

VERY Informal introduction to
**Computer
modelling of
*Carbon*Nanotechnology**

CPD 2012

Manuel Melle Franco
CCTC (DI)
University of Minho

who am I?

- **Researcher in the HPC group of DI UMinho**
- CV: Natural scientist:
 - Ph.D. Physics
 - M.Sc. Materials Science
 - First Degree in Physical Chemistry
 - Large experience in scientific computing:
 - **Research: computer models for NANOTECHNOLOGY**

**I am here for you so PLEASE DO INTERRUPT ME
AT ANY TIME!!!**

Introducion

- I could speak hours about very technical an obscure stuff **(this guy rules!)** that would be very difficult to follow and you would not get much out of it
- I will try show you something, useful from my point of view (a physicysts working with computer scientist).
- IT might BE TOO MUCH INFORMATION SO INTERRUPT ME WHEN YOU HAVE QUESTIONS!

Experiment and Theory

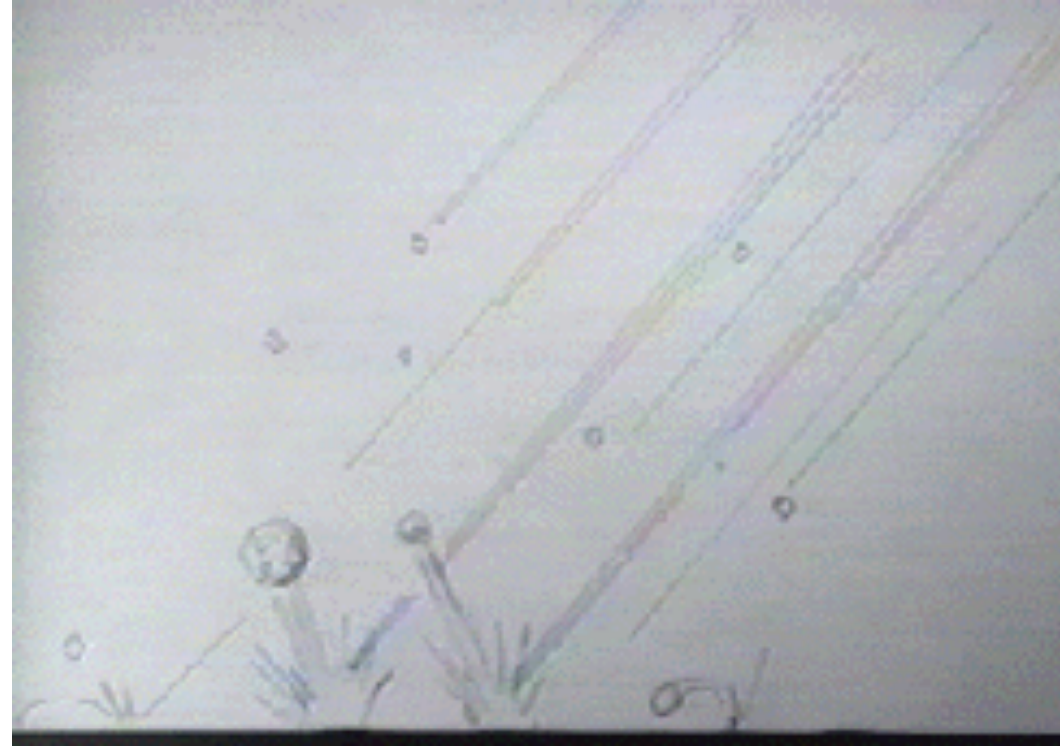
Mathematical models

Experiment vs. theory

- Experiment: WHAT WE OBSERVE
- Theory: HOW WE EXPLAIN/RATIONALIZE WHAT WE OBSERVE

Example: Galileo's Experiment

- Aristotle's theory: heavier objects fall faster
- Galileo in a hail storm: all hail sizes touch the ground at the same time, NO PREFERENCE with size or weight
- Galileo found a way to find how this thing really worked! (designed an EXPERIMENT!)



Galileo's experiment (17th century)

- Made **experiment** that found Aristotle was wrong (A. did not check, HE ASSUMED, *we do the same most of the time!!!!*)
- Proposed a simple MATHEMATICAL model that could reproduce his experimental data and **predict** what would happen in other



Why theory?

