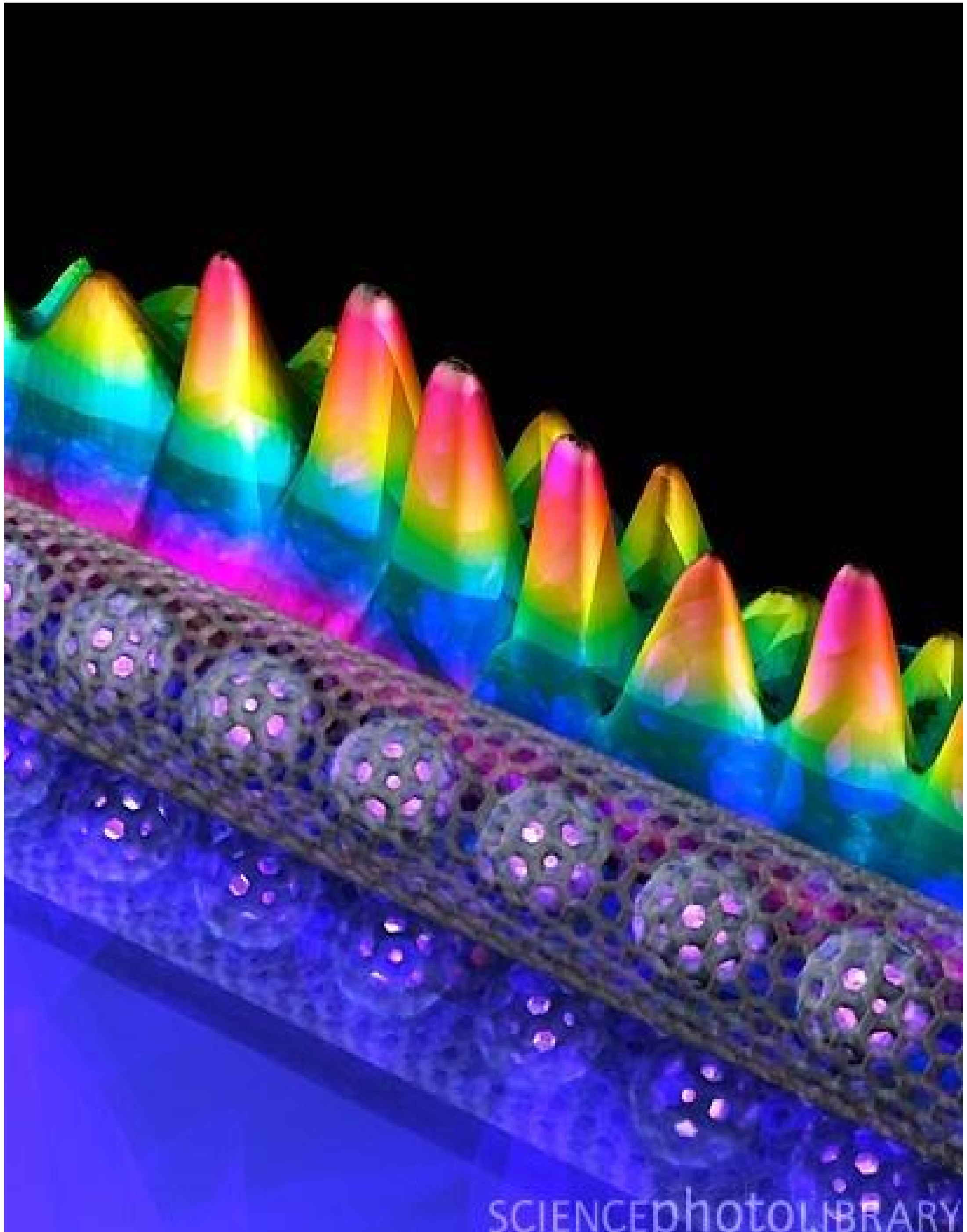


VERY Informal introduction to

Computer modelling of *Carbon* Nanotechnology

CPD 2013

Manuel Melle Franco
DI, HPG group
University of Minho

who am I?

- **Researcher in the HPC(G) group of DI**
- CV: Natural scientist:
    - Ph.D. **Physics**
    - M.Sc. **Materials Science**
    - Degree in **Physical Chemistry**
    - Research:
        - **HPC and scientific computing:**
        - **NANOTECHNOLOGY**
        - **chemistry**
        - **physics...**

PLEASE <u>INTERRUPT ME</u> AT ANY TIME!!!

Experiment and Theory

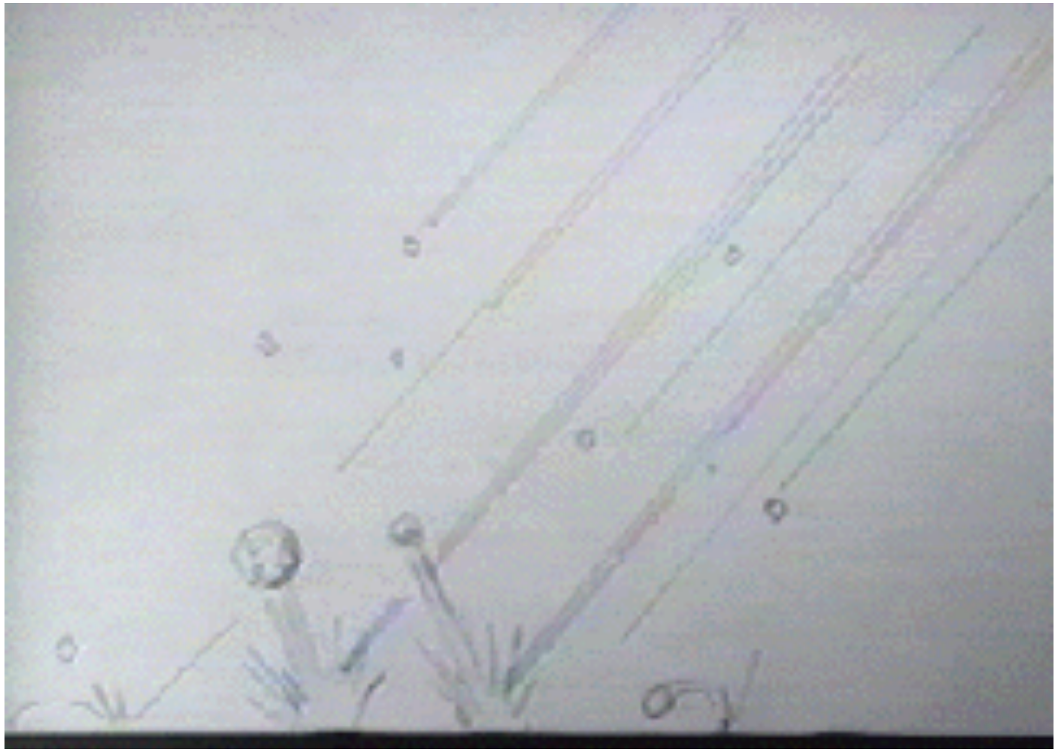
Mathematical models

Experiment vs. theory

- Experiment: observation of a physical phenomenon - EMPIRICAL
- Theory: Model, typically mathematical, reproducing the observation of thar physical phenomenon

Theory needs observation!

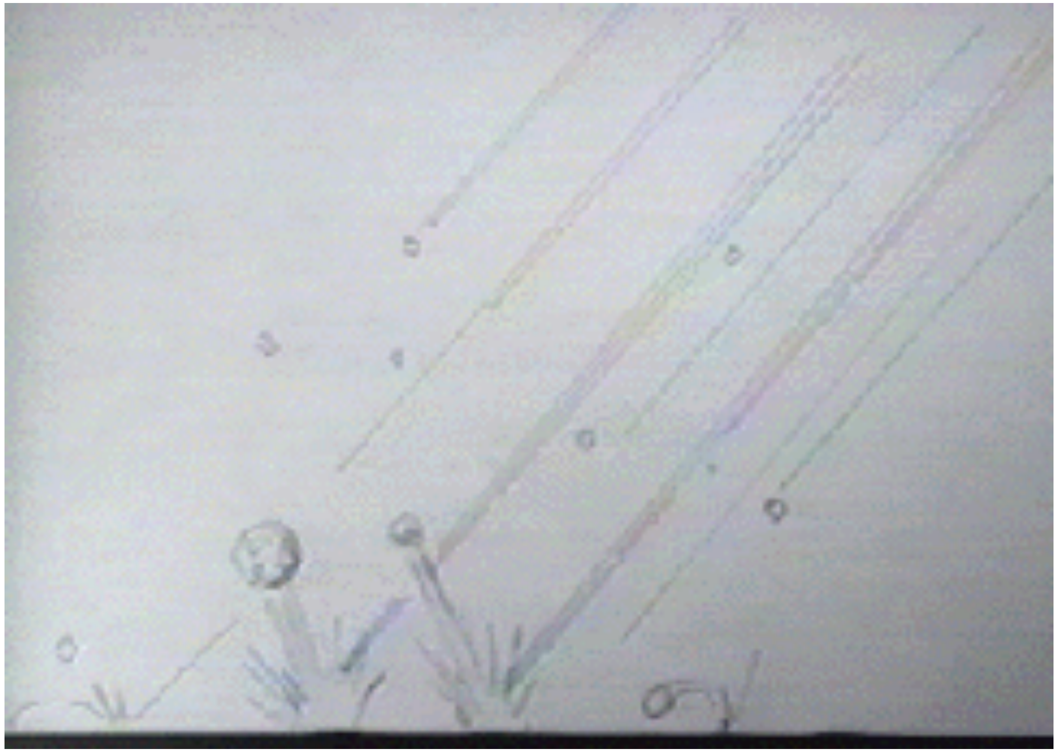
- Until 17th century: Aristotle's theory said that heavier objects fall faster



- Galileo Galilei, OBSERVED in a hail storm: small hail and big hail touched the ground at the same time
- NO PREFERENCE with size (weight)

Theory needs observation

- Galileo found this surprise and wanted to know more so he INVENTED a way to find out: he made up an **EXPERIMENT**

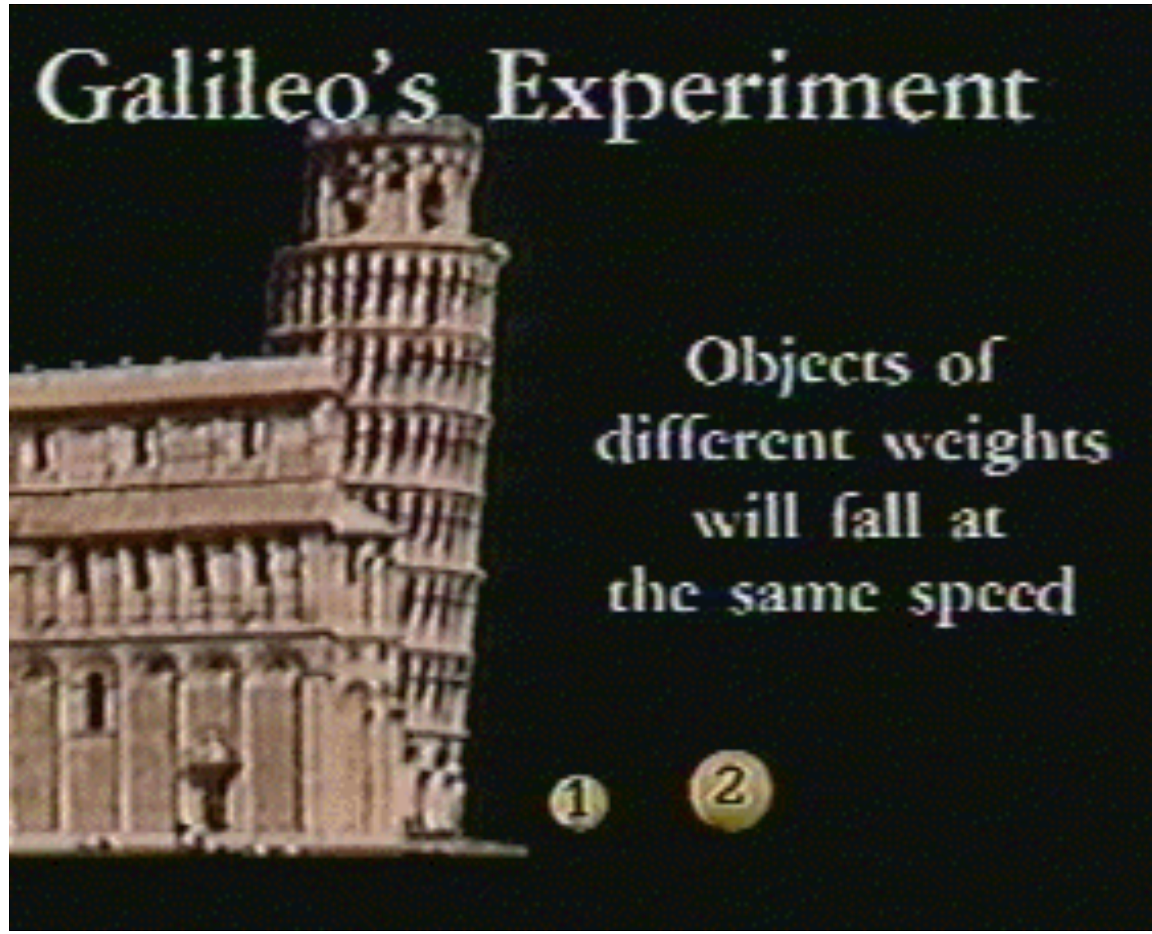


Galileo's experiment (17th century)

- Galileo's **experiment** showed **Aristotle was wrong**
- Aristotle did not check his theory. HE thought it was obvious trough common sense (we do the same most of the time!!!!)

Galileo's experiment (17th century)

- G. proposed a MATHEMATICAL model:
  - to reproduce the experimental data he collected
  - **to predict** what would happen in other cases.



Experiment vs. theory

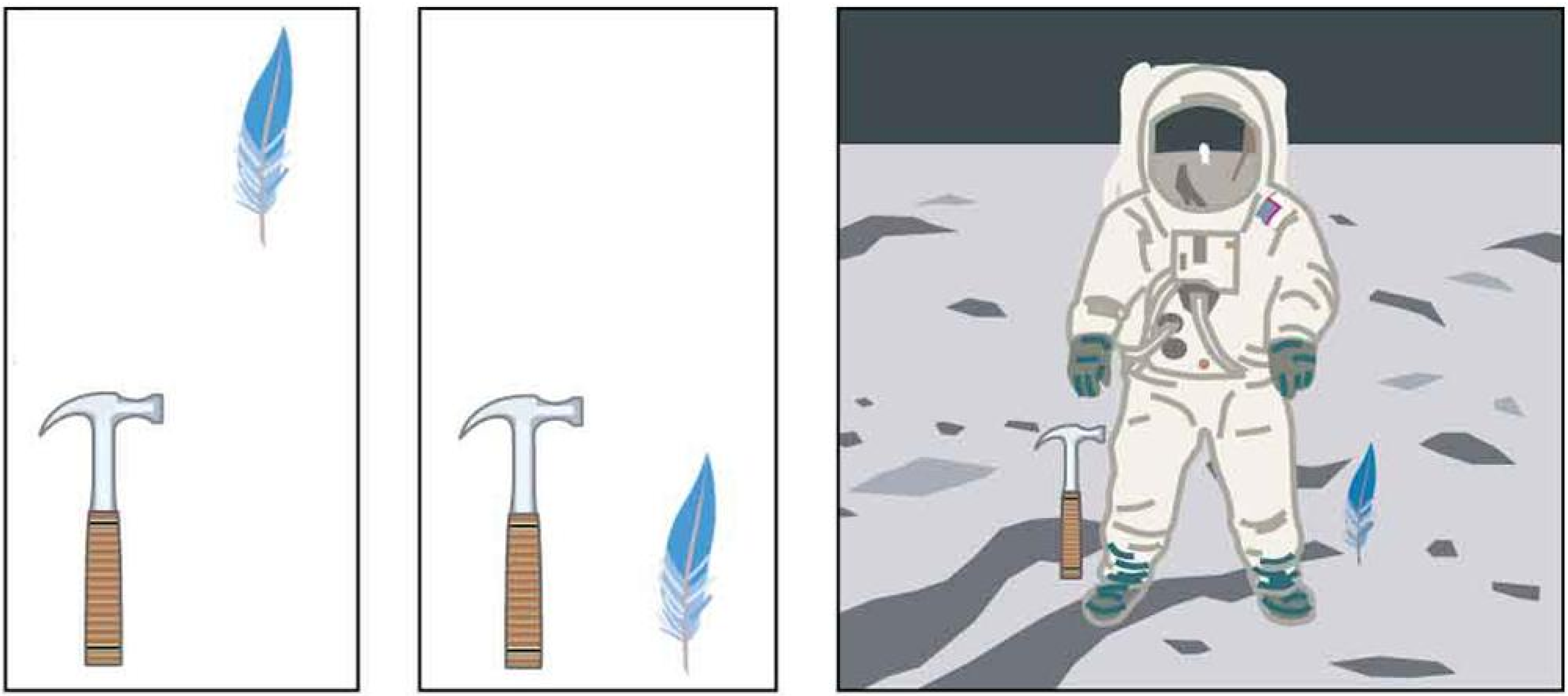
- What does fall faster a hammer or a feather?

