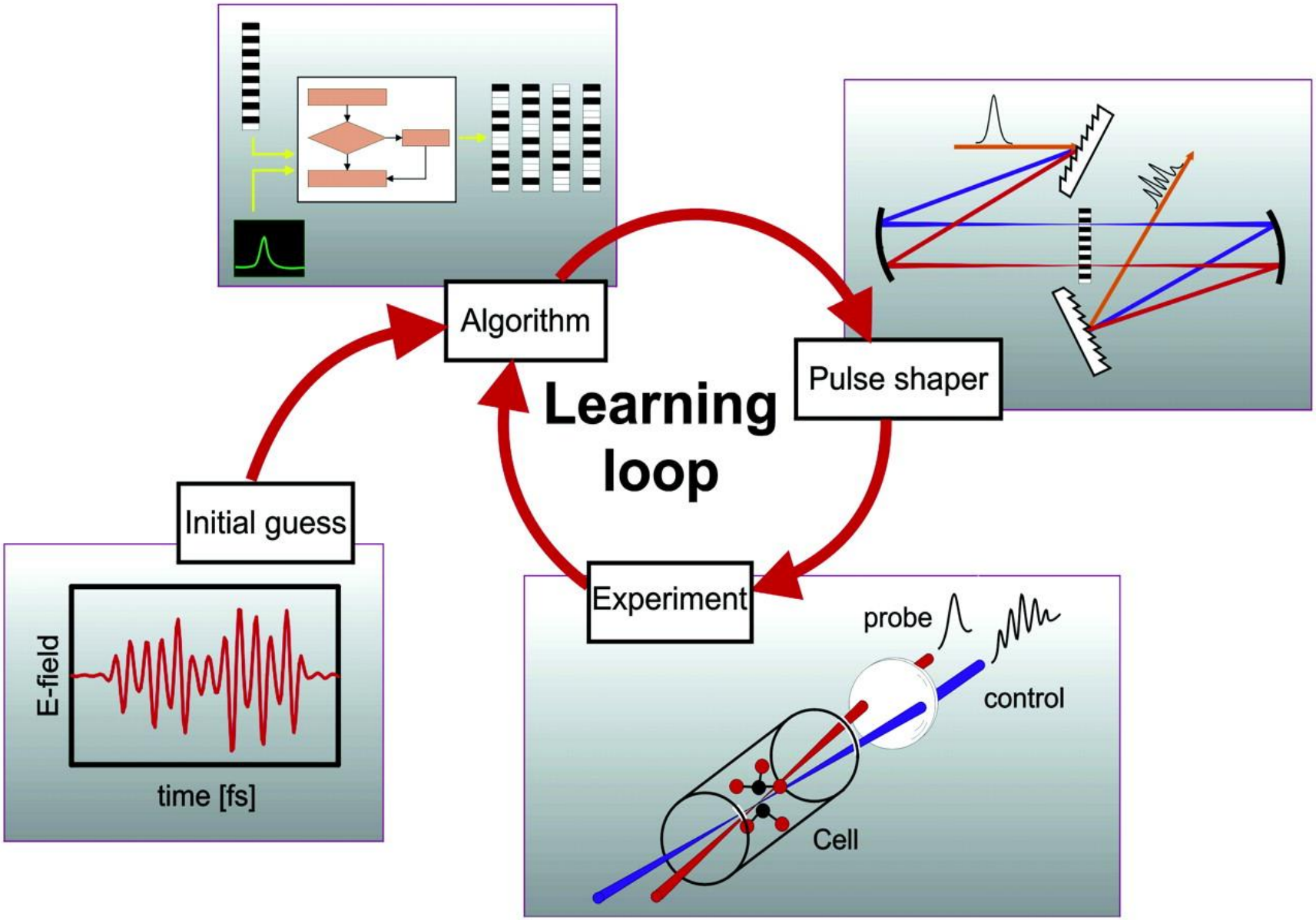


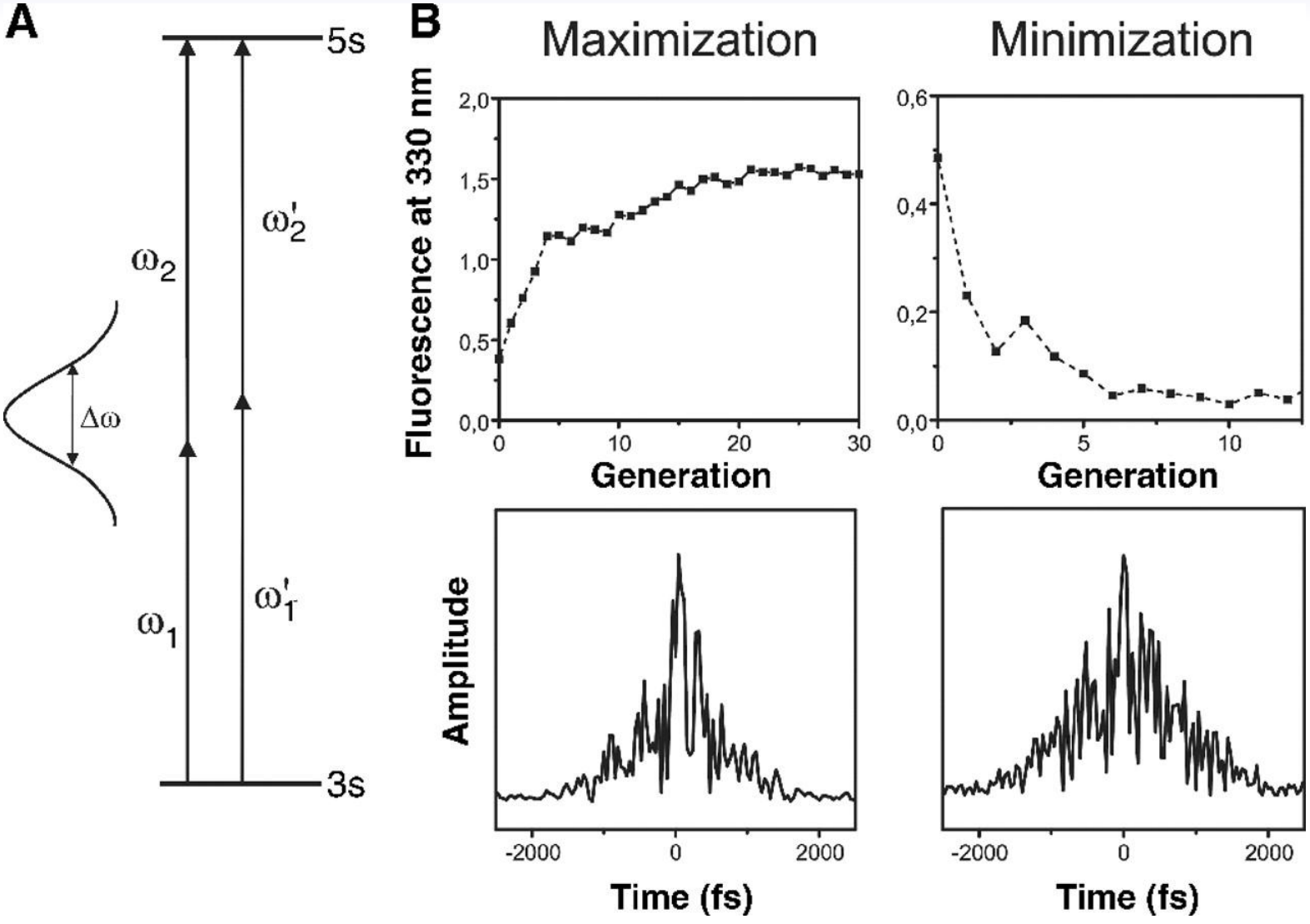






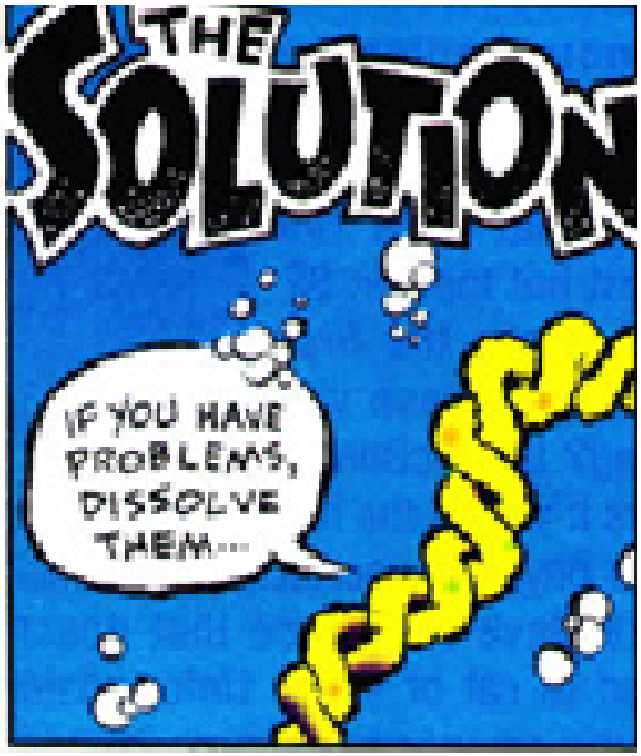



Algorithm
Pulse shaper
Learning loop
Initial guess
Experiment
E-field
time [fs]
probe
control
Cell


A
5s
ω_2
ω_2'
$\Delta\omega$
ω_1
ω_1'
3s
B
Maximization
Minimization
Fluorescence at 330 nm
2,0
1,5
1,0
0,5
0,0
0
10
20
30
Generation
0,6
0,4
0,2
0,0
0
5
10
Generation