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

David Hume, philosopher 18th century: **water boils when heated, but can we be 100% sure that it will boil NEXT time????** **Yes or no?**

Now that we know 100 % why water boils and what that physically means, we are 100% sure it will boil ALL TIMES, because we know the process completely, **SCIENCE says IT MUST boil and so it will!!!**

Why model something?

Mathematical model:

- Reproduction
- Extrapolation to exp. unknown cases/conditions
- Prediction

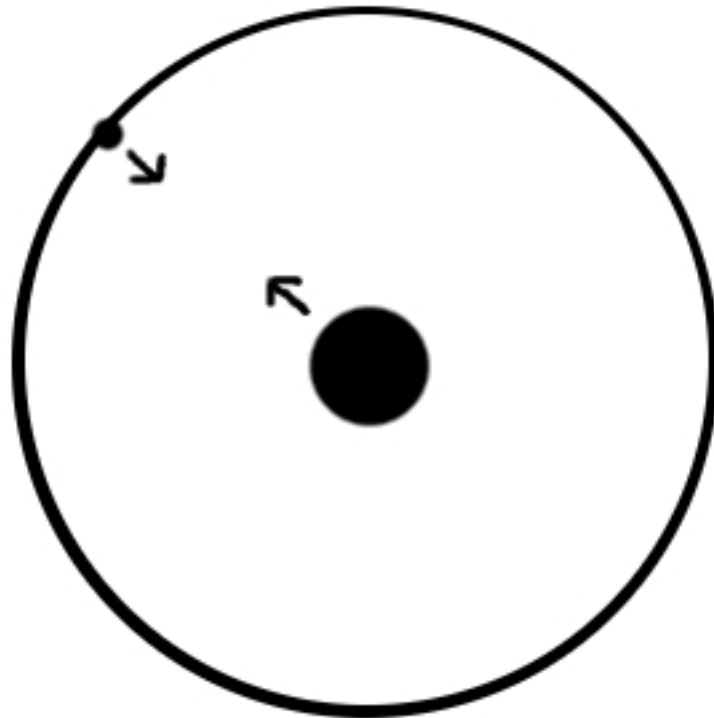
Nature follows easy rules (not obvious ones), but too many different interacting objects so nature is complex!

Theory/modelling is fundamental for advanced technological use of nature! example: semiconductor industry, etc