Experiment vs. theory

- What does fall faster a hammer or a feather in the moon?

Experiment vs. theory

- What does fall faster a hammer or a feather? (**air resistance, why aristotle “theory” was wrong!!!**)



In air — In a vacuum — In a vacuum (the hard way)

Do we need theory? nature works anyway!

- UNDERSTANDING
- Cause-effect relationship or why natural phenomena happen!!!!!!

David Hume, philosopher 18th century: heated **water boils every time we try, but how can we be sure that it will boil NEXT time????**

Why theory?

Water boils when heated, but can we be 100% sure that it will boil NEXT time????

WE know:
a) why water boils 100 % (complete theory!)
b) water boiling is a deterministic process, the same cause causes ALWAYS the same effect!

YES WE CAN BE 100 % sure it will ALWAYS boil!!!

Why Models?

Mathematical model:

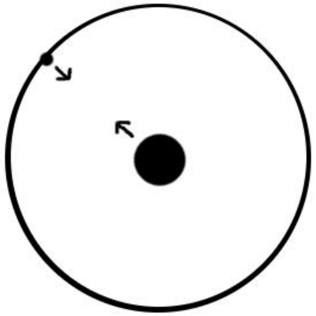
- Reproduction (Ex: Temperature water boils)
- Prediction (Ex: Temperature water boils in a Mountain)
- Extrapolation (to cases/conditions not tried Ex: Temperature water boils in another planet!)

Nature is easy and complicated:

- Easy rules
- but too many interacting complex objects! THEN **COMPUTER MODELLING**

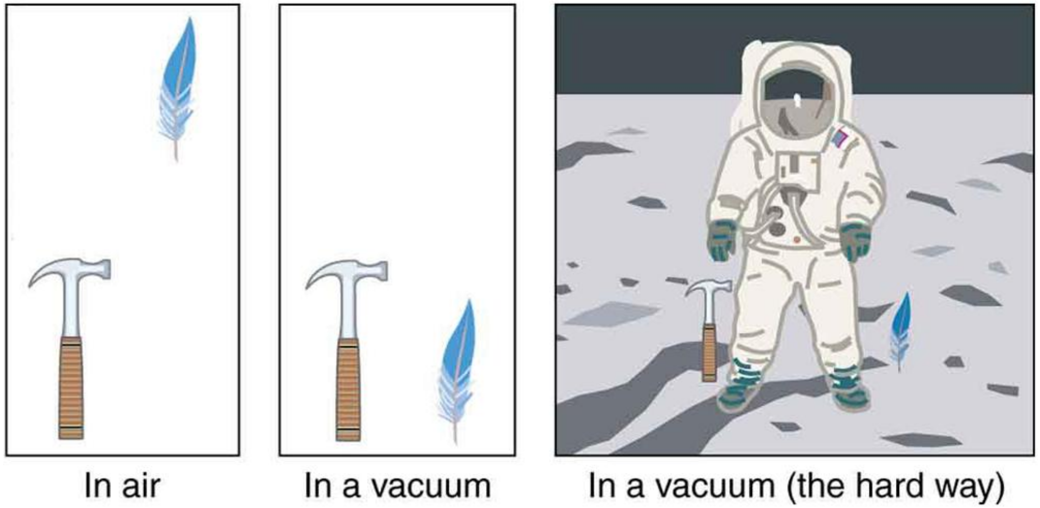
Mathematical models: The two-body problem

The **two-body problem**: motion of two bodies that interact with each other. Examples:



1. Falling object (Galileo)
2. The moon orbiting the earth
3. Electron "orbiting" hydrogen nucleus

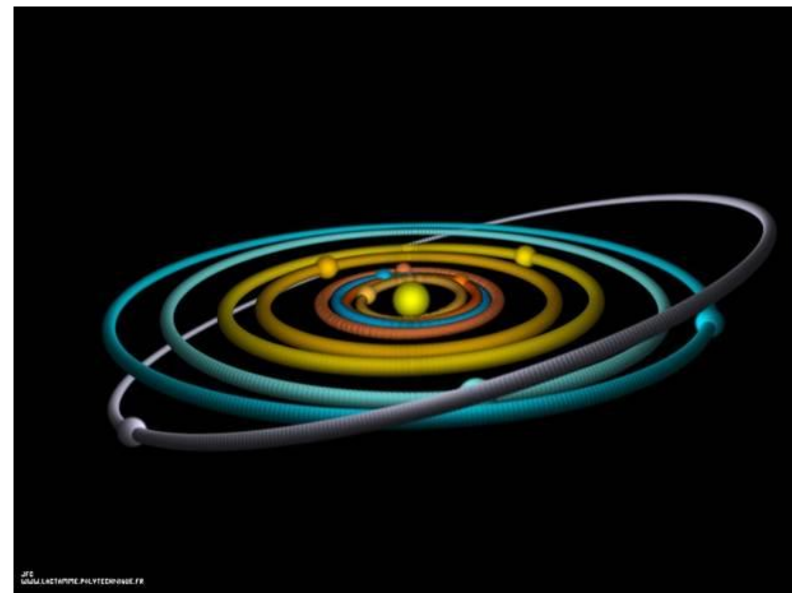
Two-body problem can be solved analytically (i.e **EXACTLY**).
GALILEO DID!



Mathematical models: The n-body problem

The **n-body problem**: motion of three or more interacting bodies. Examples:

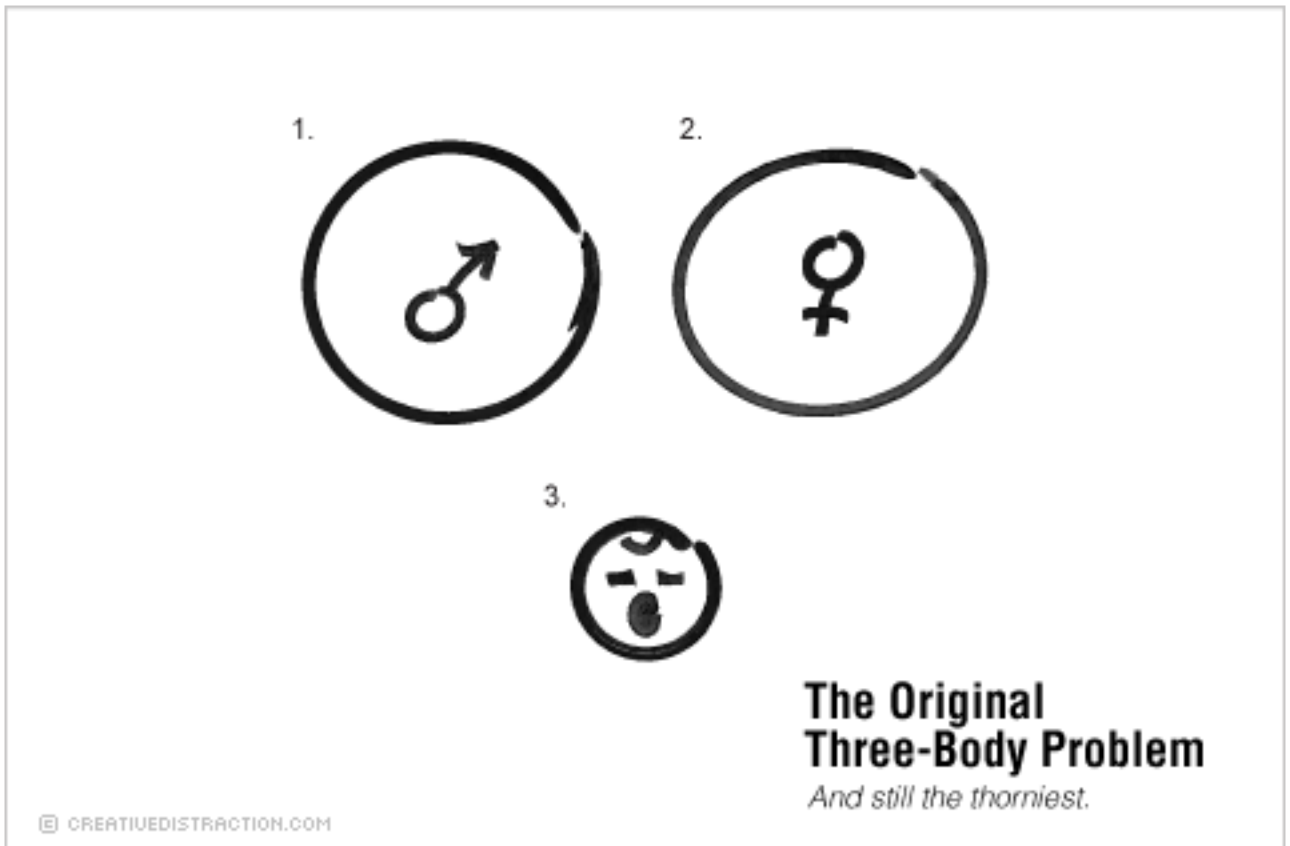
1. The solar System
2. **Electrons and nuclei of ALL atoms** > hydrogen



- n bodies **cannot be solved analytically/exactly** but in few in special cases
- they have to be solved **NUMERICALLY**

The "original" Three body problem

Mother + Father + child = No exact solution, always **approximated**!!!



Numerical vs. Analytical models

Numerical (computers)

1. Approximated
   - Relative precision
2. Only most simple cases are doable by hand (in a reasonable time of course!)
3. **"Easy" to do (with software)**

Analytical (pencil and paper)

1. Exact
   - 100 % accurate
2. Quite powerful, all basis of Quantum Mechanics was done with pen and paper
3. Difficult to do, you have to know how to do them!

Most models in scientific computing are numeric!

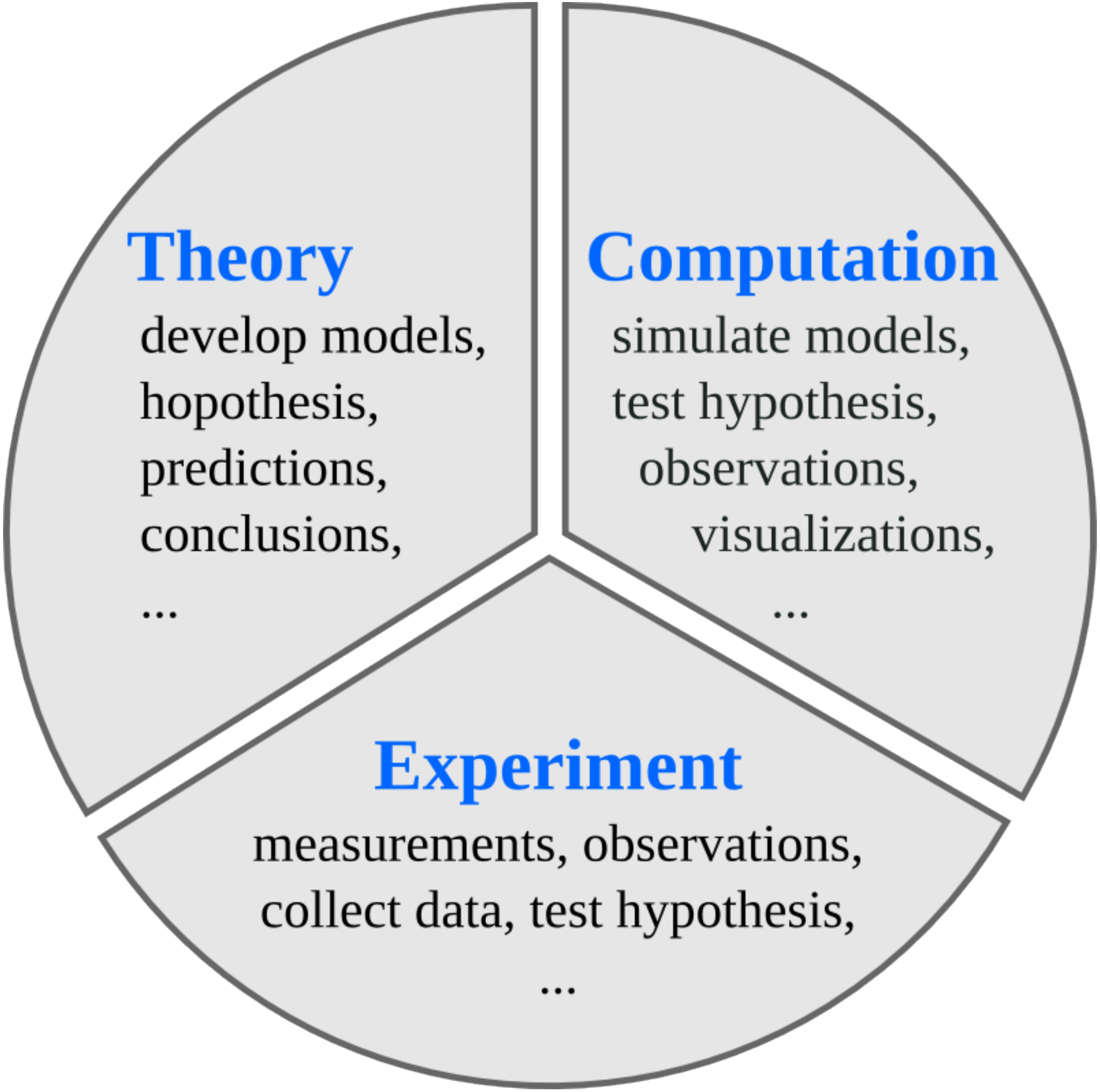
Computer simulation = automatic numerical procedure

- First computer simulation (**1945**):
  - It was a simulation of **12** **hard spheres** (BODIES) to model the process of nuclear detonation during the Manhattan Project in World War II

- State of the art **2005**: a **2.64-million-atom model** of a ribosome (Ribosome is protein that works as a molecular machine that builds proteins from genetic code! **Nature's Nanotechnology**)

- State of the art **2013**: **64 million-atom model** of HIV capsid (a protein shell that protects the virus's genetic material and is a key to its virulence, **Nature's Nanotechnology**)

http://news.illinois.edu/news/13/0529HIVcapsid_KlausSchulten.html


Theory
develop models,
hopothesis,
predictions,
conclusions,
...
Computation
simulate models,
test hypothesis,
observations,
visualizations,
...
Experiment
measurements, observations,
collect data, test hypothesis,
...

Atomistic modelling in natural sciences!

why is High Performance Computing is needed?

Computational, natural, science

- Exponential growth in commodity PC's power:
    - experimental science more EXPENSIVE than ever
    - virtual science is, in comparison, cheaper than ever

~~RESEARCH in virtual theoretical science is very complex, need typically **highly qualified, highly trained, Ph.Ds level researchers!**~~

- ~~**User-friendly software slowly appearing**~~
- ~~**Large high quality HOW-TO needed: computer model of nature can be tricky!**~~

Computational, natural, science

- Current state, amazing powerful PCs!
  - **TODAY**: This **laptop**: i5 M460 @2.53GHz = 2x4x2.53 = **20 gigaFLOPS** (theoretical)
  - **15 years ago**: One of the 500 fastest, **parallel, computers of the world!** (www.top500.org)
  - The first system to achieve **1 petaFLOPS [peta=10**15] (2007):** distributed computing using PS3 and PCs(GPUS) **folding@home** [folding proteins!]