Amplitude
-2000
0
2000
Time (fs)
-2000
0
2000
Time (fs)

"IF YOU HAVE PROBLEMS, DISSOLVE THEM"

(Larry Gonick cartoons)



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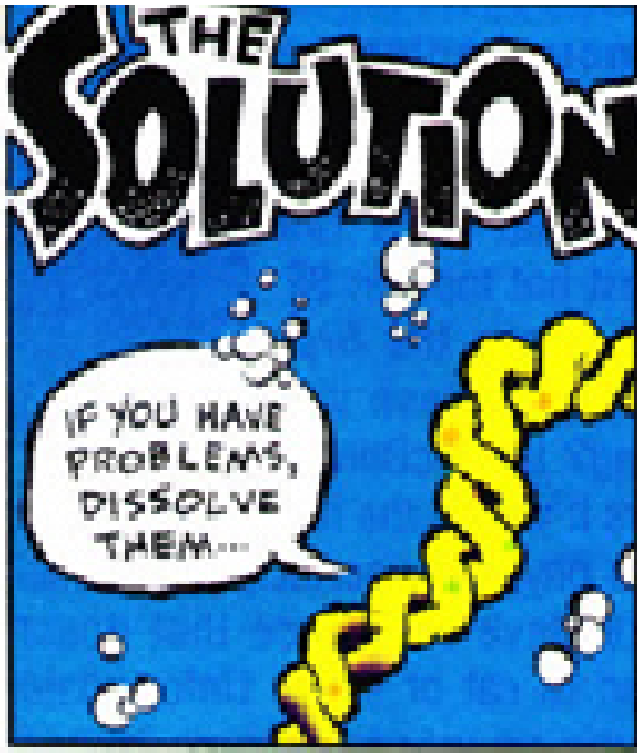

A chemical computer with indivdual molecules as working parts

Computation using DNA

Leonard Adleman: (*Science* **1994**)
Traveling Salesman problem (Hamiltonian Path problem)