Mathematical models: The two-body problem

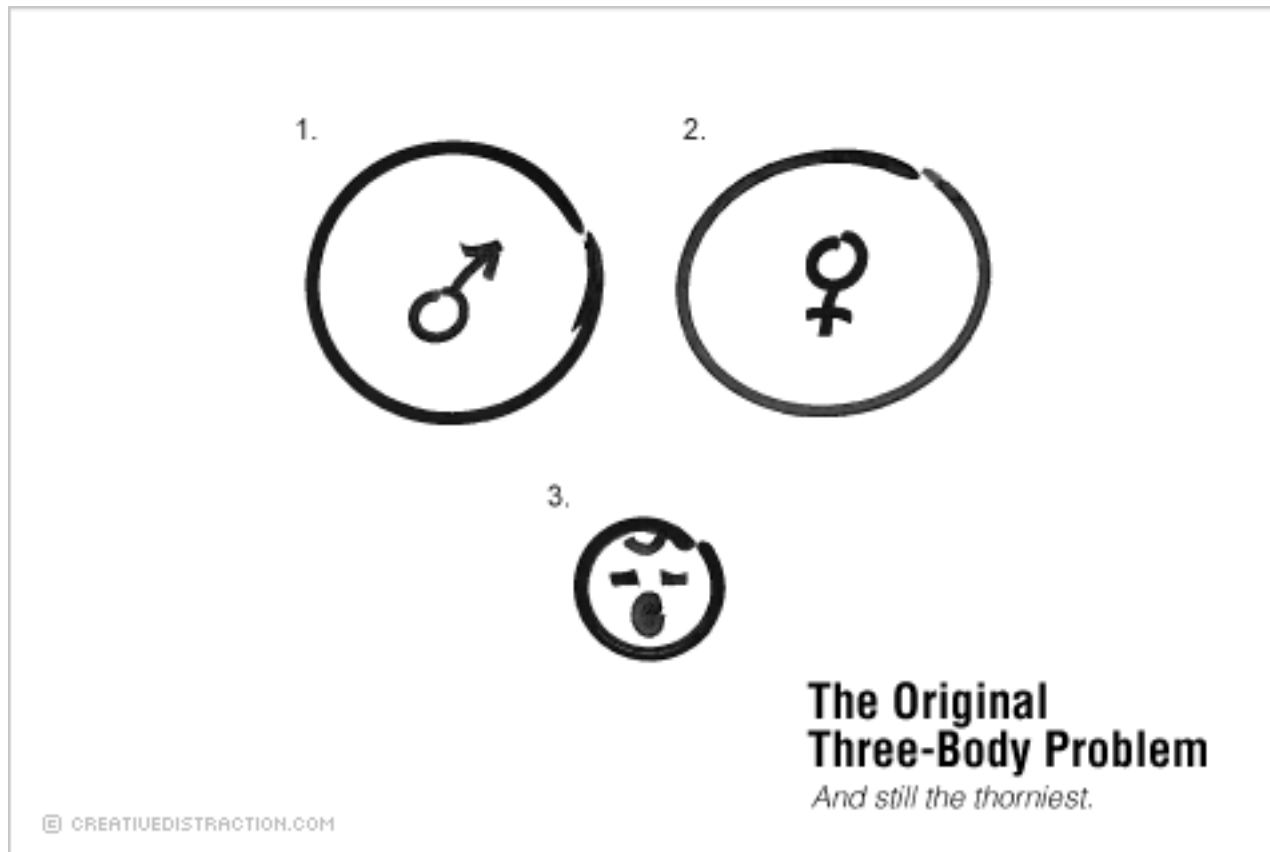
The **two-body problem** (nothing to do with sex!):
motion of two bodies that interact with each other. Examples:

1. Moon and the earth
2. Electron "orbiting" hydrogen nucleus



The "original" Three body problem

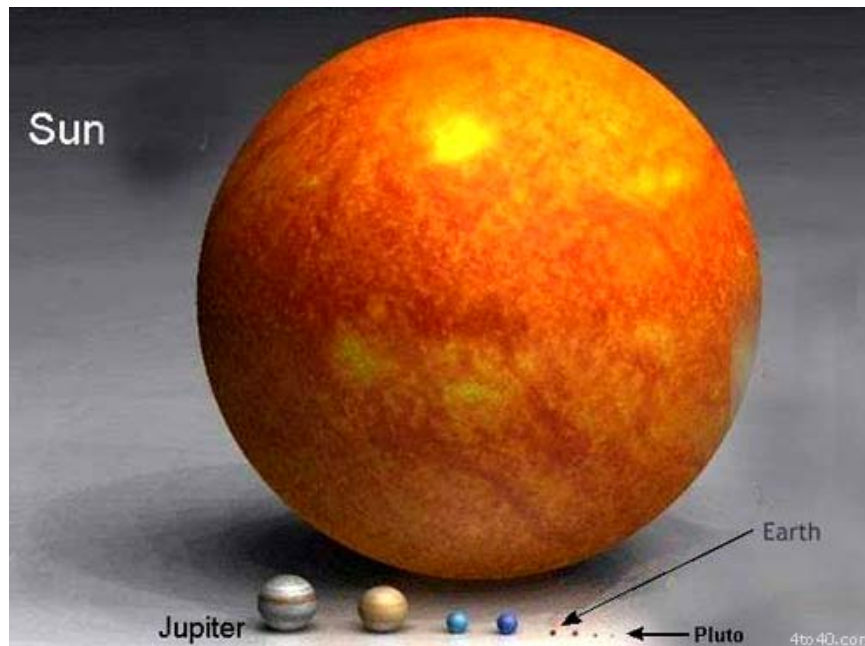
Mother + Father + child = No exact solution!!!



Mathematical models: The two-body problem

The Two-body problem can be solved analytically (i.e **EXACTLY**).