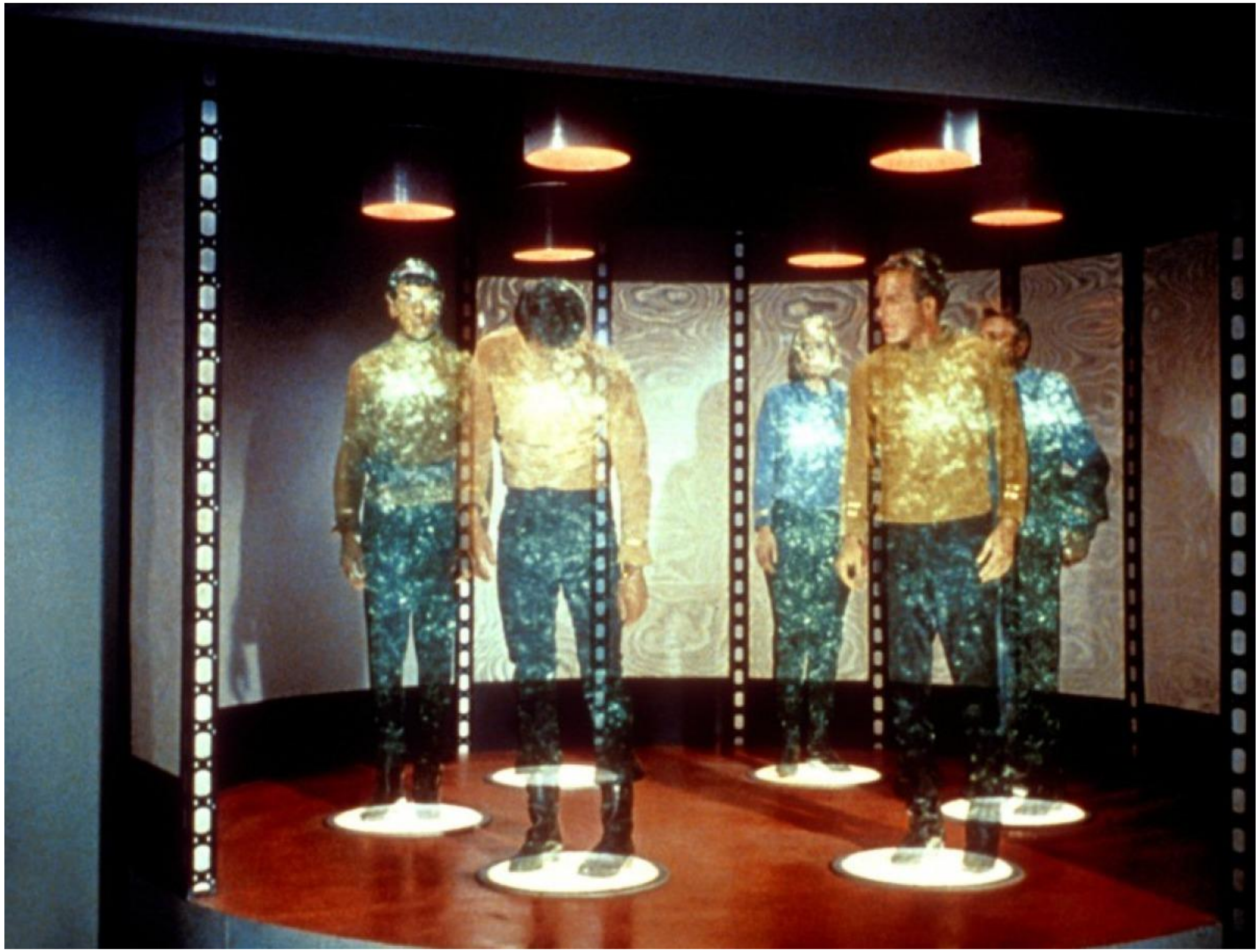
I started doing this in **1996**, **1st generation pentium PC with first linux distribution in FLOPPIES! REALLY SLOW, but revolutionary, UNIX machine really cheap!**

"Beam me up Scotty!"

Molecular Models: a way to "digitalize" matter, yet not like **Star Trek teletransport**!

Persons or non-living items would be placed on the transporter pad and are dismantled particle by particle by a beam with their **atoms being patterned in a computer buffer** and converted into a beam that is directed toward the destination, and then reassembled back into their original form (usually with no mistakes).

Possible or Science FICTION?



Digitalizing the real world (SIZE)

- Teletransport: Knowing the 3D position of all “things” that form an object or person
- At least atomic resolution (all molecules have to be right!).
- DNA wrong -> wrong biochemistry!!!
- Example:
  - The tip of a pencil: 1 gram of graphite!
  - How many hard drives??

Digitalizing the real world (SIZE)

- 1 gram of carbon has ~5 x 10^{23} atoms
- The position in space of atoms in **1 gr carbon** in single precision (4 byte):
  - 6 x 10**24 bytes = (SI) 6 yottabytes
  - **6 million millions** of hard drives (1 TB)
  - piling up laptop HDs (1km HDs= 100000 TB):
    - 1 yottabyte = 10**12 HDs=10 million kms of HDs

1 gram of carbon 10 million kms of HDs!!!

Earth diameter is ~ 12000 km

Digitalizing the real world with atomic resolution (SIZE!)

Models of graphite Impossible? **NO!**

- Due to the way atoms pack in matter (very redundantly *in many cases*):
  - Many properties of **carbon (graphite)** can be described by an infinite system:
    - **2 C atoms** + mathematical tricks!!!

- Information theory: Crystals highly ordered, very low Shannon Entropy!!!

Digitalizing the real world with atomic resolution (SIZE!)

- Interesting to model explicitly large sizes?
  - 1 gr carbon = 5 x 10^{22} atoms (modelling BORING!!!)
  - 1 human brain = 10^{11} cells (modelling **exciting!**)*.

*:http://www.guardian.co.uk/science/blog/2012/feb/28/how-many-neurons-human-brain

Digitalizing the real world with atomic resolution (TIME!)

- ~~Most molecules in our body are built with light atoms (H, C, O, N)~~

Models moving atoms?

- Atoms move very fast:
  - Time in numerical models is discrete (steps)
  - require timescales <= 1 fs (10^{-15} seconds).
  - Discretize time in steps of 1 fs!

Digitalizing the real world with atomic resolution (TIME!)

Different important molecular processes happen in different time scales:

- **1 nanosecond 10^6 iterations**.
- 1 microsecond 1**0^9 iterations**

- **Miliseconds**, like protein folding, are now reached with supercomputers for small, few atoms, systems **(10^{12} iterations)**.
- 1 second doable with a dedicated petaFLOP computer!

~~**NOTICE that it is not enough simulating a second, IT HAS TO BE a second where something very interesting**~~

Digitalizing the real world , why HPC computers? SUMMARY

- Many iterations:
  - Large scales:
    - Size: Simulations of millions of atoms
    - Time: ms simulations
    - Size & time
  - Very complex methods:
    - Quantum mechanical methods.
      - Simulation with explicit electrons can be several orders of magnitude heavier to calculate

Nobel prize of chemistry 2013
Theoretical Chemistry

- MULTISCALE MODELLING: combine classical and quantum models to study chemical reactions very in large molecules (pr

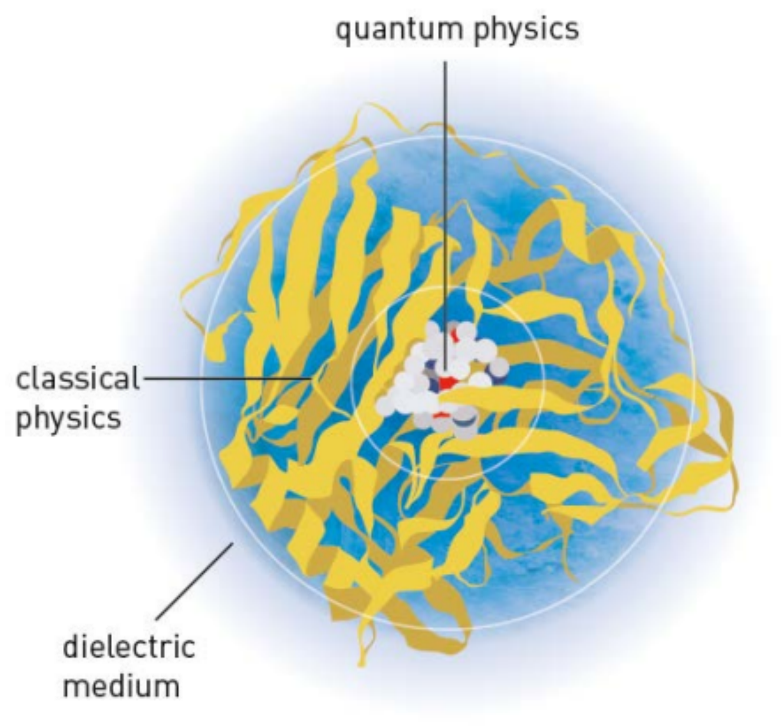


Figure 1

Figure 1 Multi-copper-oxidase embedded in water [1].

Computing natural sciences

Natural Scientists vs. computer scientists!

Computational vs computer scientists?

Computer scientists (ex):

- Formal education programming (C, C++, etc)
- Profilers, debuggers, ...
- (**Should**) understand processor architecture
- Cannot admin a unix machine!

Natural computaional scientists (ex):

- Some, cheap, self-taught programming (matlab, fortran, python, ...)
- what?
- WHAT????
- Most computational natural scientists can admin a Unix Machine.

Natural vs computer scientists?

Natural scientists (ex):

- (Should) know GOOD physics/chemistry/biology
- what algorithms are better
- Know what is the main purpose of simulations: **WHY!!!**

Computer scientists (ex):

- WHAT??????
- what????
- what??????

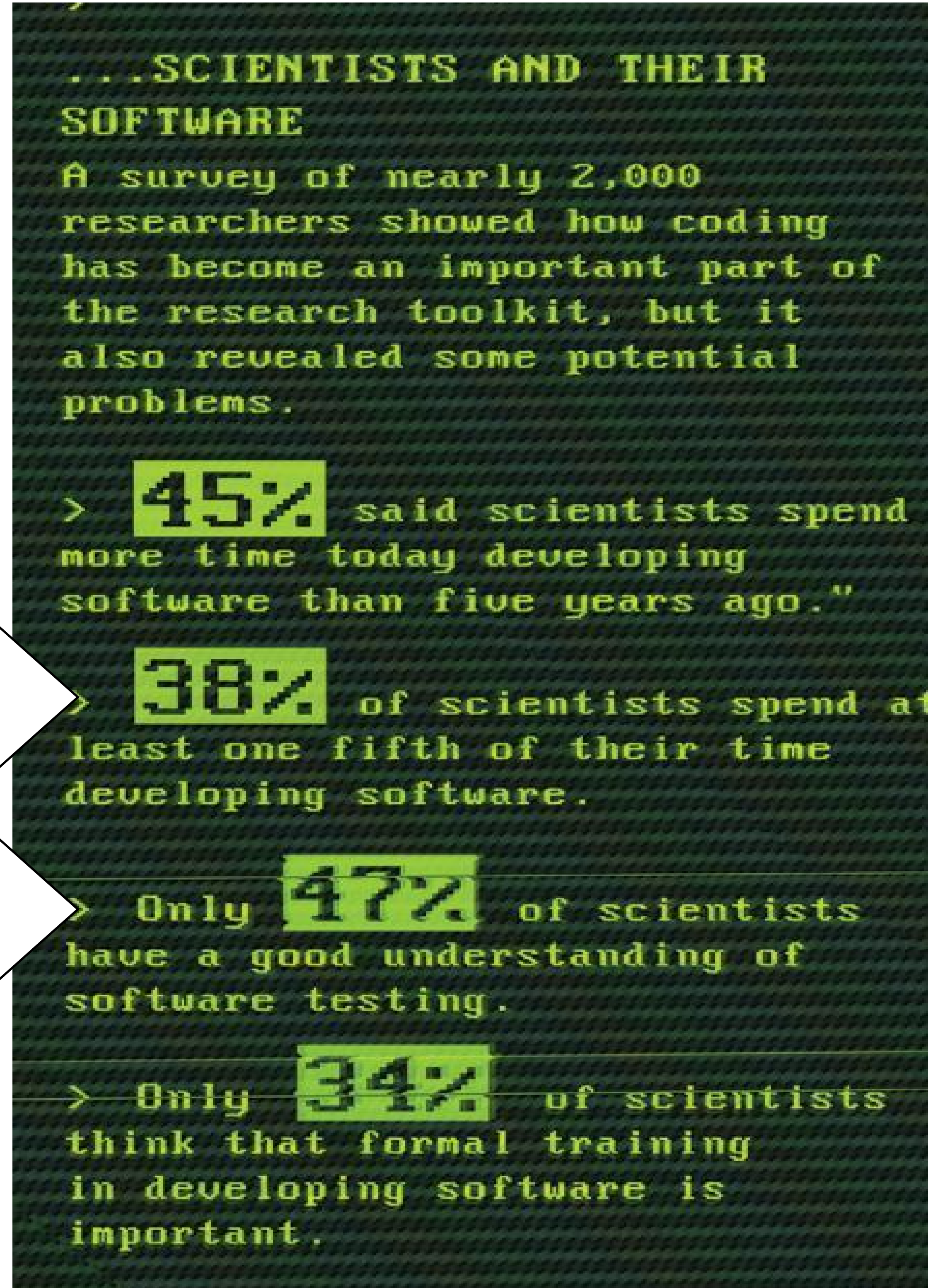
Most scientific codes are written developed and extended by

Natural scientists

Is this good?????

Computational science: ...Error …why scientific programming does not compute.

Zeeya Merali



Published online 13 October 2010 | **Nature** 467, 775-777 (2010) | doi:10.1038/467775a
News Feature

Publish your computer code: it is good enough Nick Barnes

Published online 13 October 2010 | **Nature** 467, 753 (2010) | doi:10.1038/467753a

I am a professional software engineer and I want to share a trade secret with scientists: **most professional computer software isn't very good**. The code inside your laptop, television, phone or car is **often badly documented, inconsistent and poorly tested.**

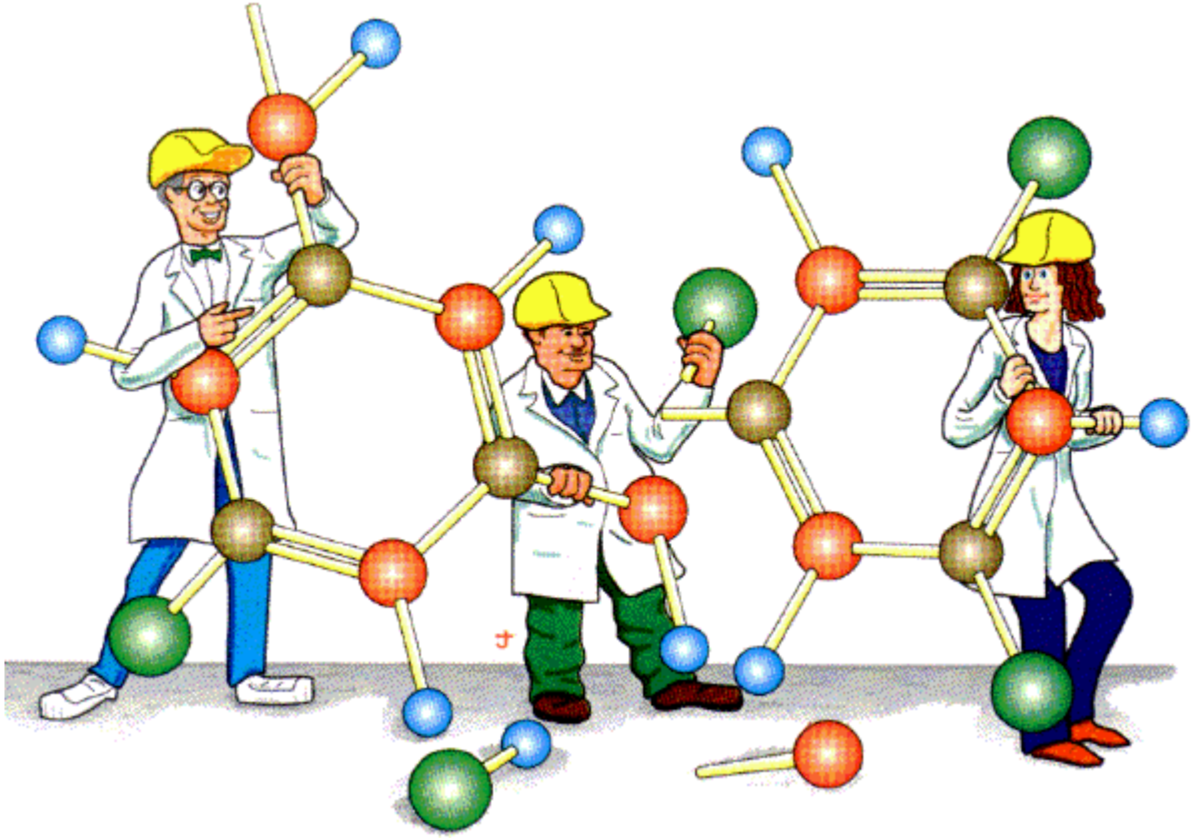
... And you scientists generally think **the code you write is poor**. It doesn't contain good comments, have sensible variable names or proper indentation. It breaks if you introduce badly formatted data, and you need to edit the output by hand to get the columns to line up. **It includes a routine written by a graduate student which you never completely understood**, and so on. Sound familiar? **Well, those things don't matter.**
That the code is a little raw is one of the main reasons scientists give for not sharing it with others. Yet, **software in all trades is written to be good enough for the job intended**. So if your code is good enough to do the job, then it is good enough to release — and releasing it will help your research and your field.