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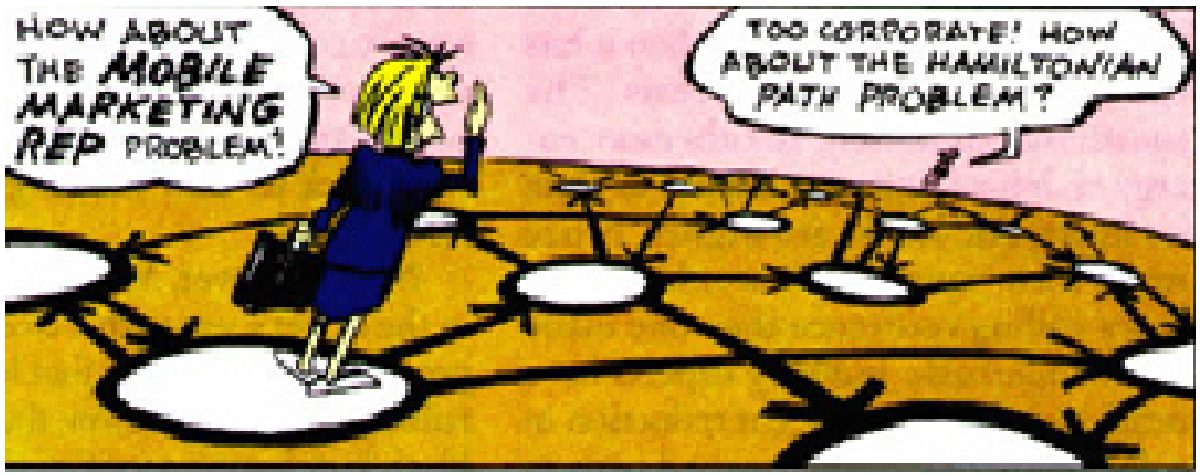
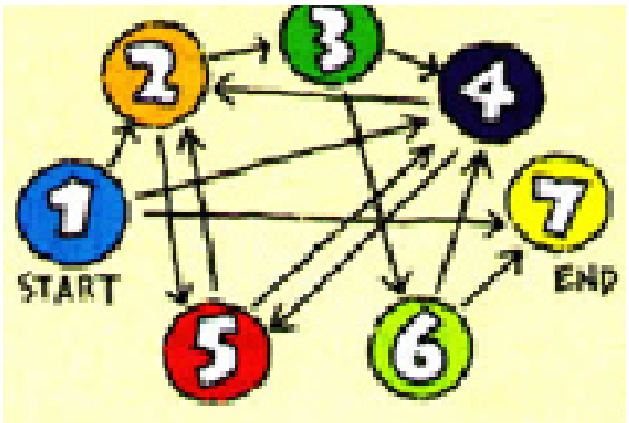
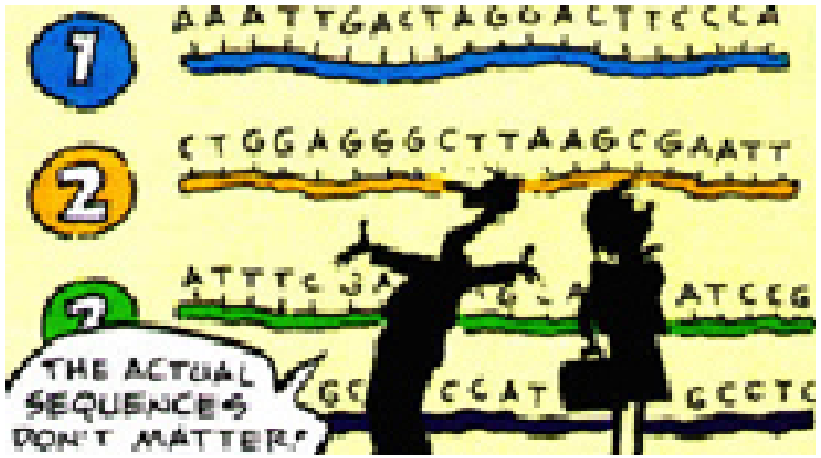
A Marketing Rep has a map of several cities with one-way streets between some of them.
Task: Find a route that passes through each city exactly once, with a designated beginning and end.



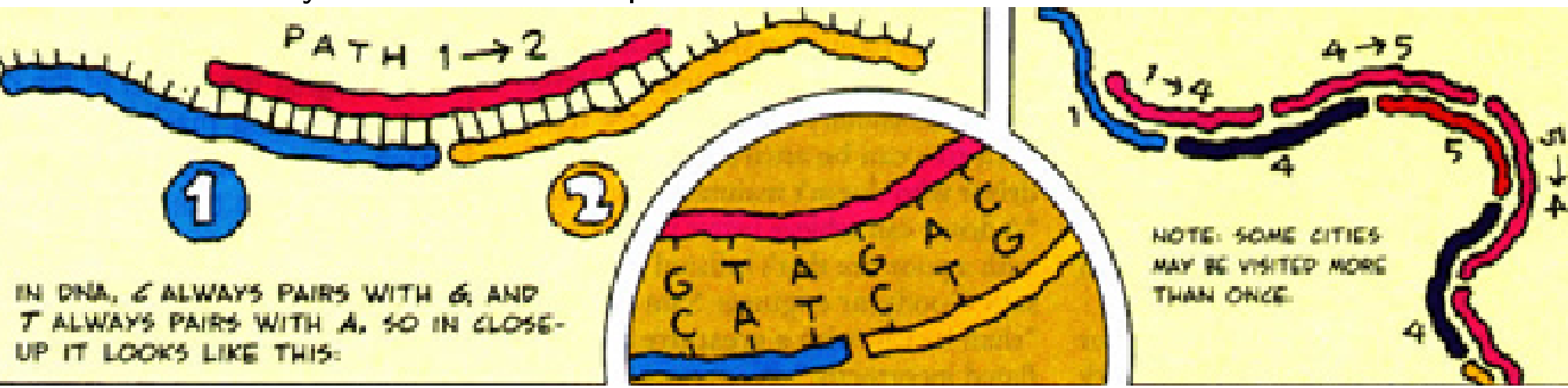
Adleman chose 7 cities and 13 streets.



Each city is represented by a ssDNA 20 bases long.



A street between two cities is the complementary 20-base strand that overlaps each city's strand halfway.
A multicity tour becomes a piece of dsDNA.



A few grams of DNA has over 10^{15} molecules. With all combinations of city and street put togetherm multiple copies of every path are created. The task is to find the paths that satisfy the conditions stated earlier. For this, Chemical techniques are used:

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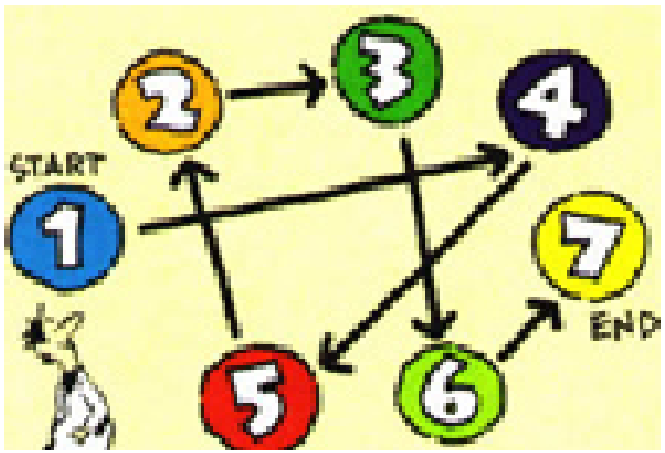
- Of those, find the ones passing through 7 cities.
- Of those, isolate paths with 7 different cities.