By contrast, larger (≥ 3 interacting bodies) bodies cannot be solved exactly, except in special cases and have to be solved **NUMERICALLY** (approximatedly). Ex: Planet orbits:



Numerical vs. Analytical models

Numerical

1. Approximated (for real numbers)
2. Relative Accuracy, typically it depends on number of iterations
3. Easy but very repetitive, only most simple cases are doable by hand (in a reasonable time) **ideal for COMPUTERS**

Analytical

1. Exact
2. Always 100 % accurate
3. Difficult (creative thought)
4. Its working can give insight in the problem at hand: **foundations of Quantum Mechanics was ALL done with pen and paper**

Computer simulation = automatic numerical procedure

- First Simulation (state of the art, 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): motion of a **2.64-million-atom model of a ribosome** on 768 parallel processors (Ribosome is a protein made molecular machine that builds proteins from genetic code! **Nature's Nanotechnology**)

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 **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

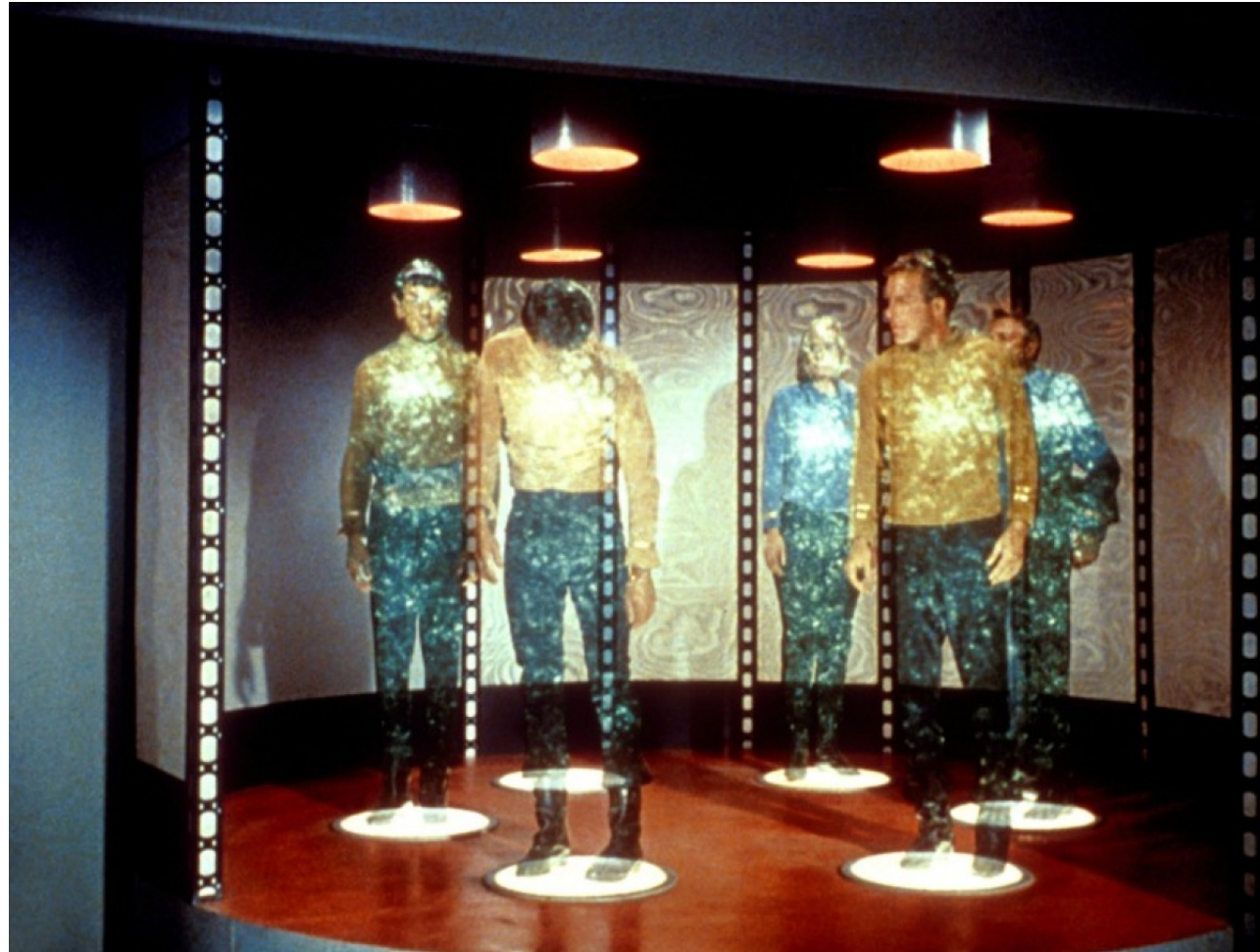
- Current state, amazing powerful PCs!
 - **TODAY**: This **laptop**: i5 M460 @2.53GHz = $2 \times 4 \times 2.53 = 20$ **gigaFLOPS** (theoretical)
 - **15 years ago**: One of the 500 fastest, **parallel, computers of the world!** (www.top500.org)
 - The first system to achieve **1 petaFLOPS [peta=10**15]** (**2007**): distributed home computers 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!**