Most scientific codes are written developed and extended by

Natural scientists

Is this good?????

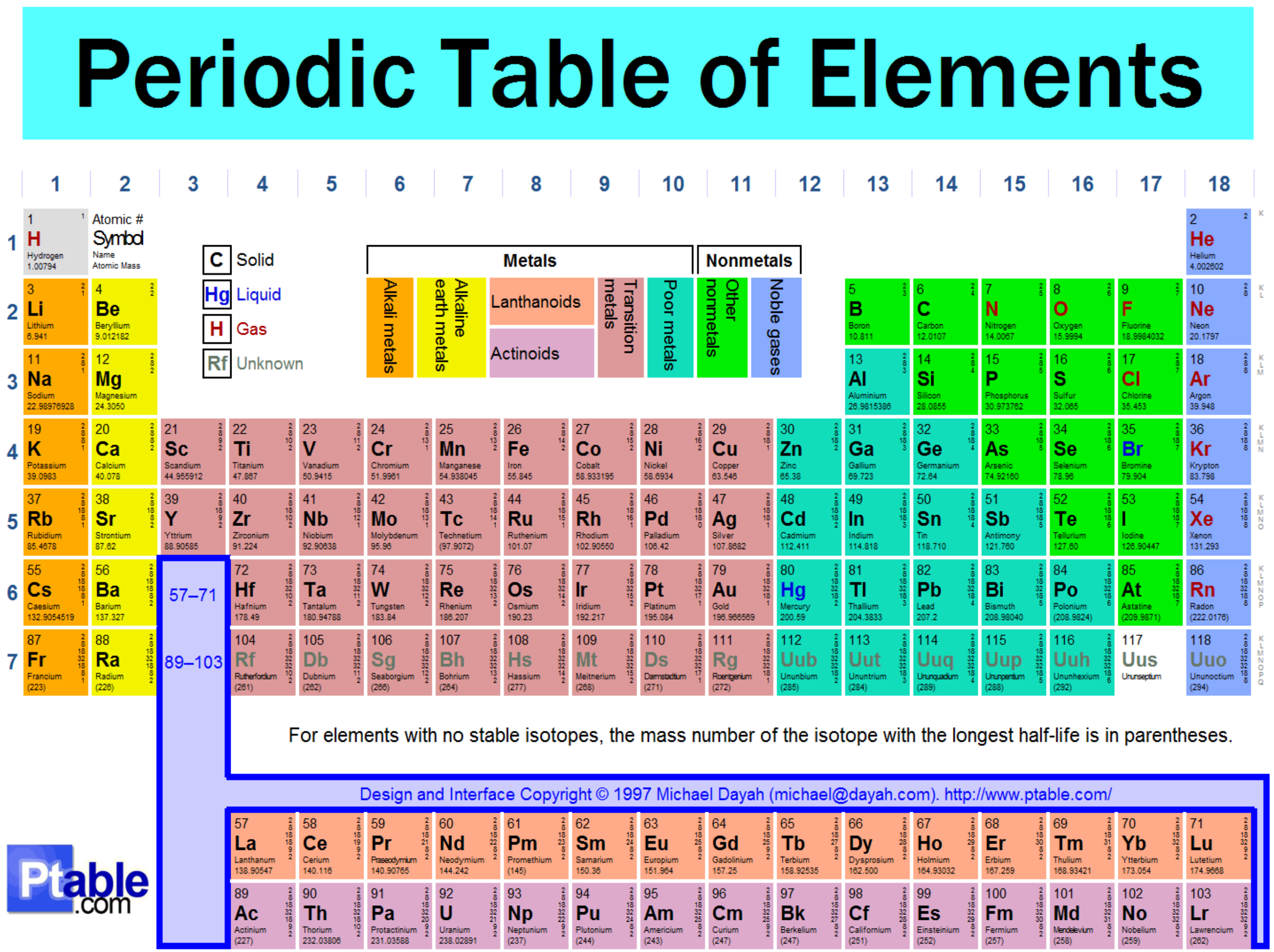
If it works, IT must be GOOD!!!!

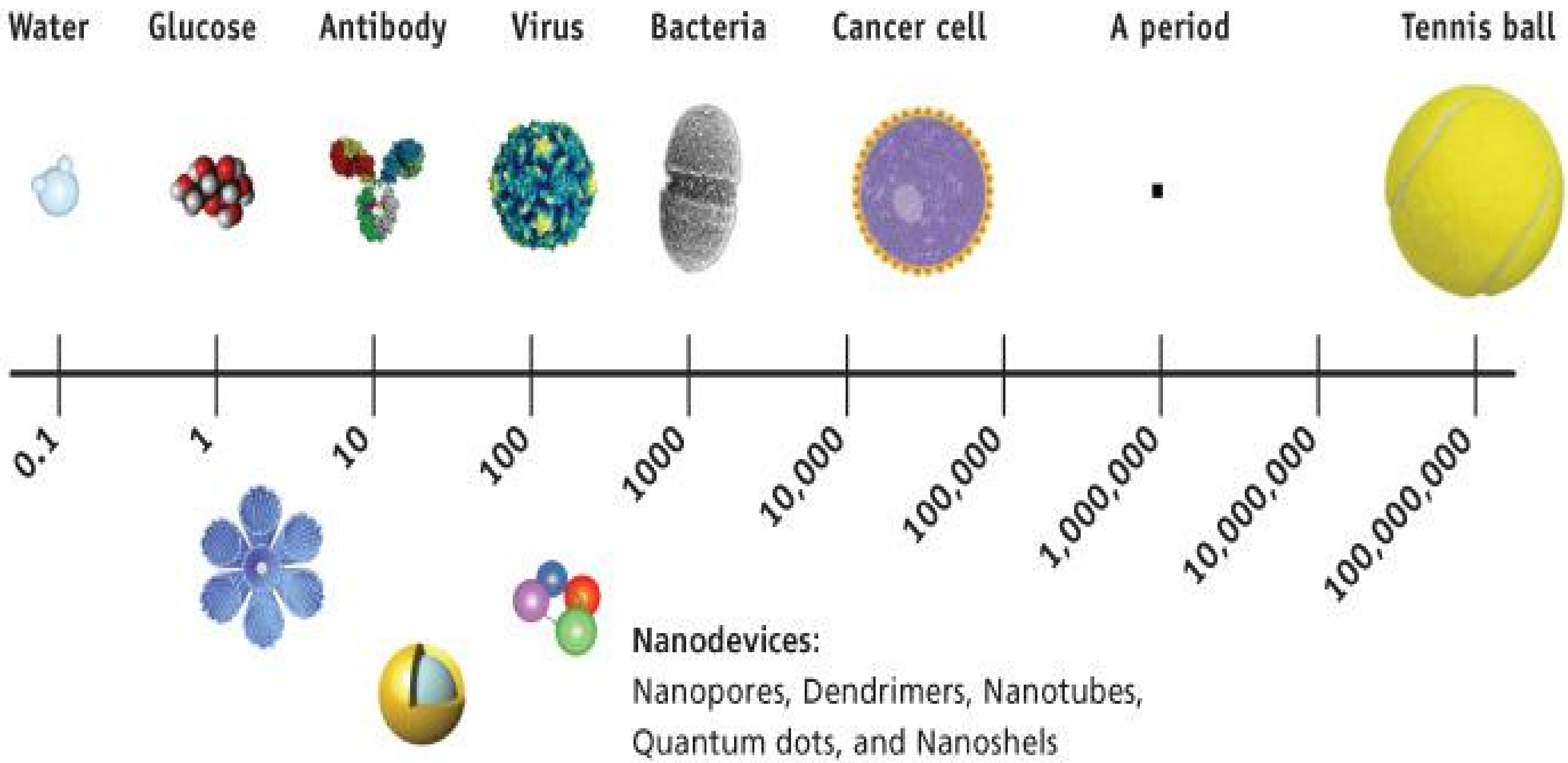


Computer modelling of carbon **nano**materials

Nanotechnology **(smallest tech!!!)**

- **Nanotechnology** is the manipulation of matter on an atomic and molecular scale (**Wikipedia).**





Nanometer **Chart**

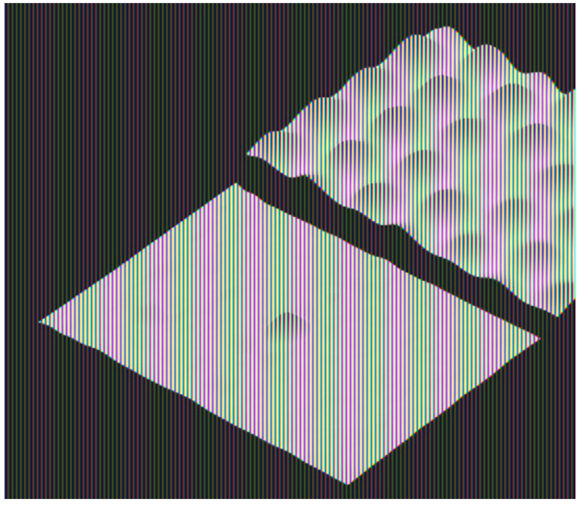
how small can we see?

- If we are to manipulate atoms we have to know and control their positions in space!
- can we see atoms?
- with a microscope?

how small can we see?

- can we see atoms with a microscope?
  - **Using light NO,** best resolution with visible light 200 nm (atom ~ 1 nm))

- But we can "feel them" like blind people reading braille!



- Electron microscopy:
  - **Electrons smaller wavelength than light**
  - **higher resolution!!**

Start of Nanotechnology

- In 1986 single atoms could be directly *imaged* for the first time with Scanning Tunneling Microscopy **(STM)**

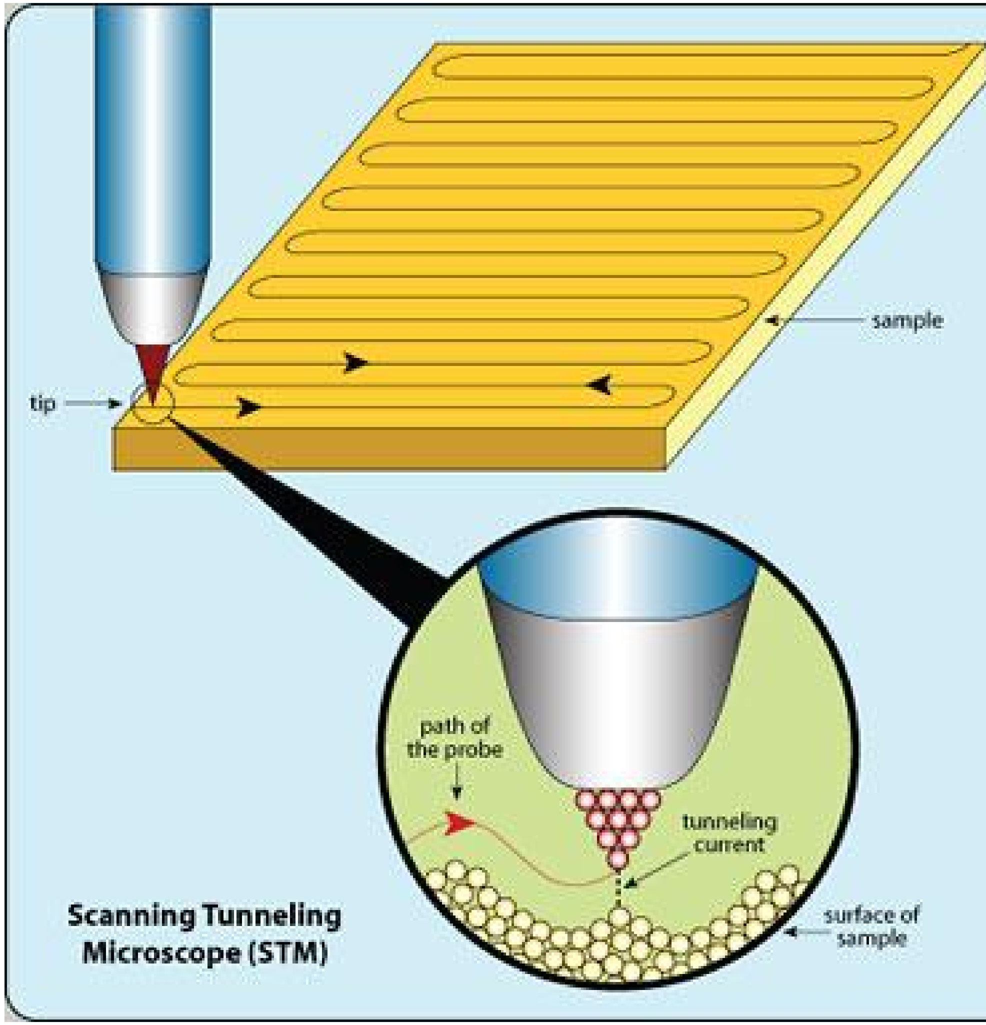
- **HUGE BREAKTROUGH:** Gerd Binnig and Heinrich Rohrer, Nobel Prize of Physics **same year!**

- Very good Description:

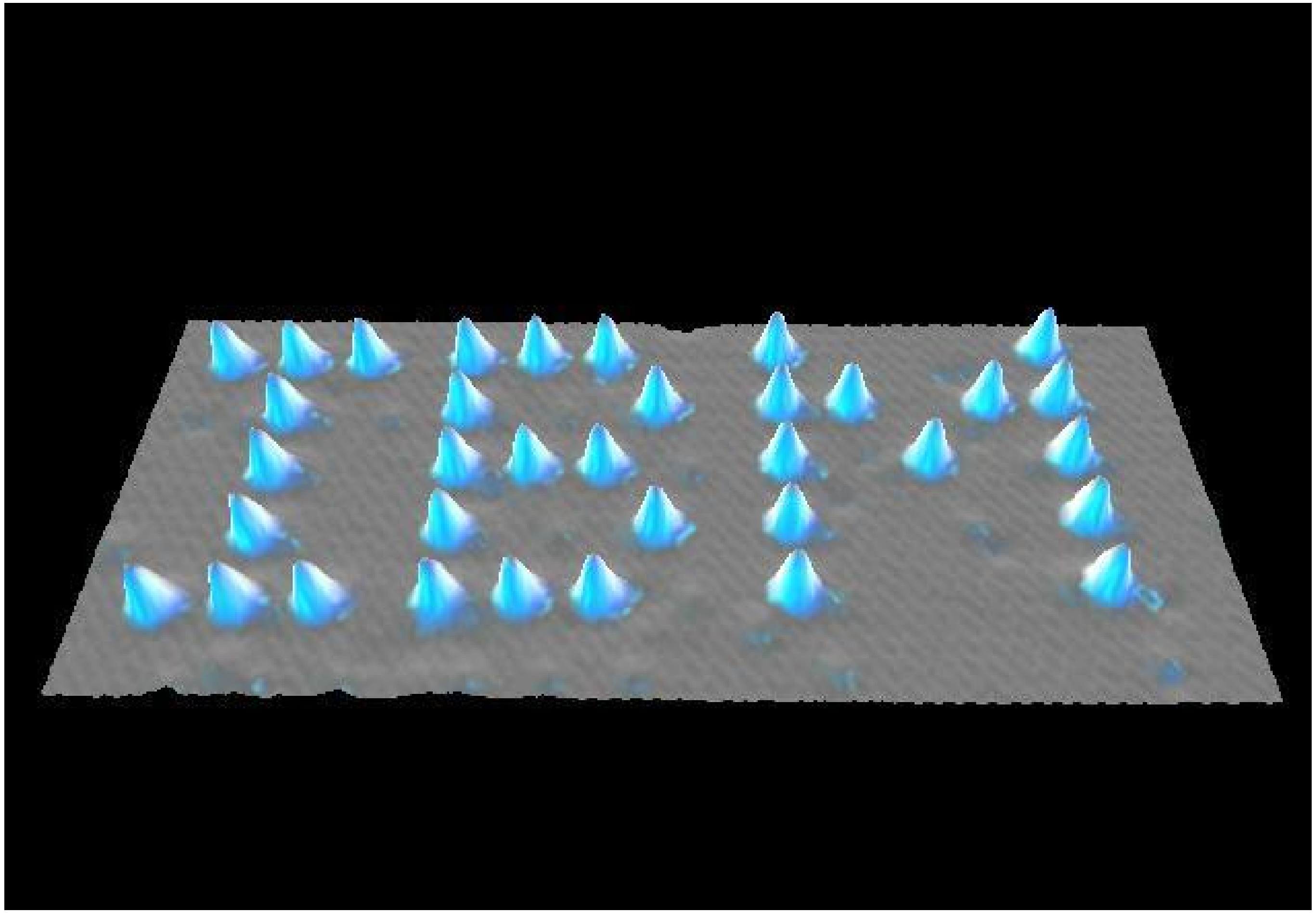
http://www.nobelprize.org/nobel_prizes/physics/laureates/1986/press.html

Scanning tunneling Microscopy

- a mechanical device is used to sense the structure of a surface like **braille-reading** (the reader's fingers that detect the impressed characters).
- the surface is traversed by a probe a distance from the surface (to not alter it) the vertical movement of which is recorded.