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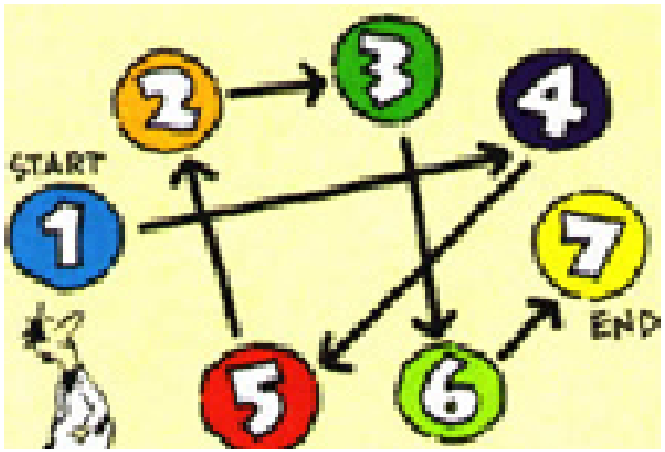

- 10^{15} parallel processors
- almost no energy required.

IT developments and scientific research have a symbiotic relationship:
•Developments in IT are most heavily used by the scientific community.

- email/internet
- visualisation
- ....
- grid-computing/ cloud computing

Chemists and climatologists (geophysical fluid dynamics researchers) are the larget users of supercomputing

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•Theoretical developments in computer science are motivated by questions of scientific research

Profound questions in theory of computing:
•What is knowable?
•Computability and universal computation

Parts of a poem by Prof Don Anderson, Professor of Geophysics, Caltech

The First Ten Million Millenia or So

In the "beginning" nothing
No time, no space, no matter.
No energy, no strings
nothing
not even a point, not even a void
nothing

No laws of physics
no myths, no Gods;
nothing, absolutely nothing
Then a singularity...
Call it a bang, call it a Big Bang, call it light, call it God
Perhaps a thought
In the beginning, the Laws of Logic begat the Laws of Physics.
The rules.
From Nothing, expansion
false vacuums, phase changes, befinning the time and space.
Potential for something, Everything Energy, potential
Waves, strings,
monopoles, sheets,threads
webs.

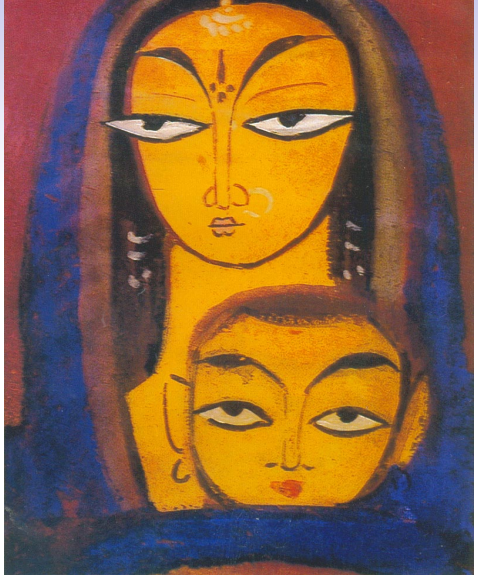
From the void, chaos
out of vacuum, Genesis.
Condensation, knots, cosmic freezing.
wrinkles in time, defects

Bubbles, foams. A detergent universe
Strong force, weak force,
symmetry breaking; machos, wimps, tubes of energy, gigantic loops.
A pasta universe
.....
Look at Earth
crust
oceans
air
Life
Cool!
a trivial speck, an afterthought
But all we got.

So here we are,
simple and meek,
Now how do we get through the rest of the week?

COMPUTER SCIENCE	$\Leftrightarrow$	NATURAL SCIENCES
• Artificial Life	soft hard wet	molecular evolution
• Artificial Intelligence		mechanics and machines
• Cognitive science		neuroscience
• ...		...

ideas of geometry inspiring Escher.



Two key terms:

Reductionism: An attempt or tendency to explain a complex set of facts, entities, phenomena, or structures by another, simpler set: For the last 400 years science has advanced by reductionism... The idea is that you could understand the world, all of nature, by examining smaller and smaller pieces of it. When assembled, the small pieces would explain the whole (John Holland).

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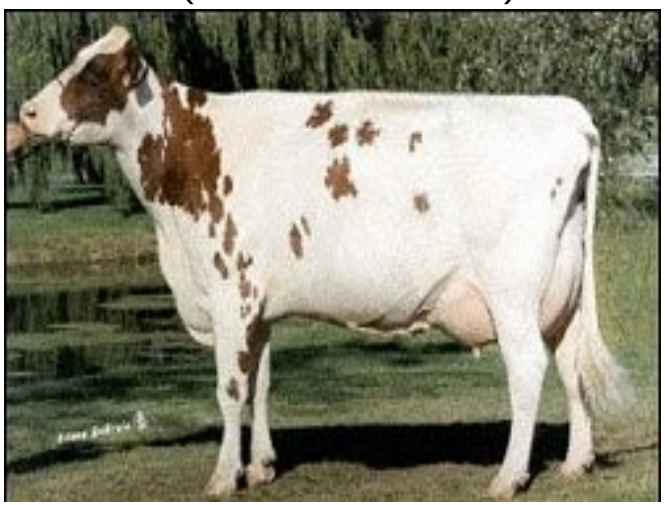

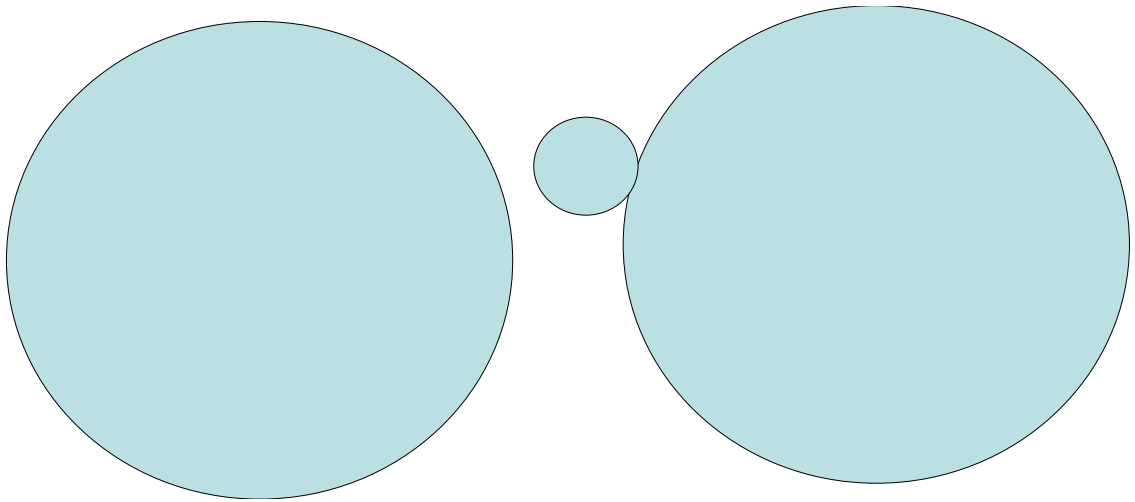

Holism: The theory that living matter or reality is made up of organic or unified wholes that are greater than the simple sum of their parts.