"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).



Digitalizing the world with atomic resolution (SIZE!)

- 1 gram of carbon has $\sim 5 \times 10^{22}$ atoms
- Store atomic positions of **1 gr carbon** atoms in single precision (4 byte):
 - 6×10^{23} bytes = (SI) **0.6 yottabytes**
 - **6 hundred thousand millions of TB harddrives**
 - piling up laptop HDs (1km HDs= 100000 TB):
 - 1 yottabyte = 10^{12} HDs=**10 million kms of HDs**
(diameter of the earth is ~ 12000 km)
- **Classic Star Trek may have weird dresses but also amazing storage density than us!**

Digitalizing the real world with atomic resolution (SIZE!)

Models Impossible? NO!

- **Most properties of crystals of carbon (graphite/diamond) can be described just by 2 atoms models**
- Most information in 1 gr of carbon is extremely redundant:
 - 1 gr carbon = 5×10^{22} atoms (BORING!!!)
 - 1 human brain = 9×10^{10} cells (**exciting!**)*.

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

Digitalizing the real world with atomic resolution (TIME!)

- Our body is mostly built by light atom molecules (H, C, O, N)
- Time in numerical models is discrete
- Atoms, being very small and very light move very fast:
 - require timescales ~ 1 fs (10^{-15} seconds).
 - Discretize time in chunks of 1 fs!

Digitalizing the real world with atomic resolution (TIME!)

Different important molecular processes happen in different time scales:

- **Miliseconds**, like protein folding, are now reached with supercomputers for small, few atoms, systems (**10^{12} iterations**, 1 tera-iterations).
- 1 second, peta-iterations, 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 **HAPPENS**.

Digitalizing the real world , why HPC computers? SUMMARY

- Many iterations:
 - Larger 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)

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
- Should be able to admin a unix/linux machine!

Natural scientists (ex):

- Some, cheap, self-taught programming (matlab, fortran, python, ...)
- what?
- WHAT????
- most computational natural scientists do

Natural vs computer scientists?

Natural scientists (ex):

- (Should) know GOOD physics/chemistry/biology
- really know why algorithms have to do that in scientific software³
- Know what is the main purpose of simulations:

WHY!!!

Computer scientists (ex):

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

Starting working in a new field, there is always more than you don't know than what you do know!!!!

is formal training needed?

- In 2003, I designed, bought and set up a **30K euros PC cluster**.
- It run flawlessly till 2009 (with a maximum, rare downtimes of one hour).
- **I never formally studied computing!**

Everybody can try to learn and do ANYTHING:
It takes time, effort, a large amount of frustration, and stubbornnes!

In other words...

If you really want to do something, there is nothing, intrinsic, to stop you!

Natural scientists are not born like that (it is not a genetic trait) neither are computer scientists, we BOTH have LEARNED to do so!

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

...SCIENTISTS AND THEIR SOFTWARE

A survey of nearly 2,000
researchers showed how coding
has become an important part of
the research toolkit, but it
also revealed some potential
problems.

> **45%** said scientists spend
more time today developing
software than five years ago."

> **38%** of scientists spend at
least one fifth of their time
developing software.

> Only **47%** of scientists
have a good understanding of
software testing.

> Only **34%** of scientists
think that formal training
in developing software is
important.