The world smallest corporate logol



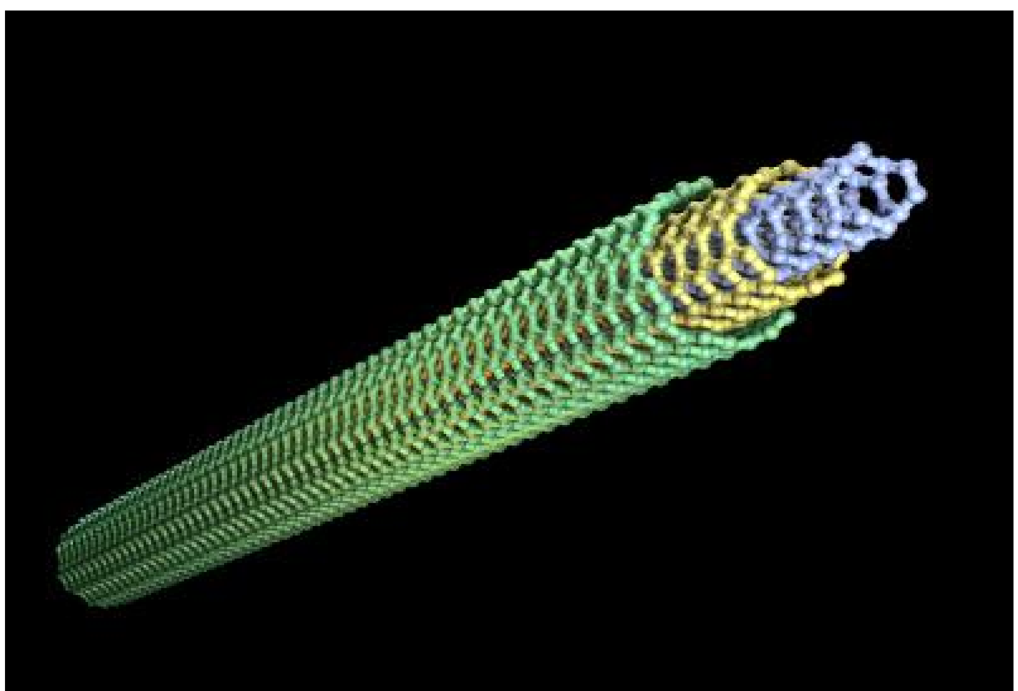
STM "images" grid data of the surface

1989 – first to controllably **manipulate individual atoms** on a surface, using the **STM** spell out "I-B-M" by positioning **35 xenon atoms** [on a Nickel (110) surface]

D.M. Eigler, E.K. Schweizer. **Positioning single atoms with a scanning tunneling microscope.** *Nature 344, 524-526 (1990)*

Nanotechnology

- Nanometer
  - 10^{-9} meters (1 millionth of 1 mm)
  - 1-2 atom diameters
- Nano-object example: carbon **nano**tube:
  - long millimeters: macroscopic (axis)
  - thick nanometers: **nano** (diameter)



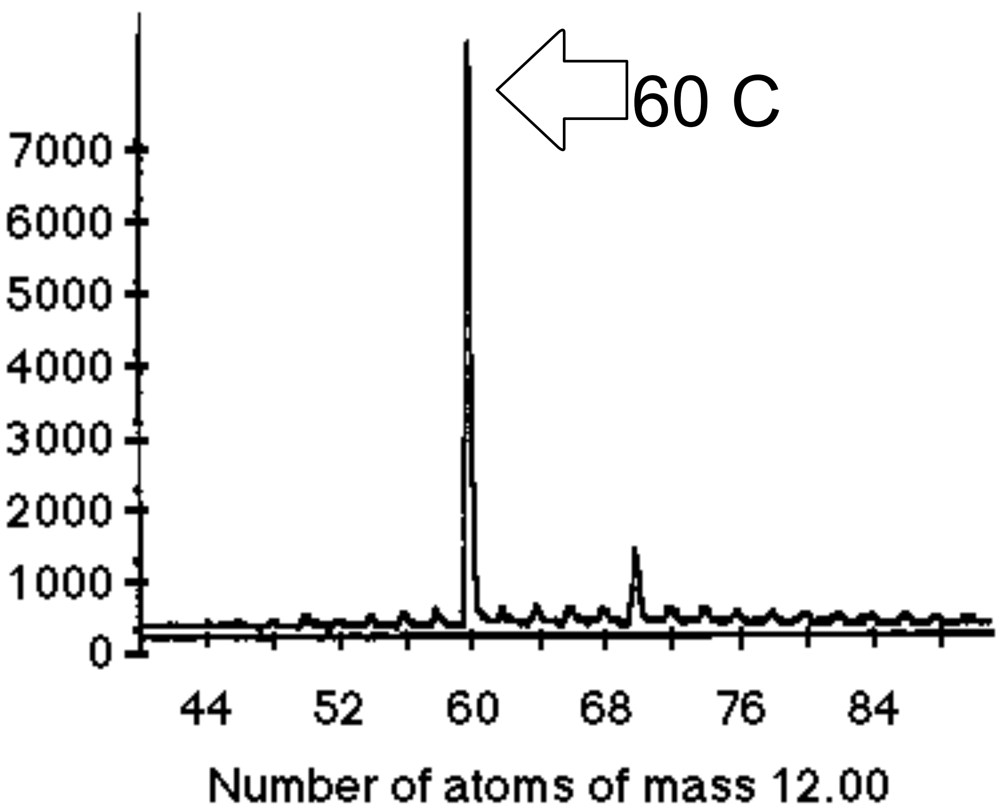
Carbon nanotechnology started in space!

- In **1985**, British chemist Harry Kroto was puzzling over strange chains of **carbon atoms** that could be **detected billions of kilometres** away in space by **radiotelescopes**. He thought that these chains might form in conditions that are found **near** red giant **stars**. **[Science is AMAZING isn't it?]**

- Kroto visited the US laboratory of Richard Smalley and Robert Curl, who were studying 'clusters' – aggregates of atoms that only exist briefly. Together they attempted to **create high-temperature conditions in the laboratory, conditions similar to those near red giants**. They vaporised graphite with a powerful laser in an atmosphere of helium gas.

Buckyballs history

- They did mass spectra of the sample and found a very large peak for **60 C atoms** (with another smaller for 70 C atoms), that was the first buckyball [(Nature 318, 162)]



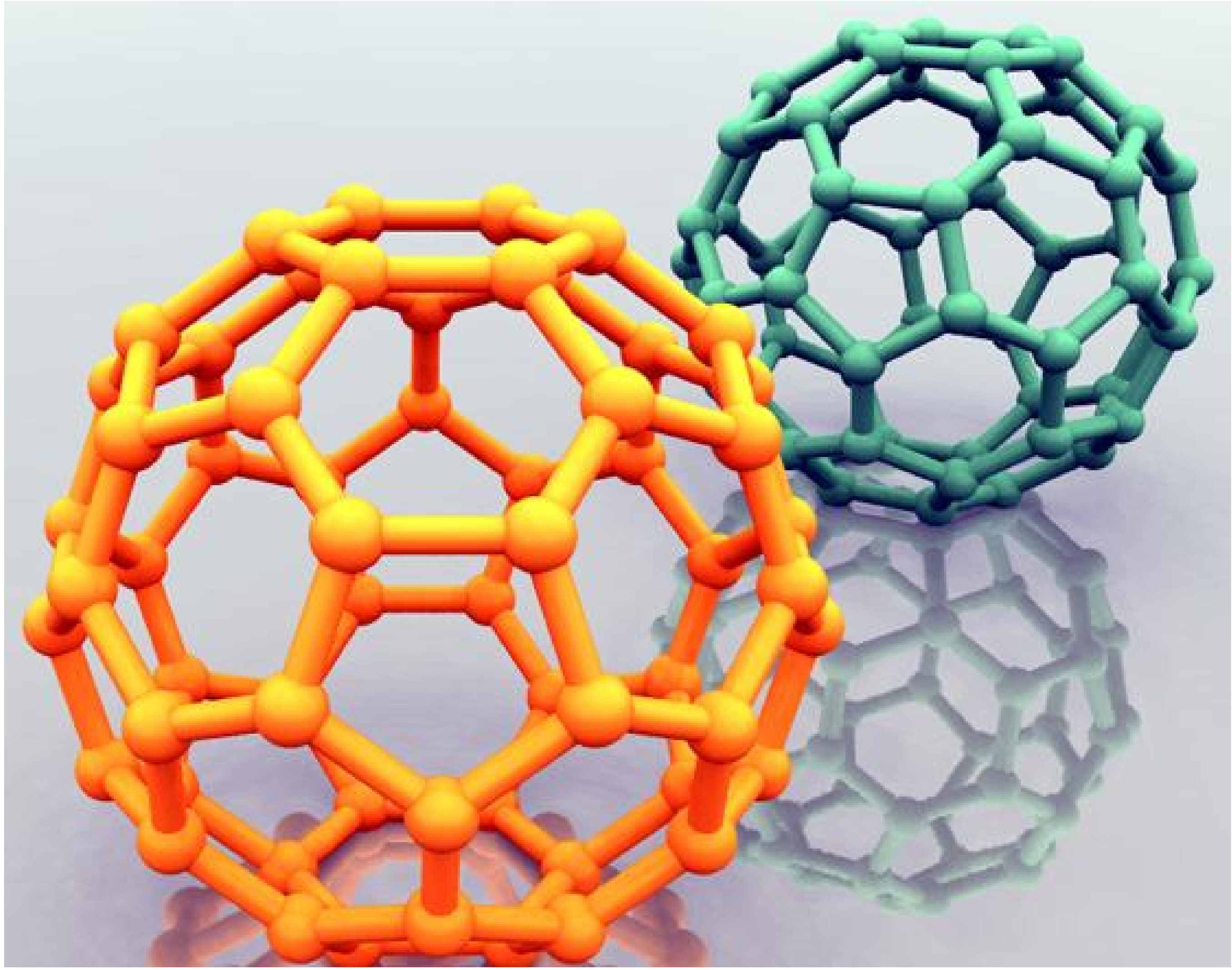
Finding the structure (how the atoms are connected in the molecule)?

They assumed the molecule was spherical ~~(as it was chemically very stable, not dangling bonds, and have only carbon)~~

Could not find the structure, as last Smalley resorted to **a paper model by cutting out paper pentagons and hexagons in which he tried to stick them together so that the figure had 60 vertices (60 atoms)**. Smalley found a sphere made out of 12 pentagons interlocking 20 hexagons to make **a football ball**. That was really the C_{60} structure, as found later, and the **nobel prize for 1996**!

Apparently Smalley did the interpretation in 11 days!

He was very lucky: really there are 1811 other possibilities he did not find (C60 is the most symmetrical



Fullerene C_{60} 1nm Diameter spherical molecule
or
the **NANO**-football ball!

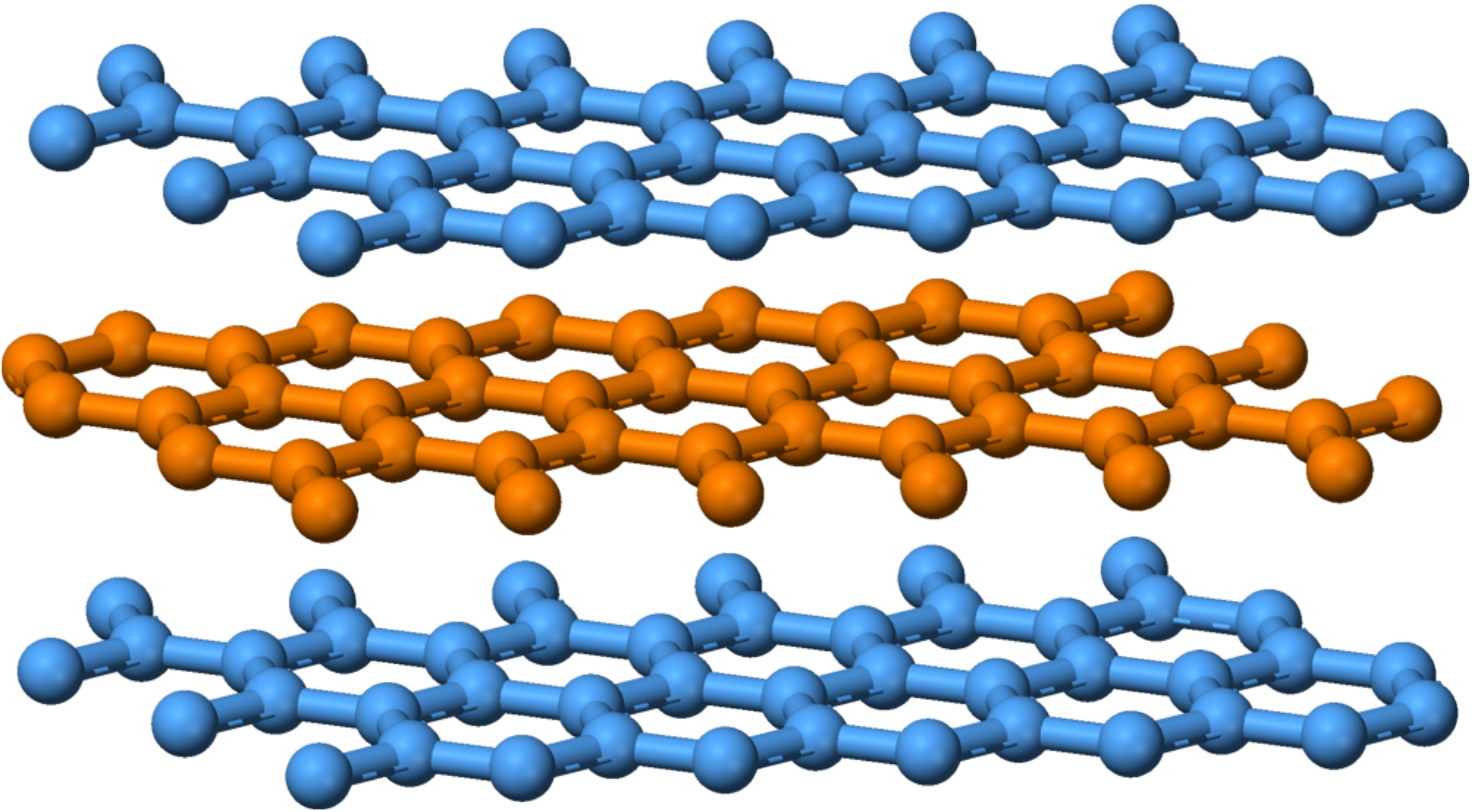
Graphite

- THE carbon Mineral
  - Thermodynamically **the most stable form of carbon**
    - Found in large quantities in nature
    - **diamond turns into graphite if you wait long enough** (extremely slowly)!!!