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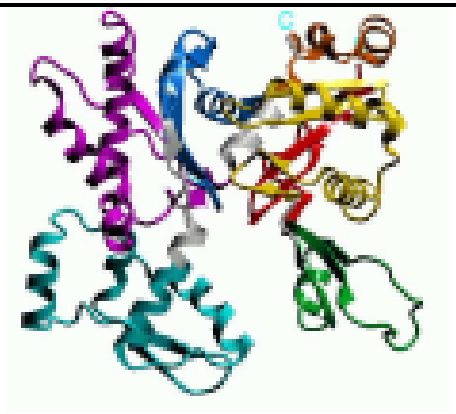
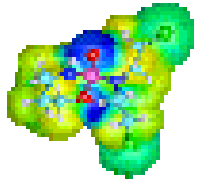
Desirable: A holistic investigation or system of treatment.

Chemical computations





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

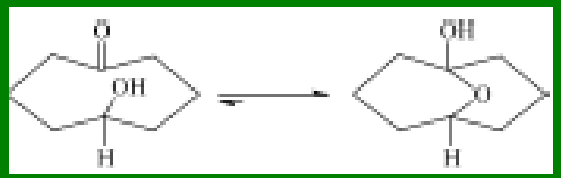
Solve Exact Schrodinger Equation

Empirical Parameters Needed

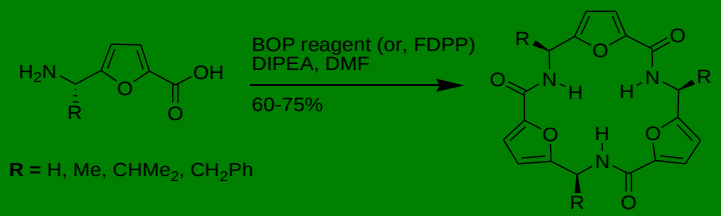
Computationally Demanding

Electronic structure and properties of molecules :

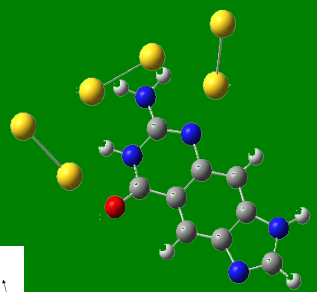
- 5-Hydroxycyclooctanone hemiacetal rearrangement



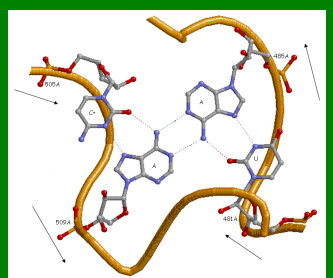
- Cyclotrimerization of furan amino acids



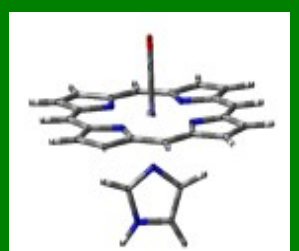
- Binding of Gold nanoclusters with size expanded DNA Bases