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

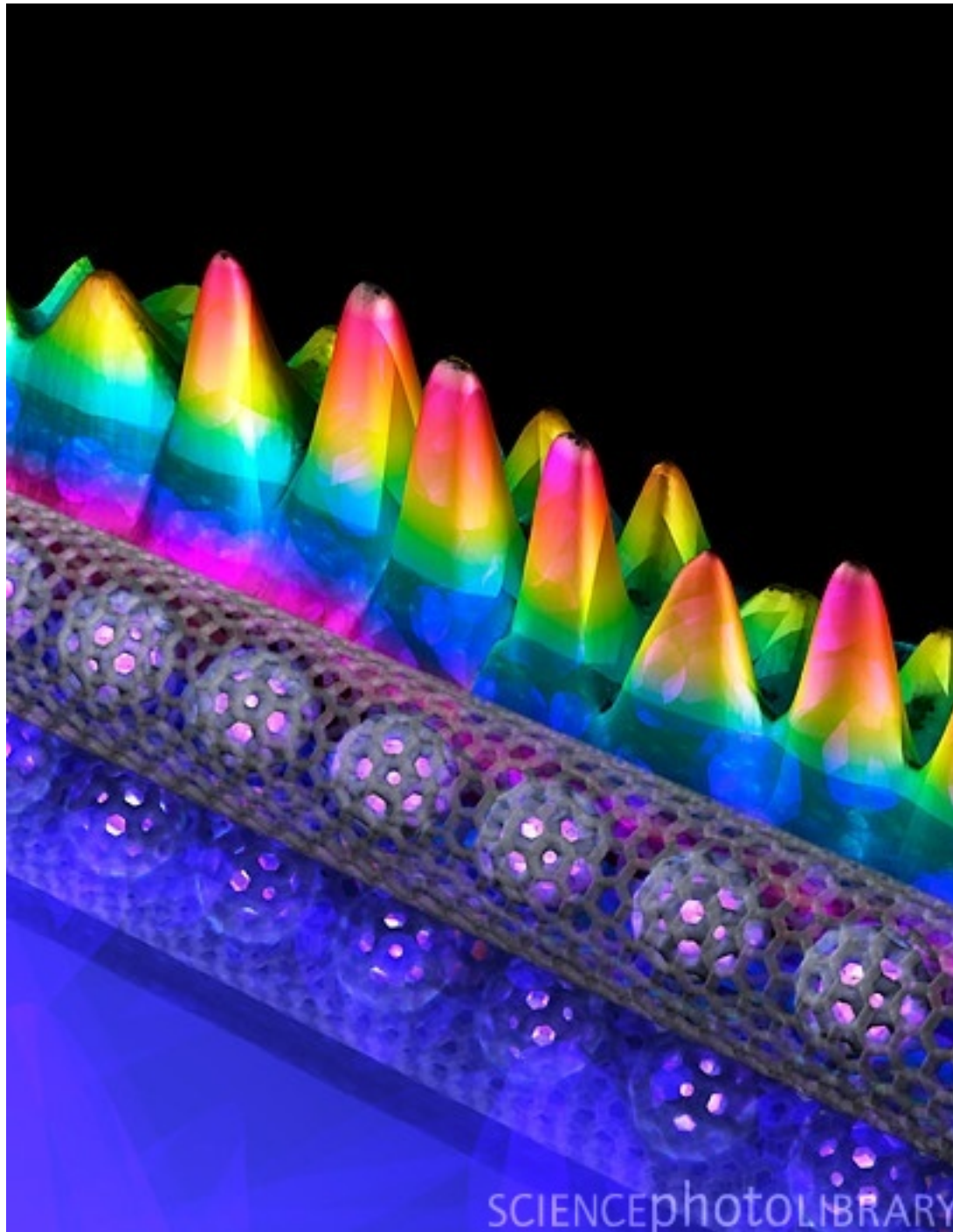
Published online 13 October 2010 | *Nature* 467, 753 (2010) | doi:10.1038/467753a

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.

Computer modelling of carbon nanomaterials



Manuel Melle Franco
CCTC (DI)
University of Minho

Nanotechnology (smallest tech!!!)