Many technological applications (historical and contemporary):

- pencils!
- electrical applications (lamps, electrodes, first speakers and microphones...)

Graphite Structure

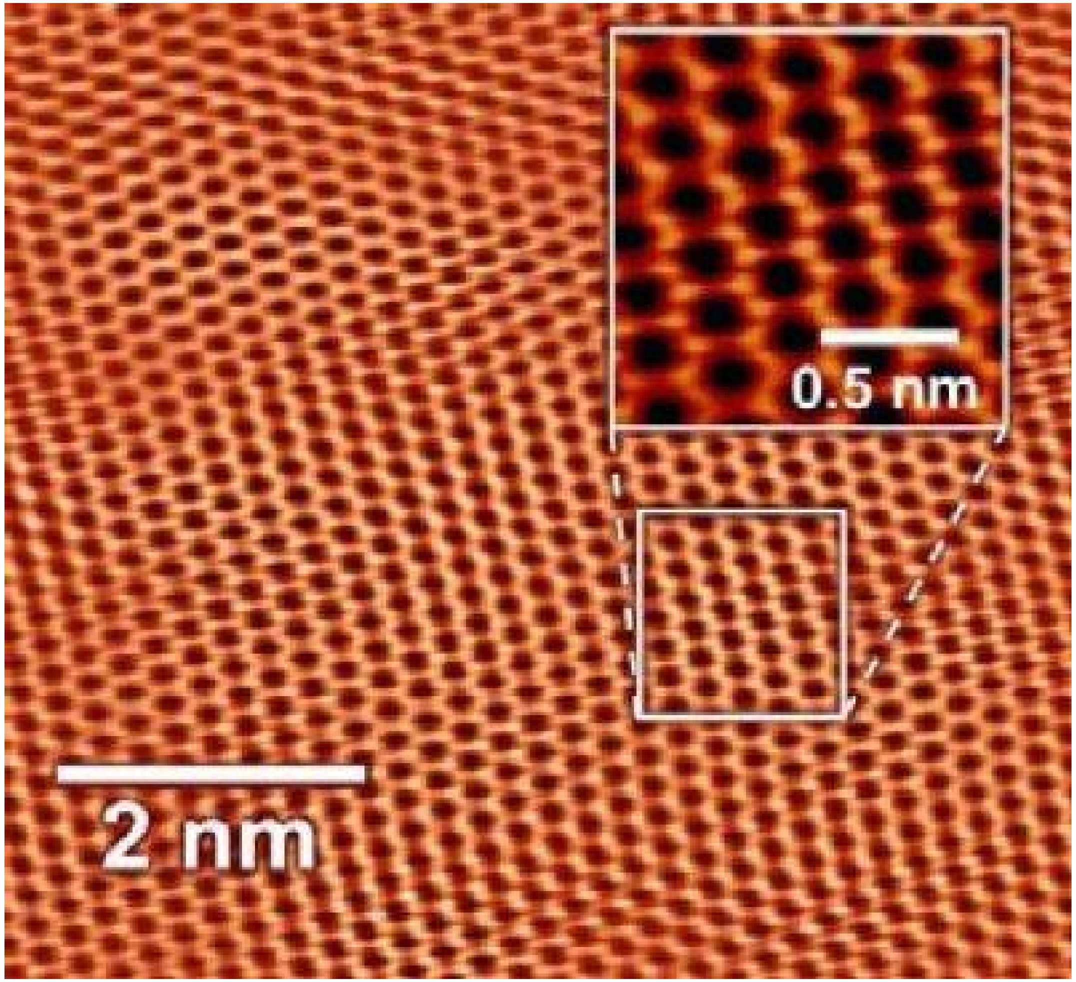


Layered structure, carbon (sp^2) layers 0.35 nm apart

The most stable form of carbon (diamond goes to graphite with time!!!)

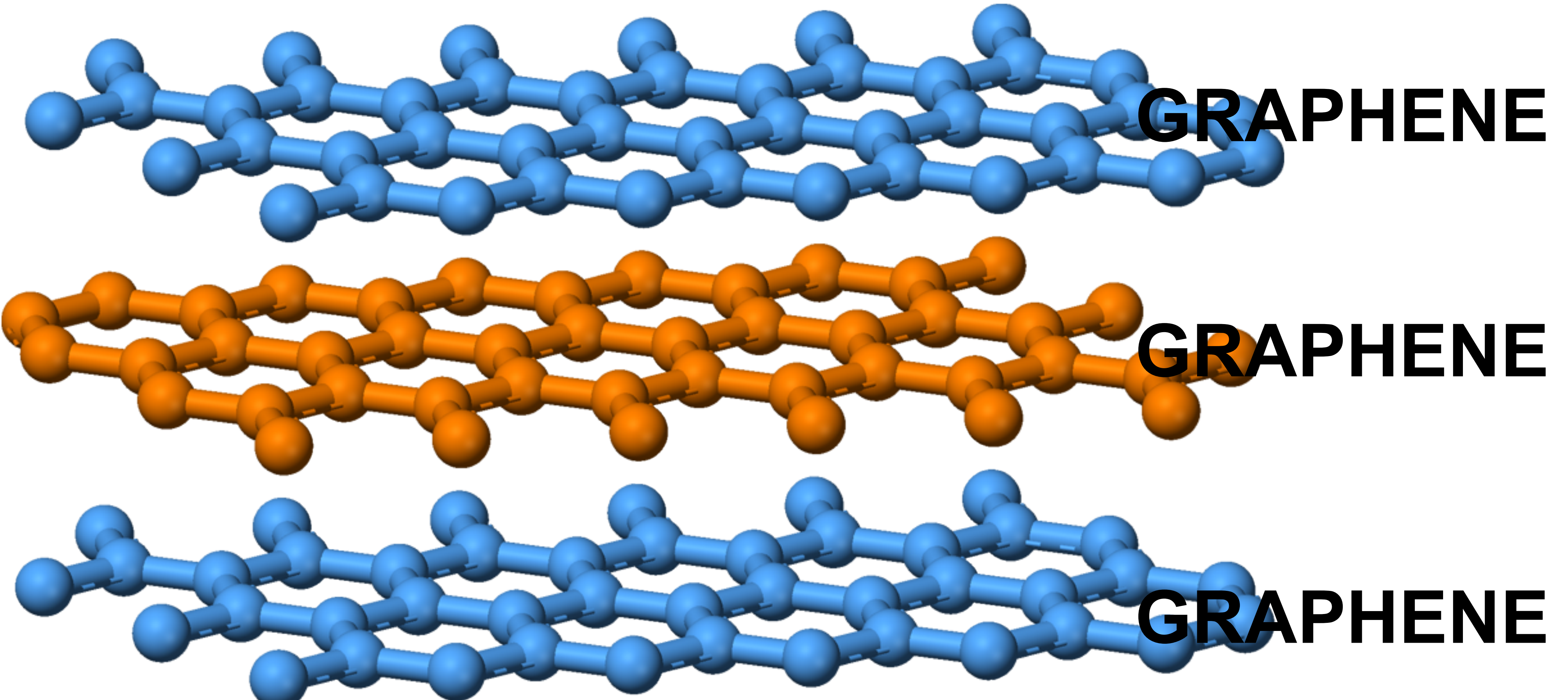
Graphite surface

- Atomic resolution STM image (easy to do in graphite!)



- Electron Microscopy great BREAKTROUGH 25 years but still a very difficult technology!
-Fullerene seen in microscopy at atomic resolution only RECENTLY (good for regular flat surfaces)

Graphite/Graphene Structure



Layered structure, carbon sp^2 layers 0.35 nm apart, **graphene 1 atom thick 2D materials (Physics NP 2011)**
Nuno Peres (U. Minho!) collaborator of NP winners!

The finding of graphene

Graphene -> 1 layer graphite

In **2004**, graphene was obtained first by **mechanical exfoliation** of graphite. They used **Scotch tape** to repeatedly split graphite crystals into increasingly thinner pieces. The tape with attached optically transparent flakes was dissolved in acetone and, after a few further steps, the flakes including monolayers were sedimented on a Si wafer. Individual atomic planes were then hunted in an optical microscope. First of a series of science and nature papers on the topic!!!!

2004? why?
Before it was "impossible"!!!! (more on a minute).

why it was impossible?

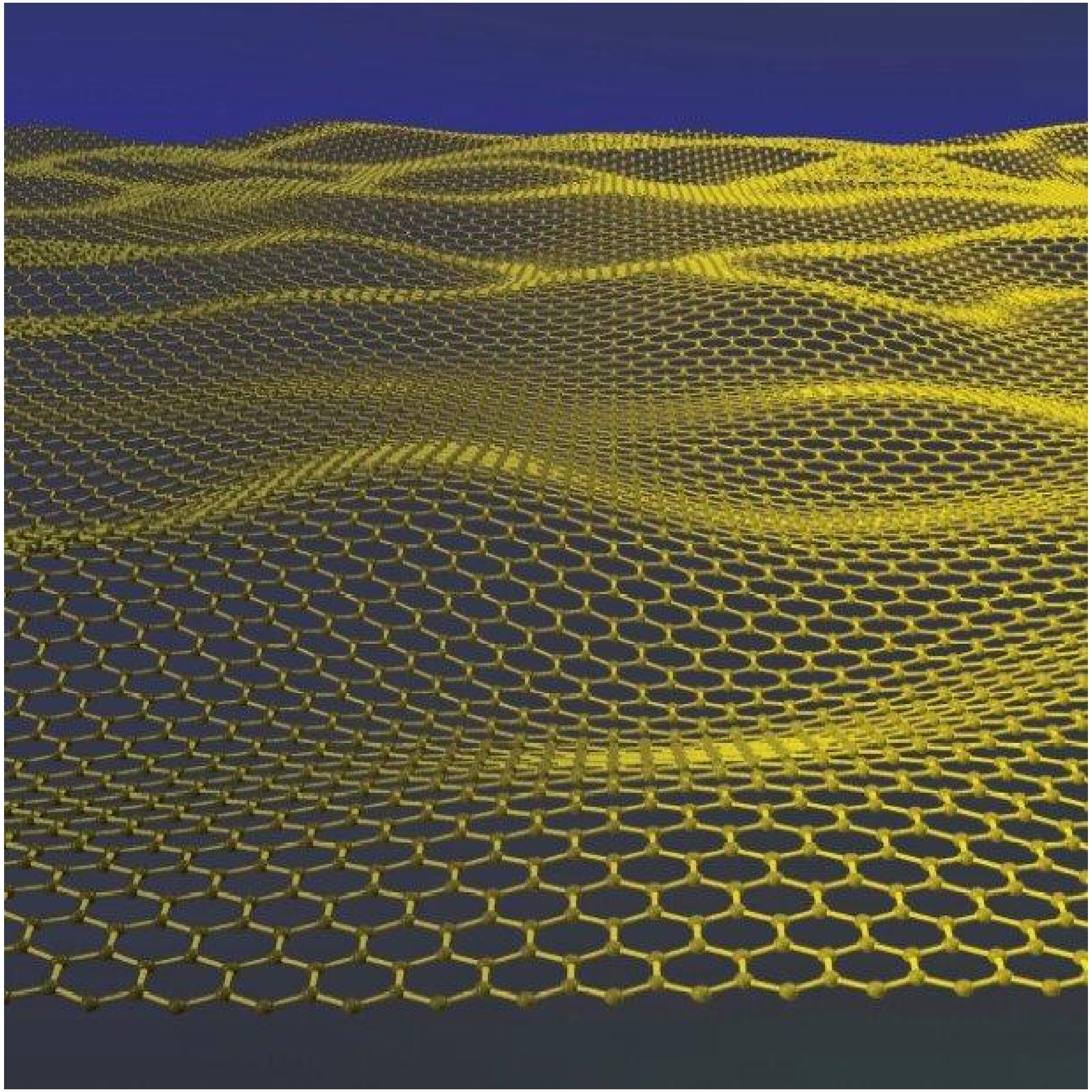
- **Perfect two-dimensional crystals cannot exist in the free state!**

Experimental evidence it was 1 atom thick material, so not impossible!

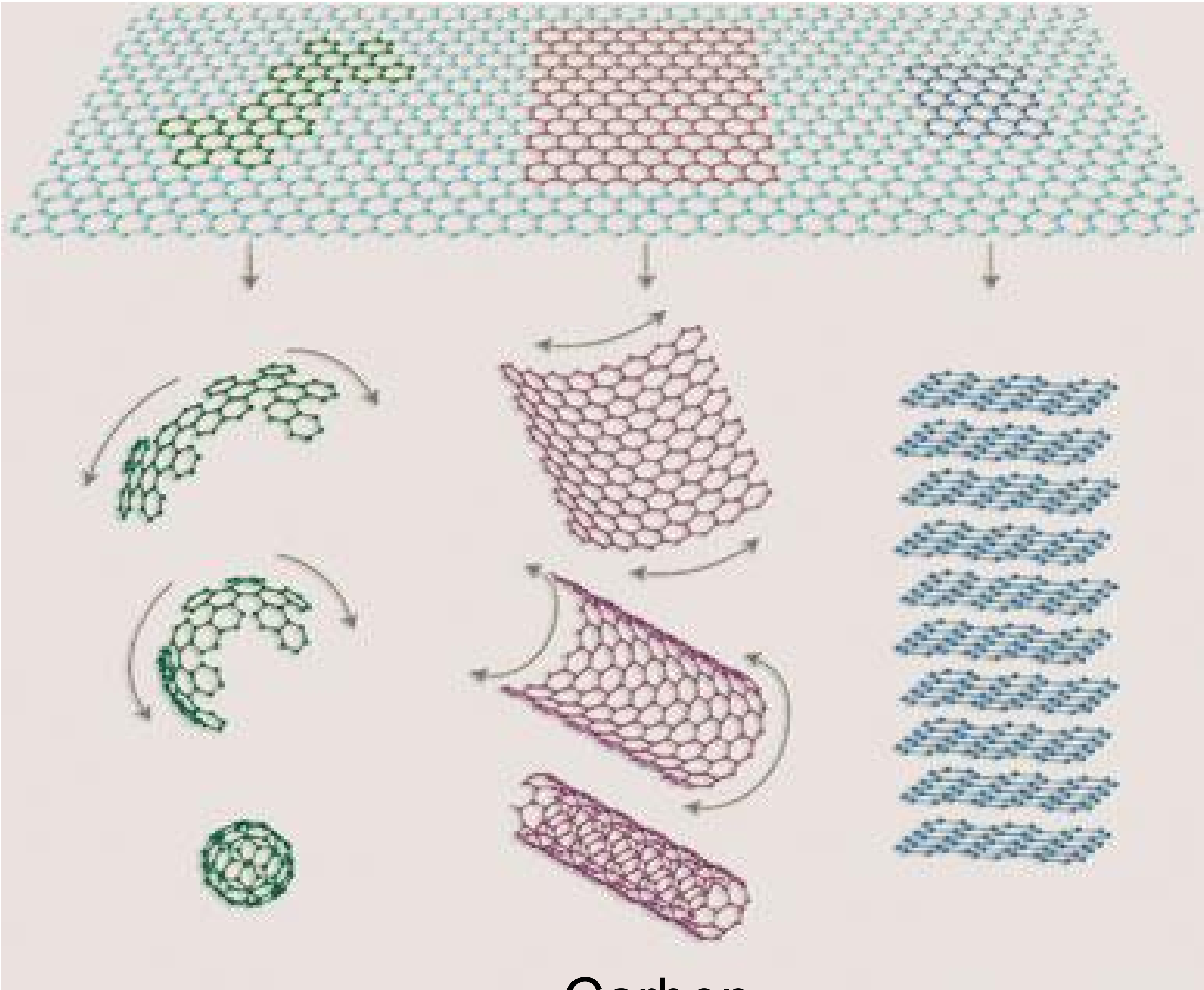
HOW?

graphene structure

- ondulated/wavy structure!
- it is not 2D but 3D!!
- Unexpected, quantum chemistry predicts graphene to be FLAT!