- Interbase binding in Noncanonical RNA Base pairs



- Controlling dynamics of Fe-C-O bond distances in monocarboxy myoglobin



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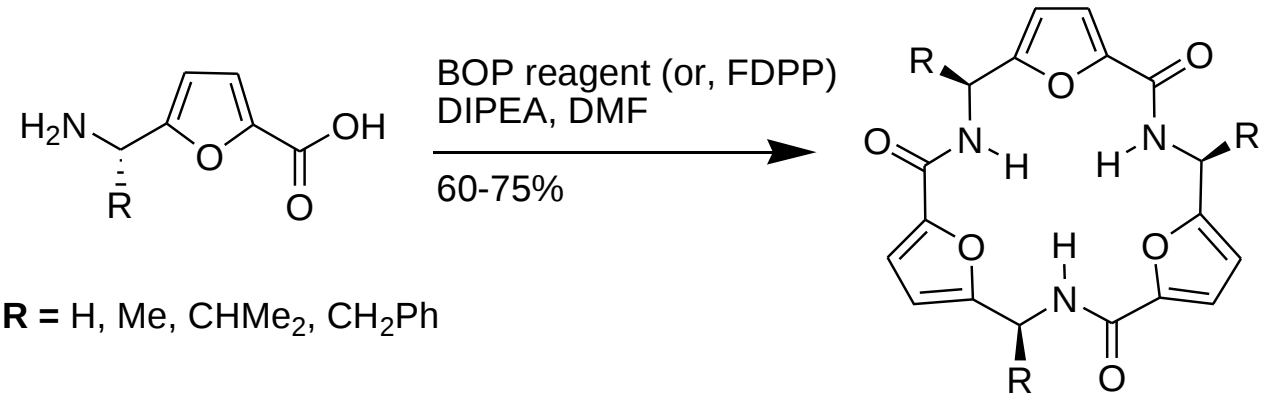