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

Periodic Table of Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																																								
1 H Hydrogen 1.00794	Atomic # Symbol Name Atomic Mass																2 He Helium 4.002602																																								
3 Li Lithium 6.941	4 Be Beryllium 9.012182	<table border="1"> <tr> <td>C</td><td>Solid</td> </tr> <tr> <td>Hg</td><td>Liquid</td> </tr> <tr> <td>H</td><td>Gas</td> </tr> <tr> <td>Rf</td><td>Unknown</td> </tr> </table>										C	Solid	Hg	Liquid	H	Gas	Rf	Unknown	<table border="1"> <tr> <td colspan="2">Metals</td> <td colspan="2">Nonmetals</td> </tr> <tr> <td>Alkali metals</td><td>Alkaline earth metals</td><td>Lanthanoids</td><td>Transition metals</td> </tr> <tr> <td></td><td></td><td>Actinoids</td><td>Poor metals</td> </tr> <tr> <td></td><td></td><td></td><td>Other nonmetals</td> </tr> <tr> <td></td><td></td><td></td><td>Noble gases</td> </tr> </table>				Metals		Nonmetals		Alkali metals	Alkaline earth metals	Lanthanoids	Transition metals			Actinoids	Poor metals				Other nonmetals				Noble gases	5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.0067	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797	11 Na Sodium 22.98976928	12 Mg Magnesium 24.3050	13 Al Aluminum 26.9815386	14 Si Silicon 28.0855	15 P Phosphorus 30.973762	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948
C	Solid																																																								
Hg	Liquid																																																								
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19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955912	22 Ti Titanium 47.887	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798																																								
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.96	43 Tc Technetium (97.9072)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.293																																								
55 Cs Cesium 132.9054519	56 Ba Barium 137.327	57-71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98040	84 Po Polonium (209.9824)	85 At Astatine (209.9871)	86 Rn Radon (222.0176)																																								
87 Fr Francium (223)	88 Ra Radium (226)	89-103 Actinoids	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)	110 Ds Darmstadtium (271)	111 Rg Roentgenium (272)	112 Uub Ununbium (285)	113 Uut Ununtrium (284)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (282)	117 Uus Ununseptium	118 Uuo Ununoctium (294)																																								