Carbon **nano**materials



Buckyball

Carbon Nanotube

Graphite

Graphene!

Common chemical bricks (Csp2!)

They all exist and are routinely synthesized!

Research in carbon **nano**materials

- Fullerenes, discovered **1985** > 10000 research articles
- Carbon nanotubes, discovered **1991**, > 70000 articles.
- Graphene, discovered **2004**, > 10000 articles.

Two nobel prizes:
- chemistry (1996)
- physics (2011)

Discovered = Clearly observed (latest development in high atomic resolution microscopy, crutial tool for nanotechnology)

1 hundred thousand PR papers, in 25 years, extremely active fields of research, why?

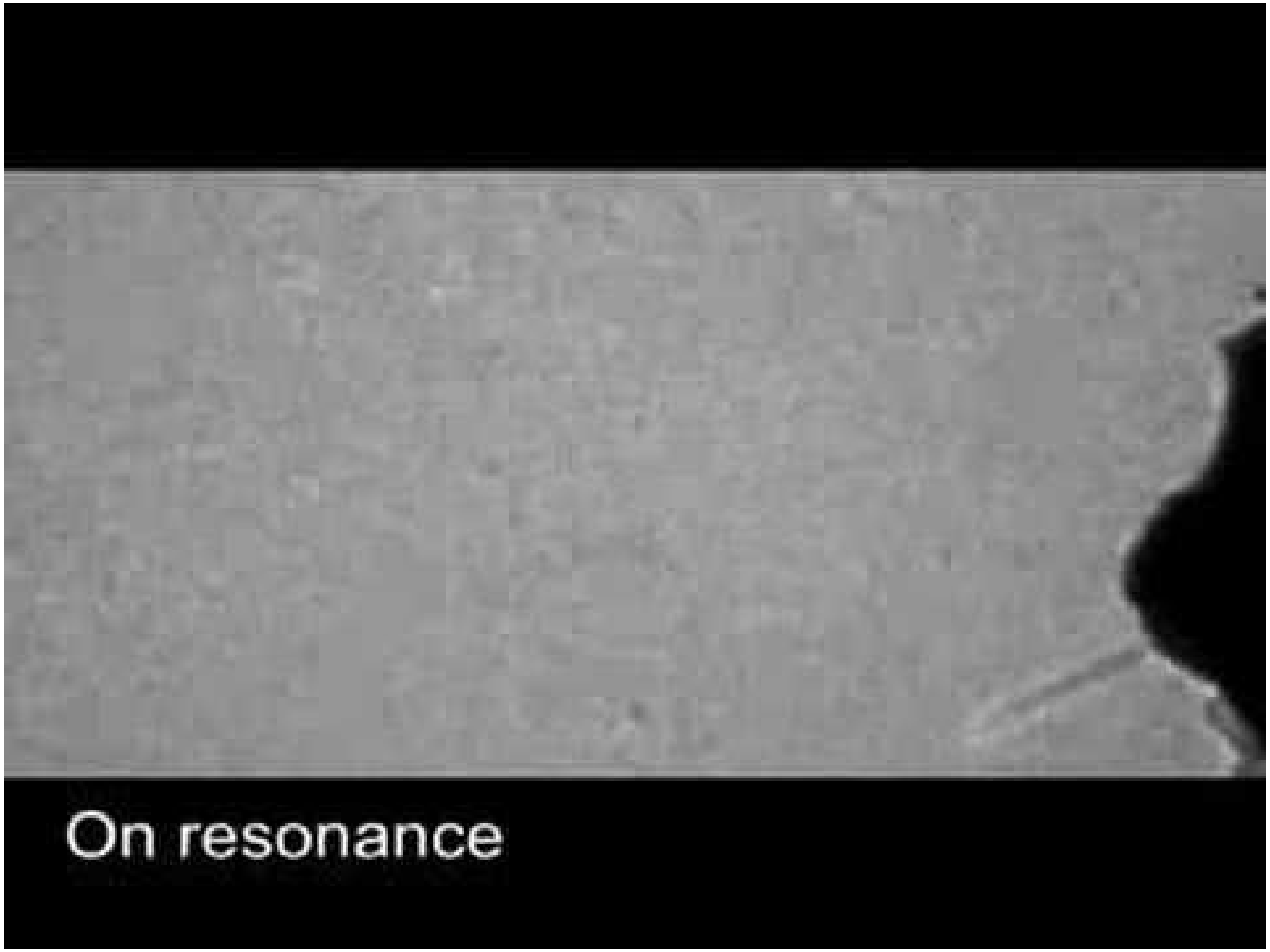
HIGH TECHNOLOGICAL POTENTIAL for **NANOTECHNOLOGY (and they are difficult and fun!)**

Carbon NanoTechnology, Sci-Fi? The Nanoradio

A few amazing devices have appeared recently in literature involving the Professor Zetll group in Berkeley and carbon Nanotubes. Specially striking, the nanoradio (K. Jensen, J. Weldon, H. Garcia, and A. Zettl. Nano Letters 7, 11, 3508-3511 (2007) a **fully functional fully integrated radio receiver made with a single nanotube**.

nanodevices

"Good vibrations..." (VIDEO!)



Nanoradio Details

We have constructed a fully functional, fully integrated radio receiver, orders-of-magnitude smaller than any previous radio, from a **single carbon nanotube**. The single nanotube serves, at once, as:

- antenna
- tuner
- amplifier
- demodulator

The antenna and tuner are implemented in a radically different manner than traditional radios, receiving signals via high frequency ***mechanical*** **vibrations of the nanotube** rather than through traditional electrical means.

Carbon Nanotechnology, NOT SciFi, everyday life?

Nanoradio: amazing, yet **proof of concept (i.e. experiment shows it can be done, but it is VERY DIFFICULT to do so!)**

industrially produced? NO, to the best of my knowledge!**!!!!!**:

- Fullerenes used for plastic solar cells (not commercially yet!!!)
- No real world application for graphene (high potential for nanoelectronics, **graphenium inside**).
- Carbon nanotubes are used JUST like carbon fibers for reinforcing COMPOSITE materials

- ALL OF THEM FOR **PLAIN MARKETING!!**

Why not **industrial** applications yet?

- **Carbon nanotechnology is very difficult**:
  - polidispersity (intrinsic):
    - all materials made with same building blocks (Csp2):
      - difficult to produce controlled materials
      - characterization problems
      - product separation problems

- No solution yet!!!!
- It needs complex **JOINT experimental and theoretical techniques** and analysis **GOOD FOR ME!**

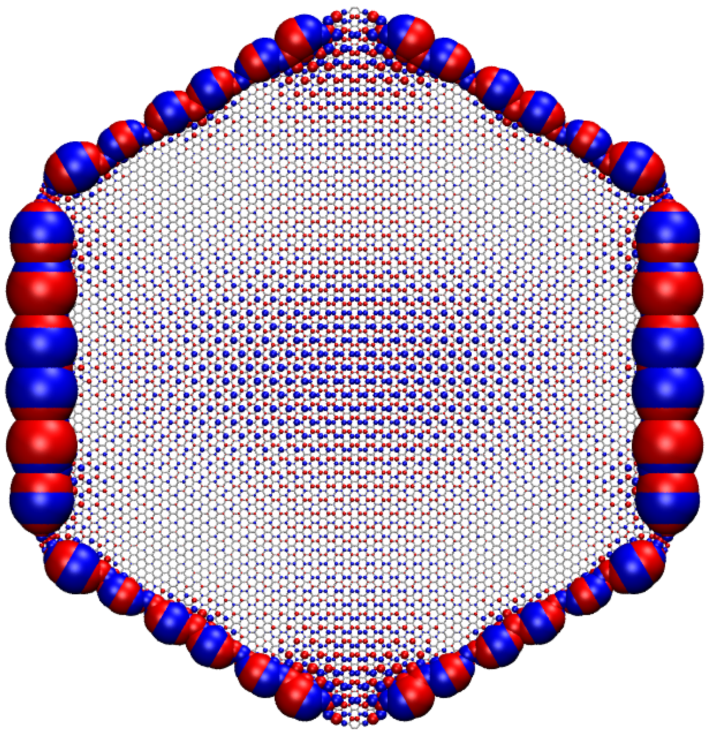
Real Research
Computer models aid COMPLEX experiments

Electronic and mechanical properties of carbon nanomaterials!

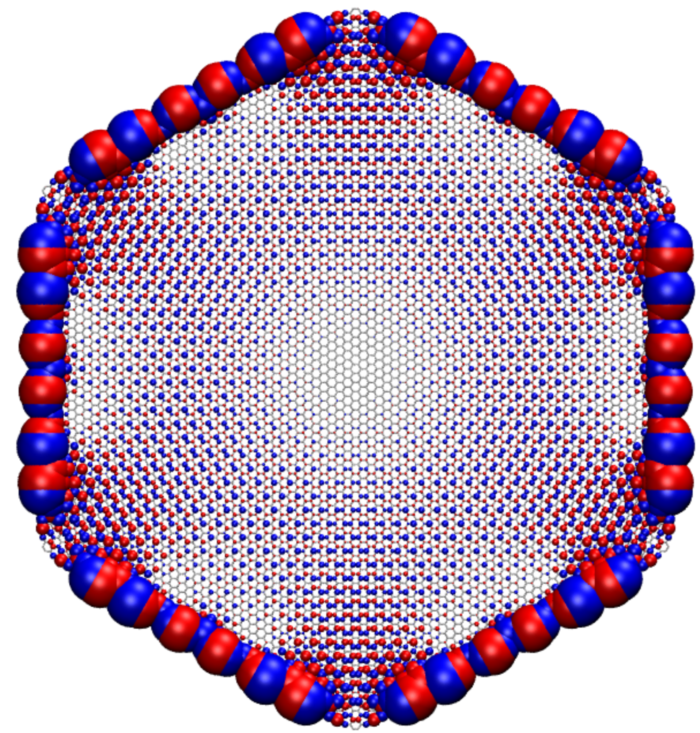
Developing QM software for carbon

- Quantum chemistry models are based on matrices
- Matrices have sizes proportional to the number of electrons
- C has 6 electrons, but most interesting properties depend only on 1 electron:
  - 1 electron matrices are 1/36th in size so allow for larger sizes
  - Still, memory use (explicit full matrix):
    - 10^4 electrons/C atoms -> 0.74 GB memory (Done)
    - 10^5 electrons/C atoms -> 74 GB memory (doable)
    - 10^6 electrons/C atoms -> **7400 GB!**

Orbitals of 9600 C/e^- graphene flake (calculation only takes 24 hours!)



HOMO



LUMO

Each DOT in graph is AN ATOM!!!!

Balls represent diffuse electrons -> these borders are very reactive! IMPOSSIBLE WITH MOST SOFWARE

Possible CPD projects in QM of carbon

- Computing huge systems with QM:
    - Matrix free project (Lanzcos): Huge QM systems without matrices [some easy mathematical Programming with Rui Ralha]
    - Alternative free matrix methodologies: testing and measuring performance of new matrix libraries
- Faster performance:
    - GPU diagonalization libraries: testing and measuring performance CUDA libraries
    - Intel PHI: testing and measuring performance with MKL inside PHI

Computer models aid COMPLEX experiments (II)
3D structure of Graphene (on going very preliminary)

Molecular dynamics: 3D structure of Graphene

- From results of master students of CPD modified algorithm way to make very fast calculations of graphene in serial computers
- Results with molecular dynamics give an stable wavy structure at room temperature (100,000 atoms for 1 ns (10^6 iterations, in 24 hours):

- **PRELIMINARY,** It is reproducible, but not in all conditions, yet, :(
- Is it real (physics) or arising from a numerical artifact ? very subtle computation!!!
- **It scales linearly so I am trying now much larger systems**

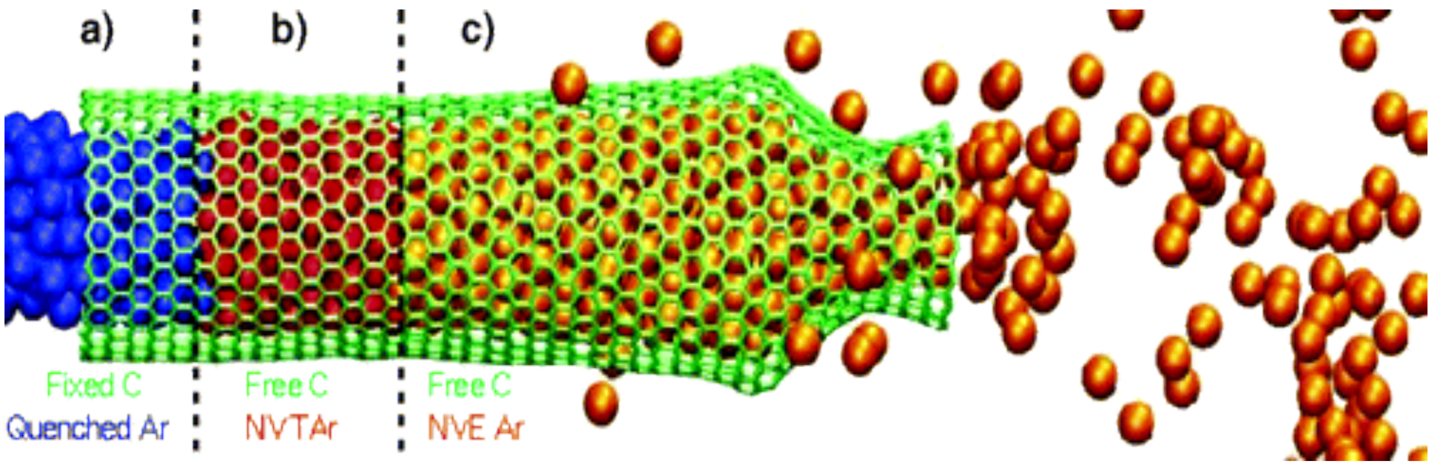
Virtual/in silico experiments

Do things that are impossible experimentally and see what happens

Nanonozzles Virtual Experiments

Liquid Argon at hight pressure trough carbon nanotube nozzle, Molecular dynamics NANO-FLUIDICS!