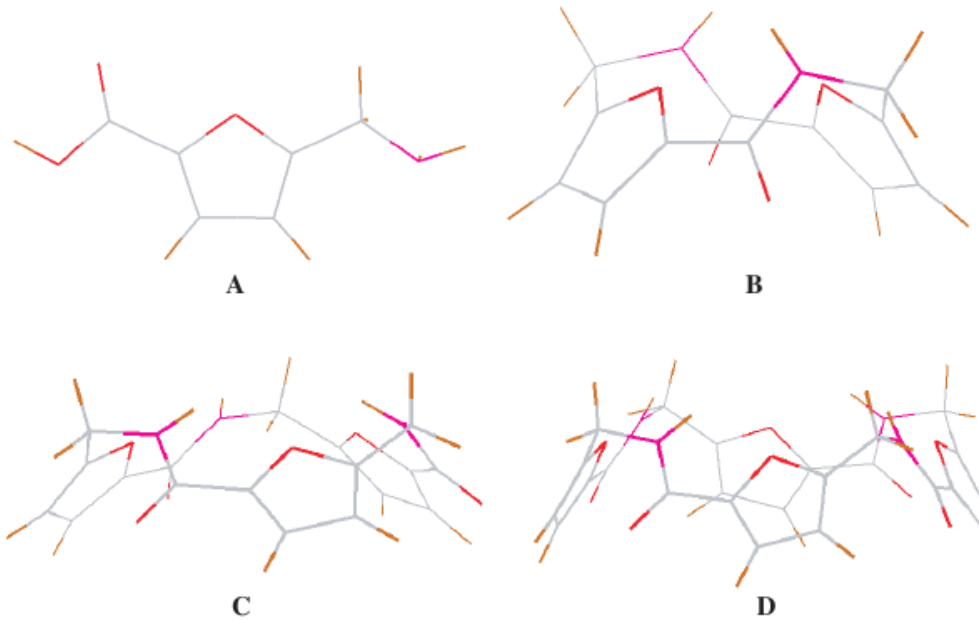
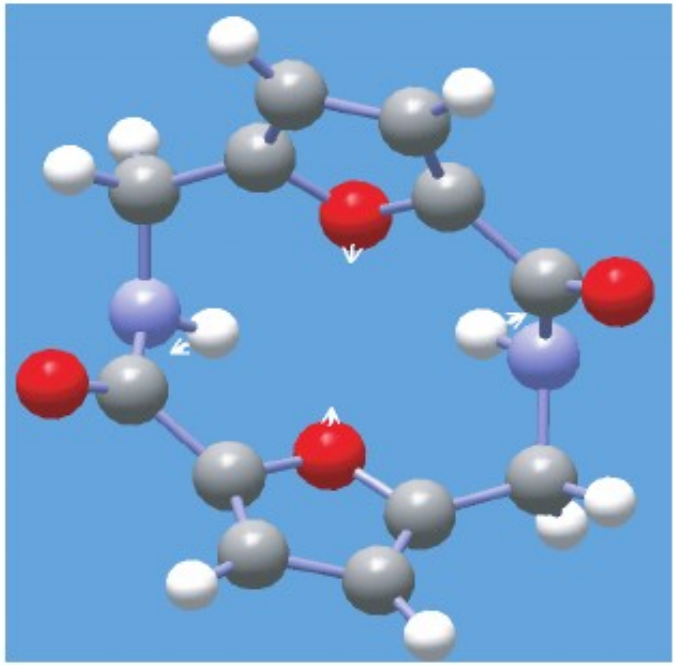
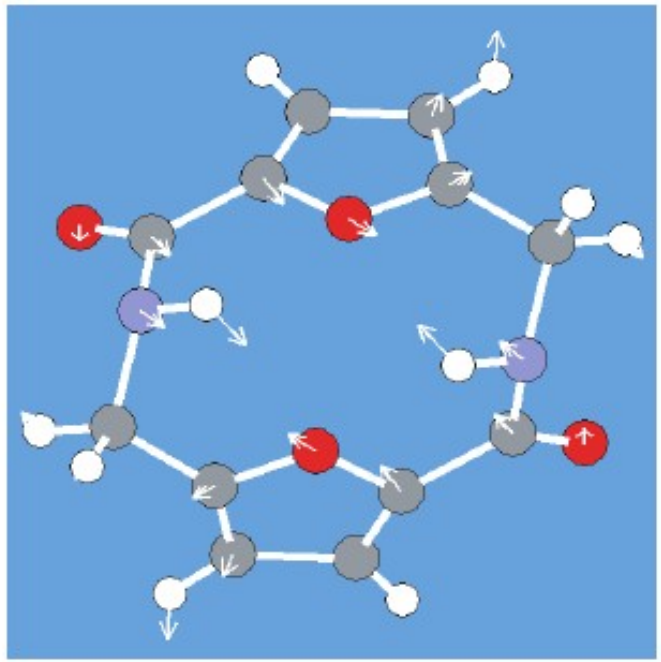
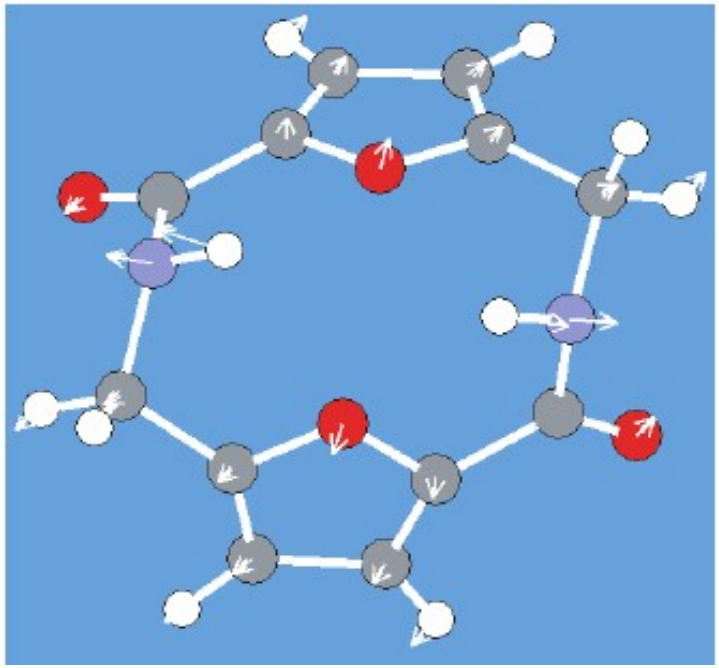
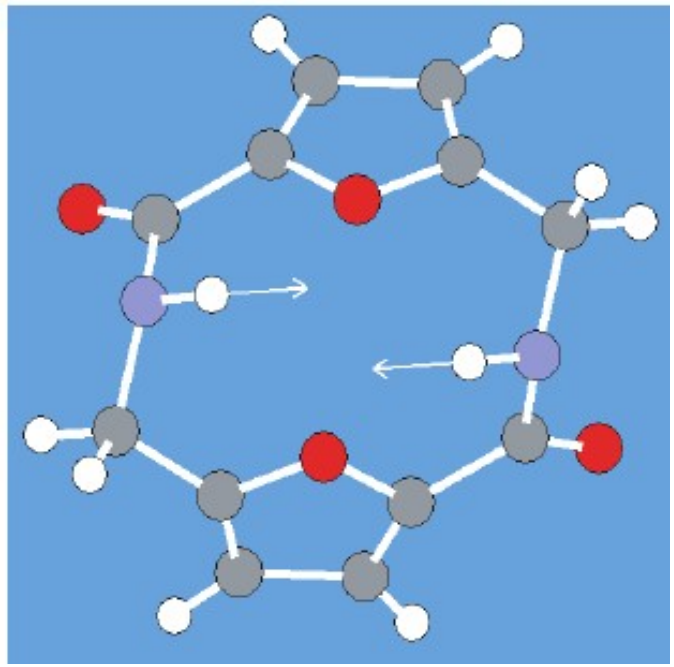
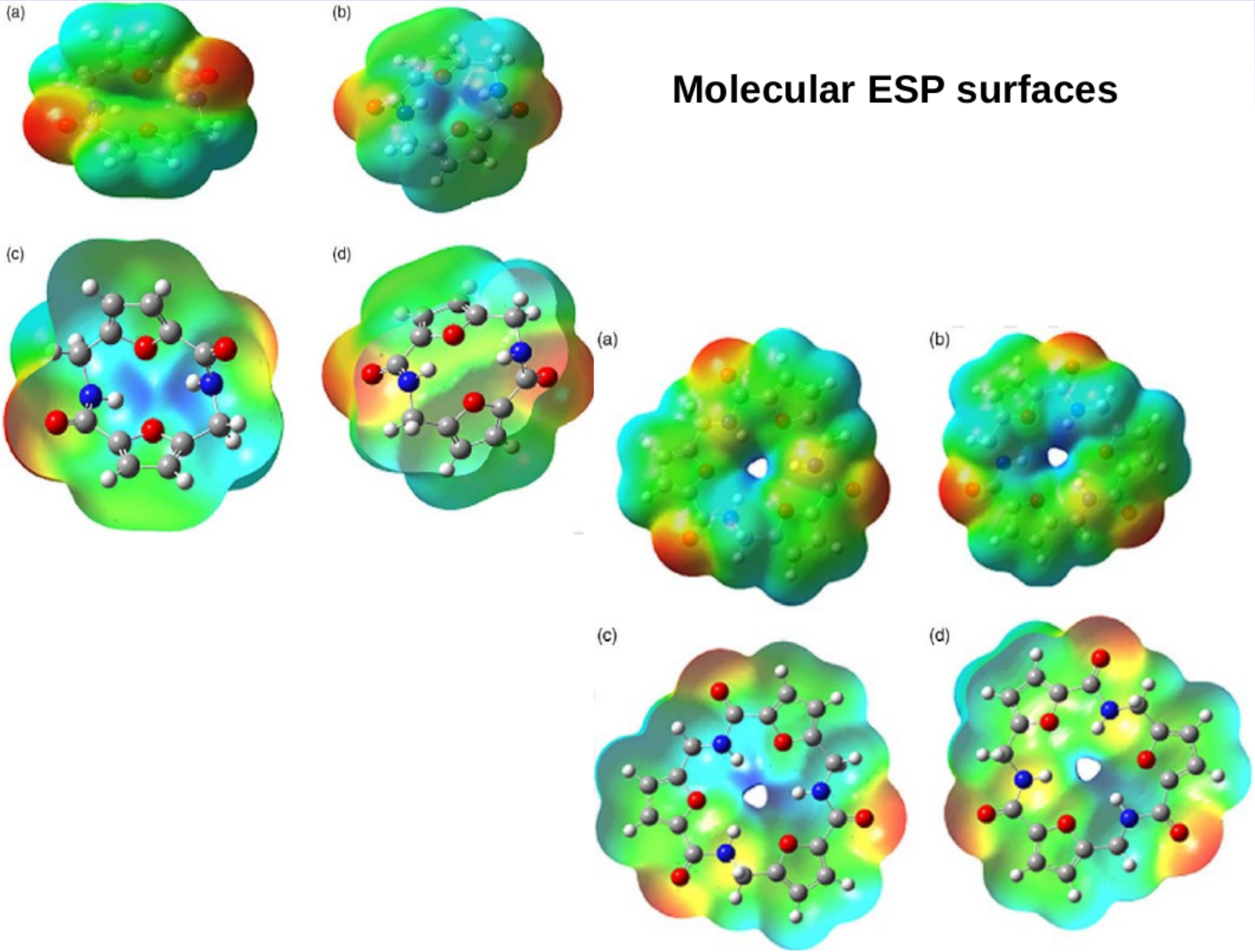