- **2 years programming**
- 2 weeks simulations



I WROTE my MD software to do this!
Very challenging algorithms and physics. **VIDEO!**

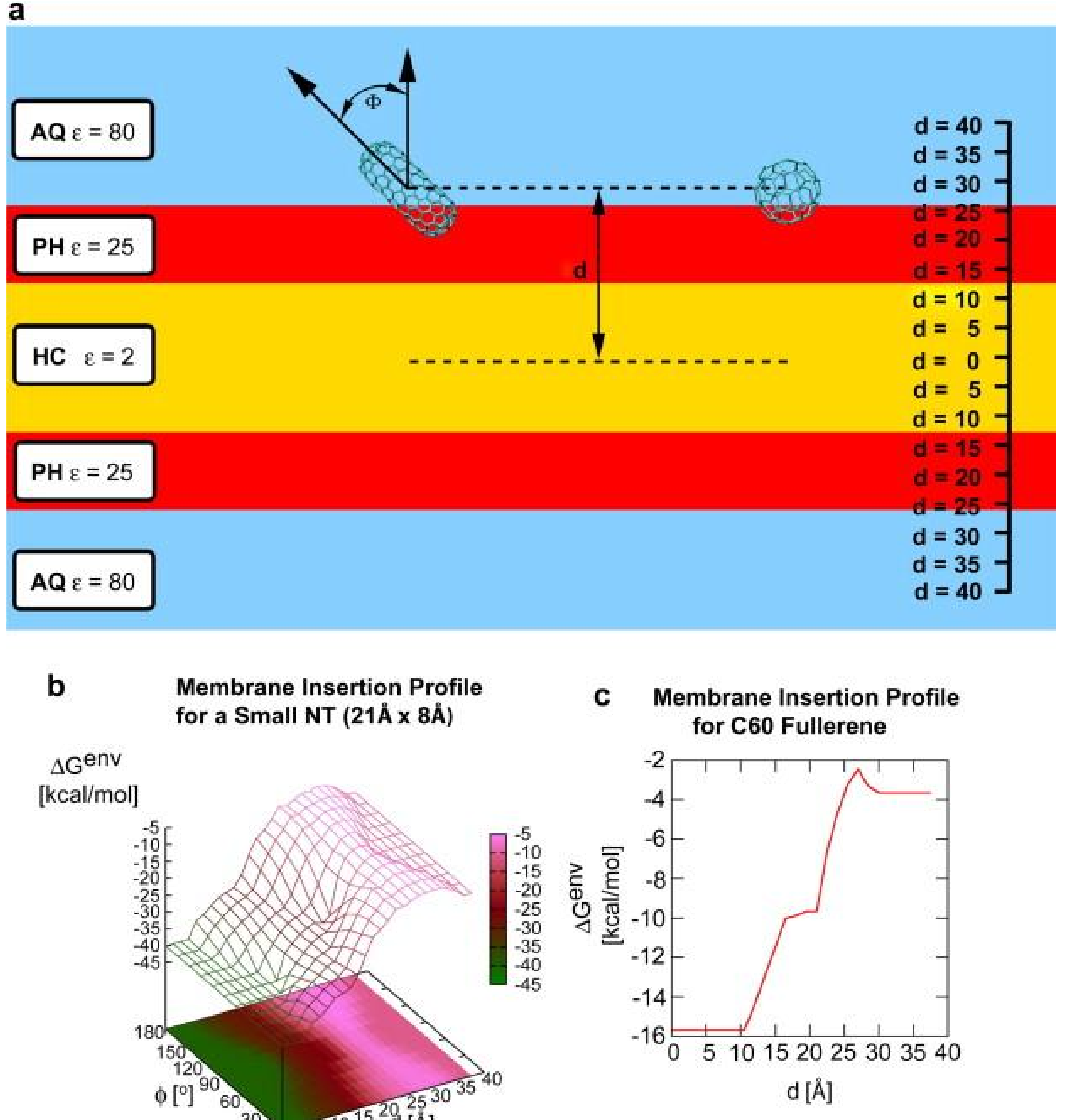
Ejection Dynamics of a Simple Liquid from Individual Carbon Nanotube Nozzles

Manuel Melle-Franco*†‡ and Francesco Zerbetto*‡-Nano Lett., **2006**, *6* (5), pp 969–972

Molecular dynamics simulations show that the flow of a high pressurized atomic liquid inside carbon nanotube “pipets” occurs in one-atom-thick well-defined laminae. Fluxes and velocities at ejection are a function of the inlet diameter and the type of outlet. In the conditions investigated here, the force of the ejected liquid is similar in value to that of biomotors, while the output per second is of the order of picoliters.

Nanocarbon and membranes

- Membrane (Spanish flag)
- Energetics for a C_{60} and small nanotubes. entering the membrane (yellow apolar part: MORE STABLE than outside)



A computational analysis of the insertion of carbon nanotubes into cellular membranes

Biomaterials Volume 32, Issue 29, October 2011, Pages 7079-7085

Siegfried Höfinger[a, b], , , Manuel Melle-Franco[c], Tommaso Gallo[a], Andrea Cantelli[a], Matteo Calvaresi[a], José A.N. F. Gomes[c], Francesco Zerbetto[a]

Carbon nanotubes have been proposed to serve as nano-vehicles to deliver genetic or therapeutic material into the interior of cells because of their capacity to cross the cell membrane. A detailed picture of the molecular mode of action of such a delivery is, however, difficult to obtain because of the concealing effects of the cell membrane. Here we report a systematic computational study of membrane insertion of individual carbon nanotubes and carbon nanotube bundles using two entirely different and unrelated techniques. First a static scan of the environmental free energy is carried out based on a membrane mimicry approach and different insertion geometries are assessed. Then the dynamics is investigated with a coarse-grained approach that was previously used in the study of the integration dynamics of nanoparticles into the bilayer. The results of both models point, for unfunctionalized carbon nanotubes, at a preference for the horizontal orientation inside the internal hydrophobic layer of the cell membrane. Finally, the energetics of the formation of bundles of carbon nanotubes is studied. The cellular membrane promotes aggregation of carbon nanotubes in its hydrophobic core and modifies the structural stability of the bundles.

Nanotoxicity

- Nanotoxicity is fundamental issue in nanotechnology!!!!
- Exp. PURE fullerenes and nanotubes are VERY TOXIC for cells!!!
  - High citotoxicity -> molecular cause:
    - Fuls and CNTs **spontaneously** enter membranes and **accumulate** there **(VIDEO*)**

~~***:Mesoscopic MD Simulations, not ATOMIC RESOLUTION (sizes and timescales!!!!)**~~

Summary I

- Computer simulation is a very powerful tool for chemistry and physics (nobel prize of chemistry 2013)
- Very complex problems need specific software and approaches
- Needed to complement / explain / justify experimental results
- Nowadays ALL state of the art studies HAVE ALSO a computational part!!!!
- Can be used, with care, to do VIRTUAL , impossible, experiments

Summary II (for you!)

- Computer modelling is a FUNDAMENTAL TOOL FOR physics and chemistry !!!!!
- HPC is fundamental for computer modelling!!!
- Parallel computing is fundamental for MUCH science!

More computing-like

Compressed sensing!

Compressed sensing

Using a mathematical concept called sparsity, the compressed-sensing algorithm takes **very noisy** data and transforms them into clean data.

It turns out that out of all the HUGE possible reconstructions, the simplest, or sparsest, image is almost always the right one or very close to it.

With a Photograph:

h /1

Compressed sensing

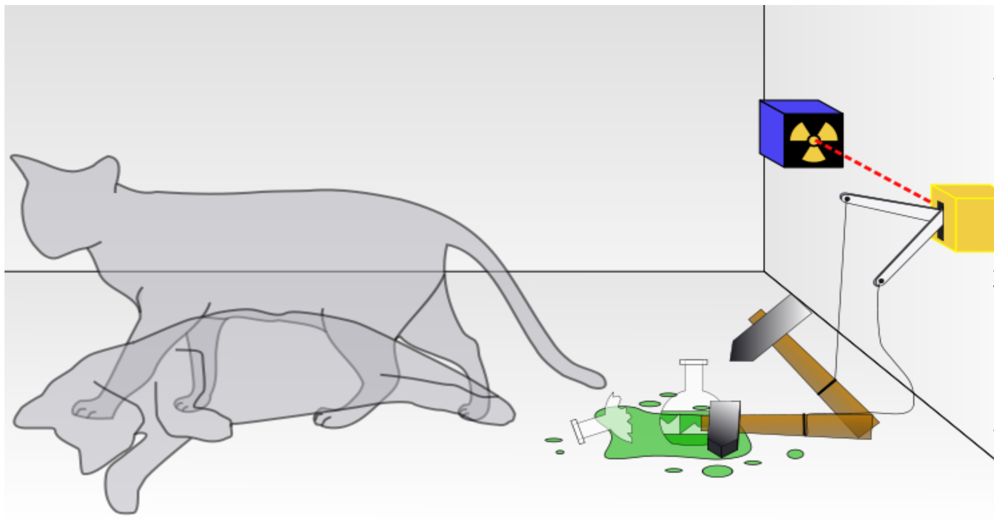
Compressed sensing used for DSP and image processing:

- Fourier transforms (FT) with much less input data

- Can it be used for molecular modelling?
  - Indirectly, FT with less data, implies less calculations

Very challenging!!!
Many interesting and amazing possibilities!

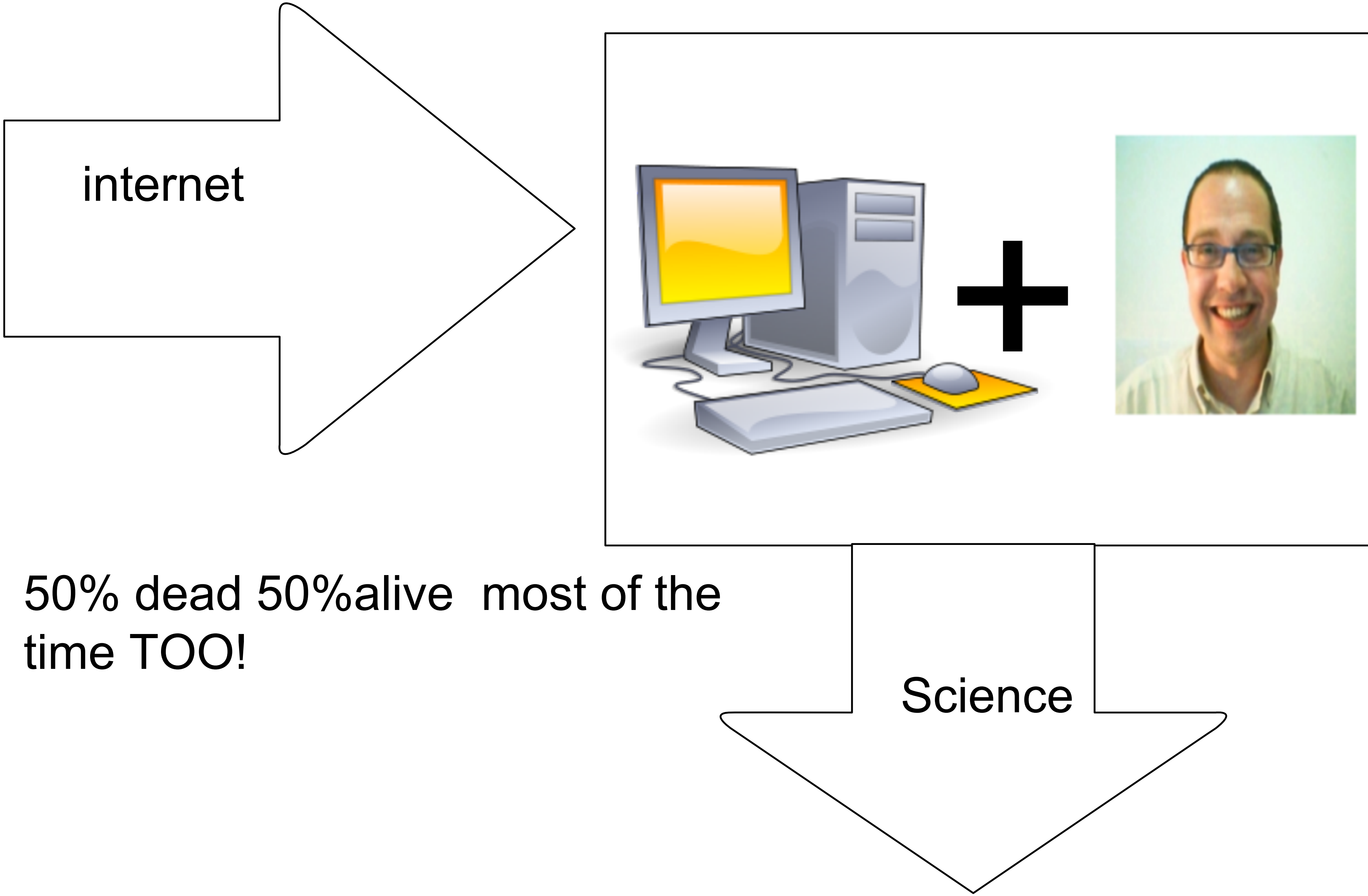
Schrödinger's cat in box



One can even set up quite ridiculous cases. A cat is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter, there is a tiny bit of radioactive substance, so small that perhaps in the course of the hour, one of the atoms decays, but also, with equal probability, perhaps none; if it happens, the counter tube discharges, and through a relay releases a hammer that shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The psi-function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts. It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks

Paradox thought experiment in which a cat, based on a QM event, is 50% dead and %50 alive!

Manuel in a box



50% dead 50%alive most of the time TOO!

Feel free to contact me for any reason!

Advice for projects:

a) Try to work with people that program the software you have to improve!

b) Be humble, REMEMBER that it is very unlikely that you can fix a complicated problem with some days work. PEOPLE ARE NOT STUPID!

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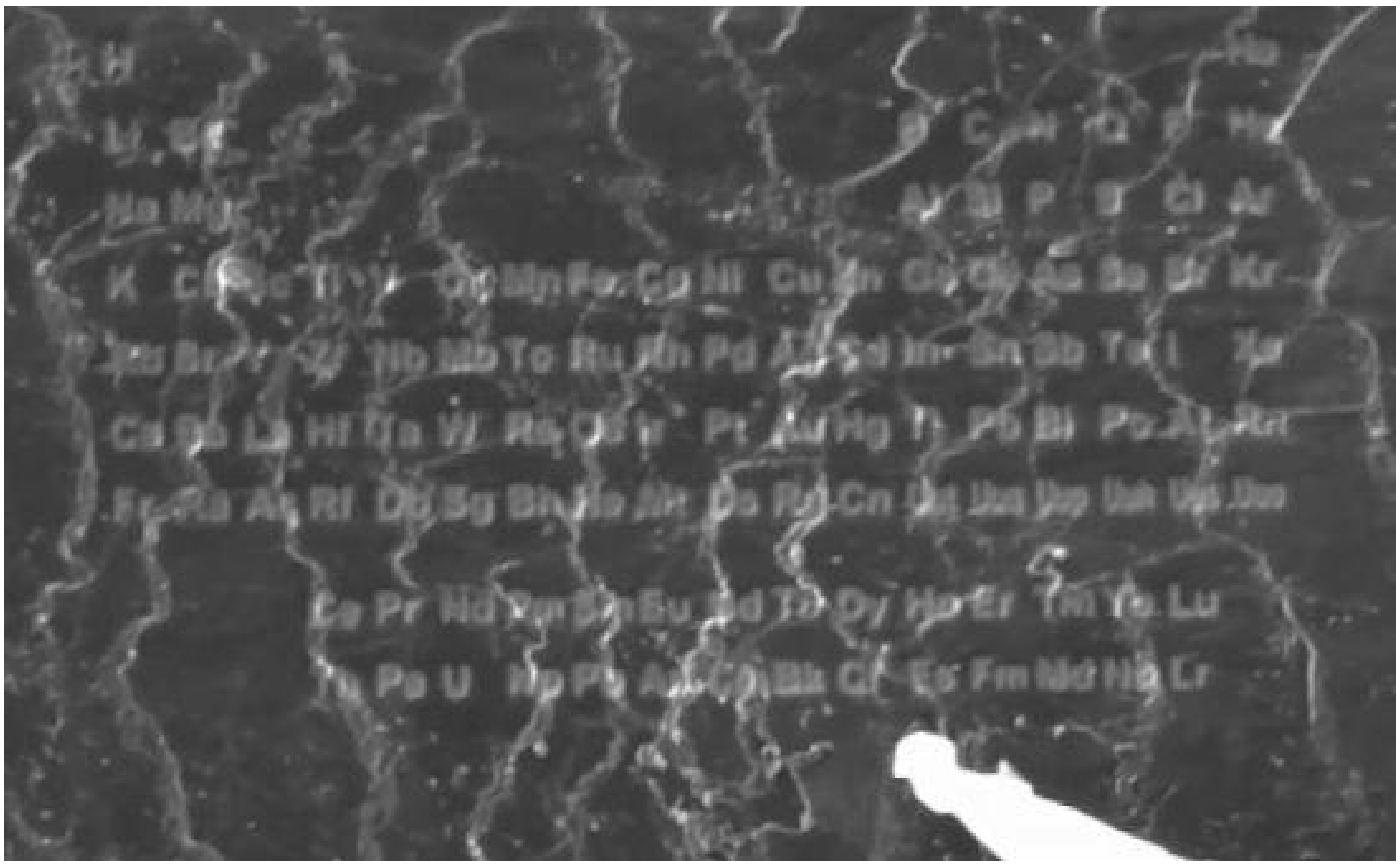
Nanotechnology: better Storage of information:
Smallest Periodic table on a hair!!!!!



0.046 mm

0.088 mm

On a human hair!!!