R = H, Me, $CHMe_2$, CH_2Ph



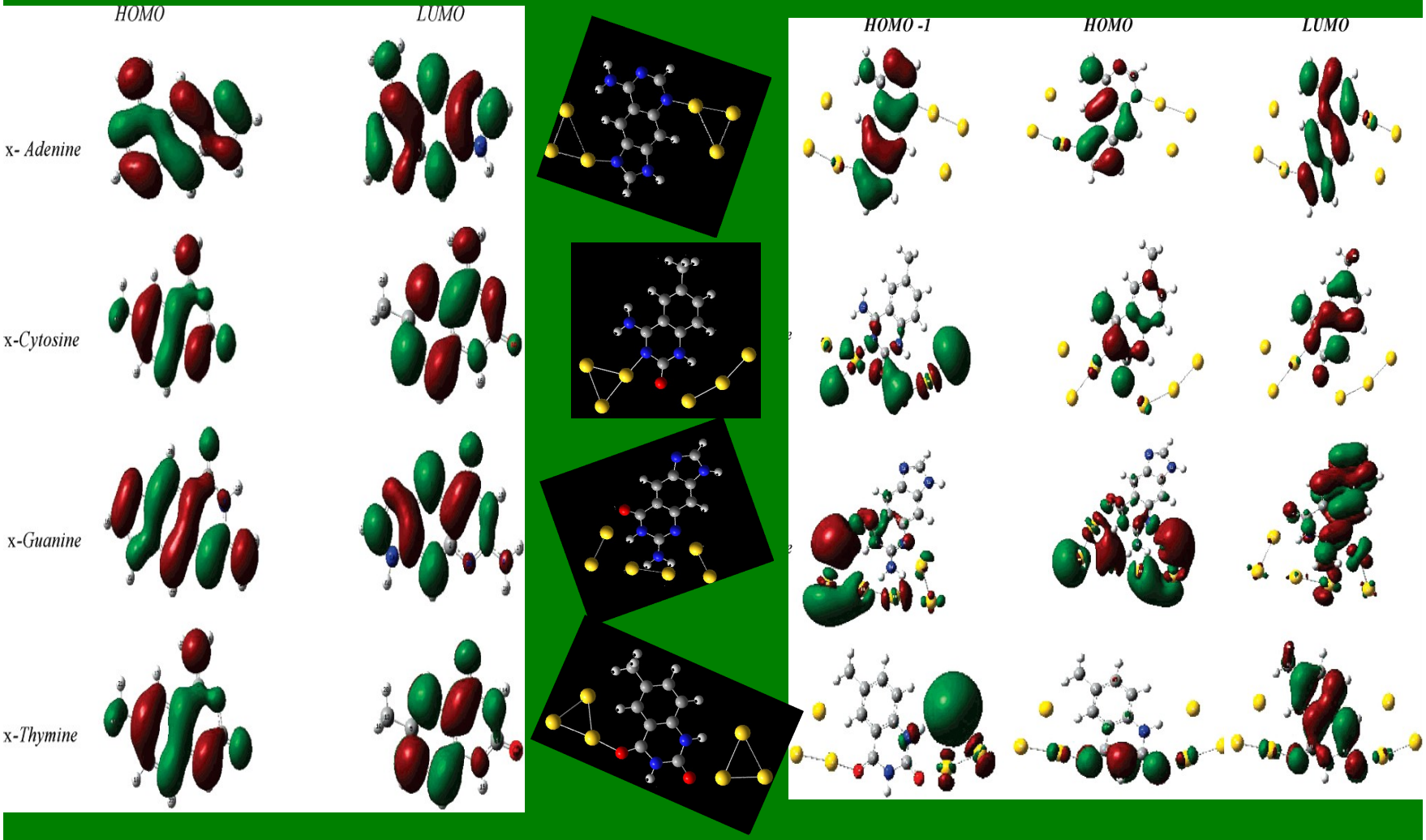
Molecular ESP surfaces



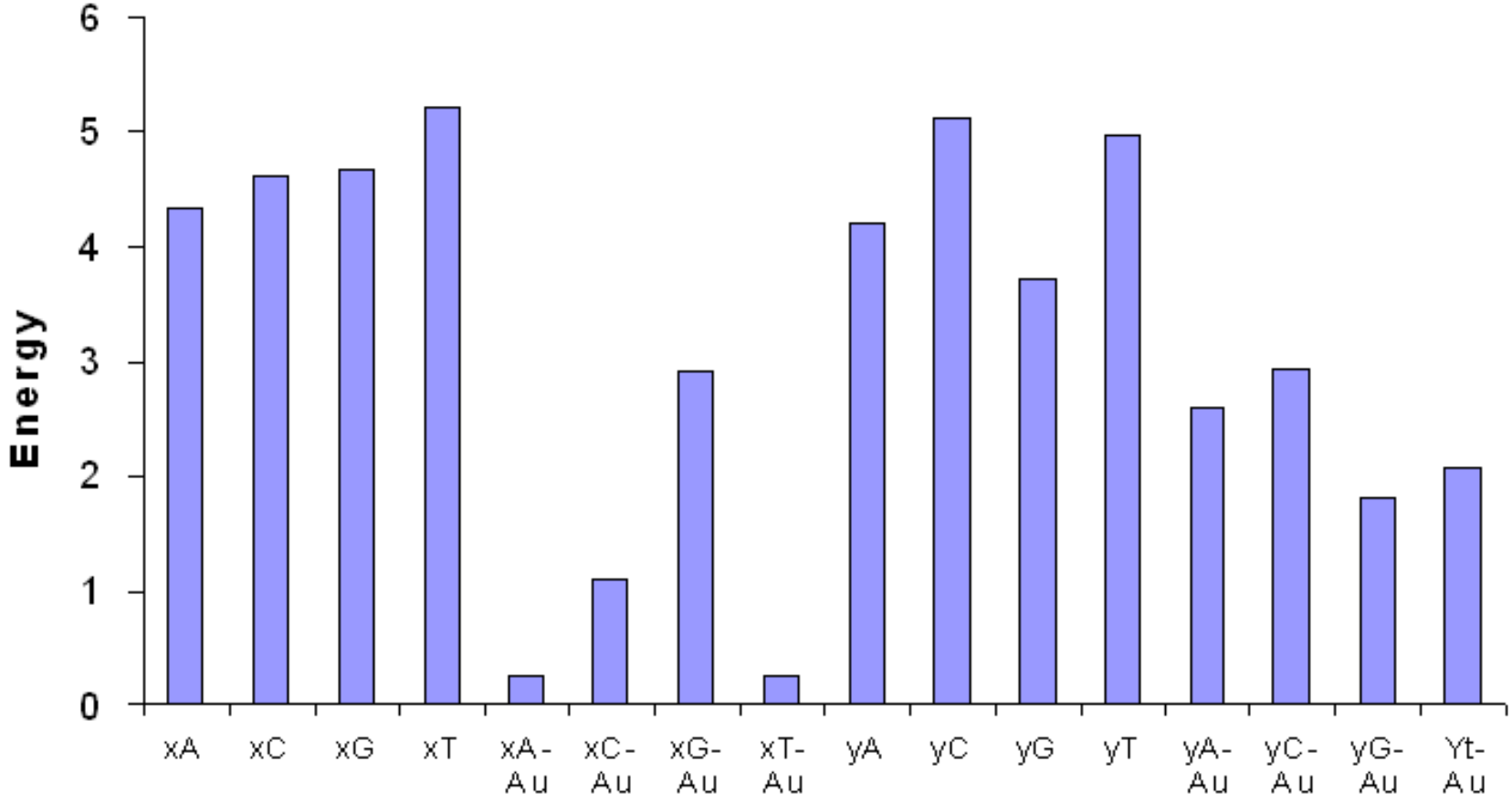
Free bases

Optimized geometires

Gold complexed bases



HOMO-LUMO gaps



Grand challenges in physical sciences today

1. Control processes at the level of electrons
2. Design and perfect atom- and energy-efficient syntheses of new forms of matter with tailored properties.
3. Understand and control the remarkable properties of matter that emerge from complex correlations of atomic and electronic constituents
4. Master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things
5. Characterize and control matter away especially far away from equilibrium.

Grand challenges in biological sciences today

1. Synthesizing Life-Like Systems
2. Understanding the Brain
3. Predicting Individual Organisms Characteristics from Their DNA Sequence
4. Interactions of the Earth, Its Climate, and the Biosphere
5. Understanding Biological Diversity

It from Bit

Hypothesis: every item of the physical world, be it particle or field of force, ultimately derives its very existence from apparatus-solicited answers to binary, yes /no questions

-John Wheeler