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

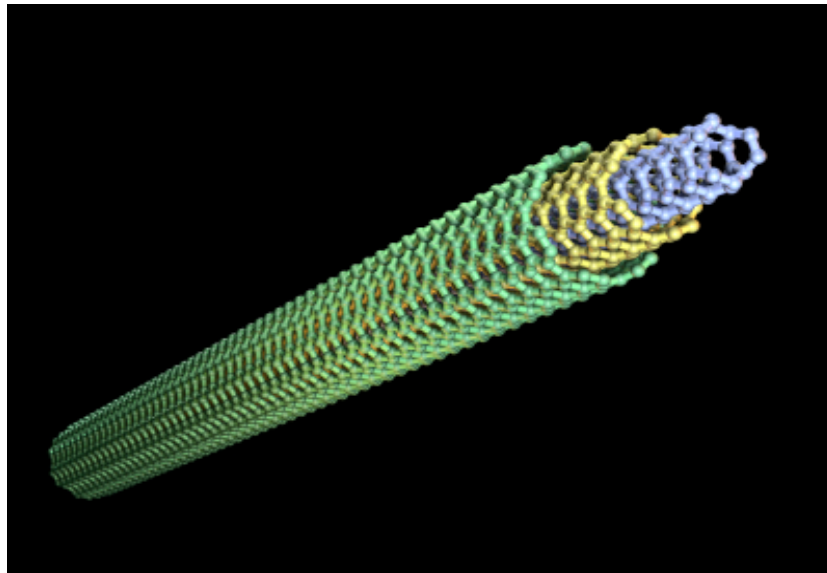
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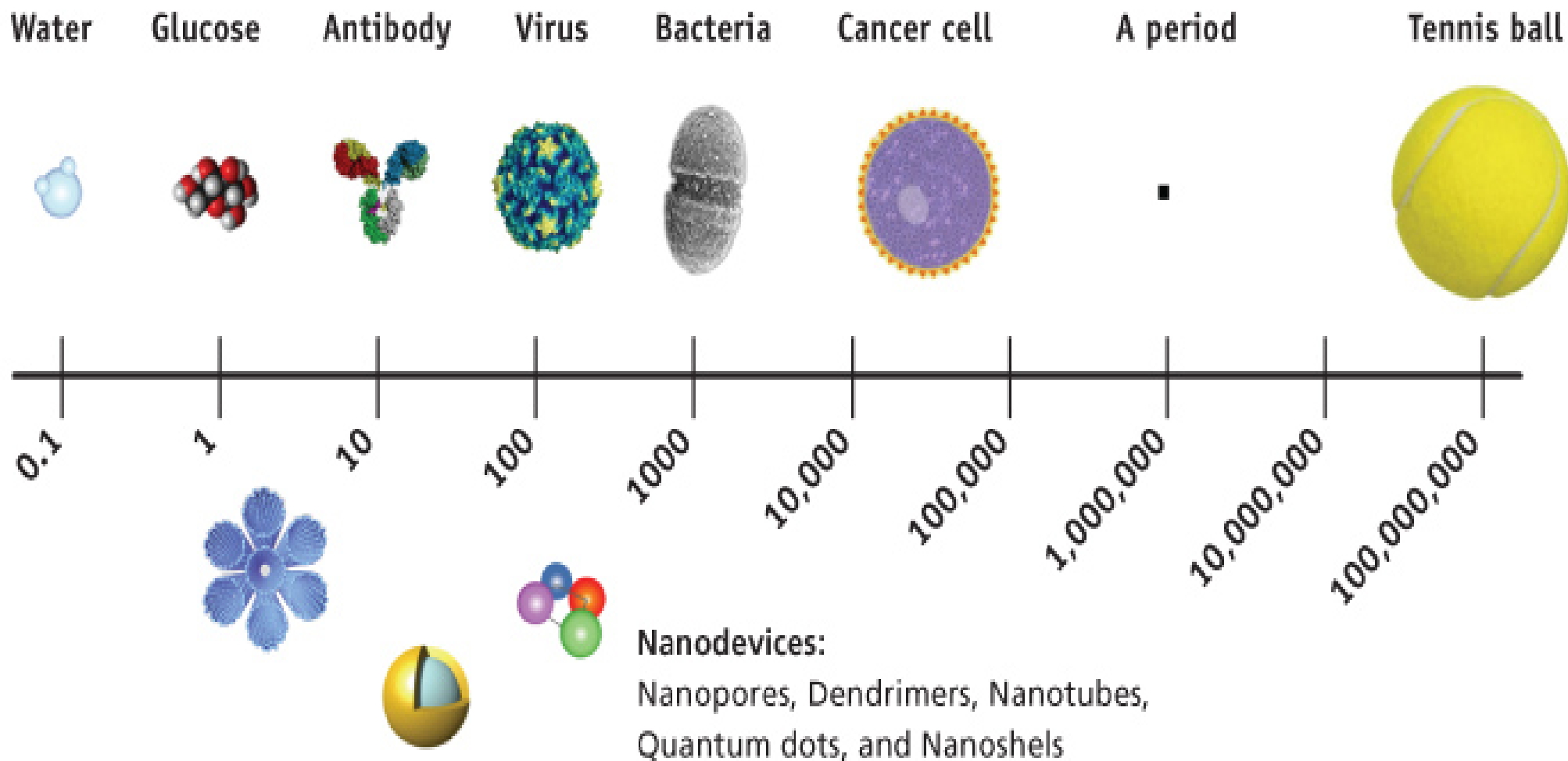


57 La Lanthanum 138.90547	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93032	68 Er Erbium 167.259	69 Tm Thulium 168.93421	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.9668
89 Ac Actinium (227)	90 Th Thorium 232.03806	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

Nanotechnology

- Nanometer
 - 10^{-9} meters (1 millionth of 1 mm)
 - 1-2 atom diameters
- Nanoobjects < 1000 [nanometers](#) in at least one dimension, i.e. carbon **nanotube**:
 - long millimeters: macroscopic (axis)
 - thick nanometers: **nano** (diameter)





Nanometer Chart

Can we see nanobjects?

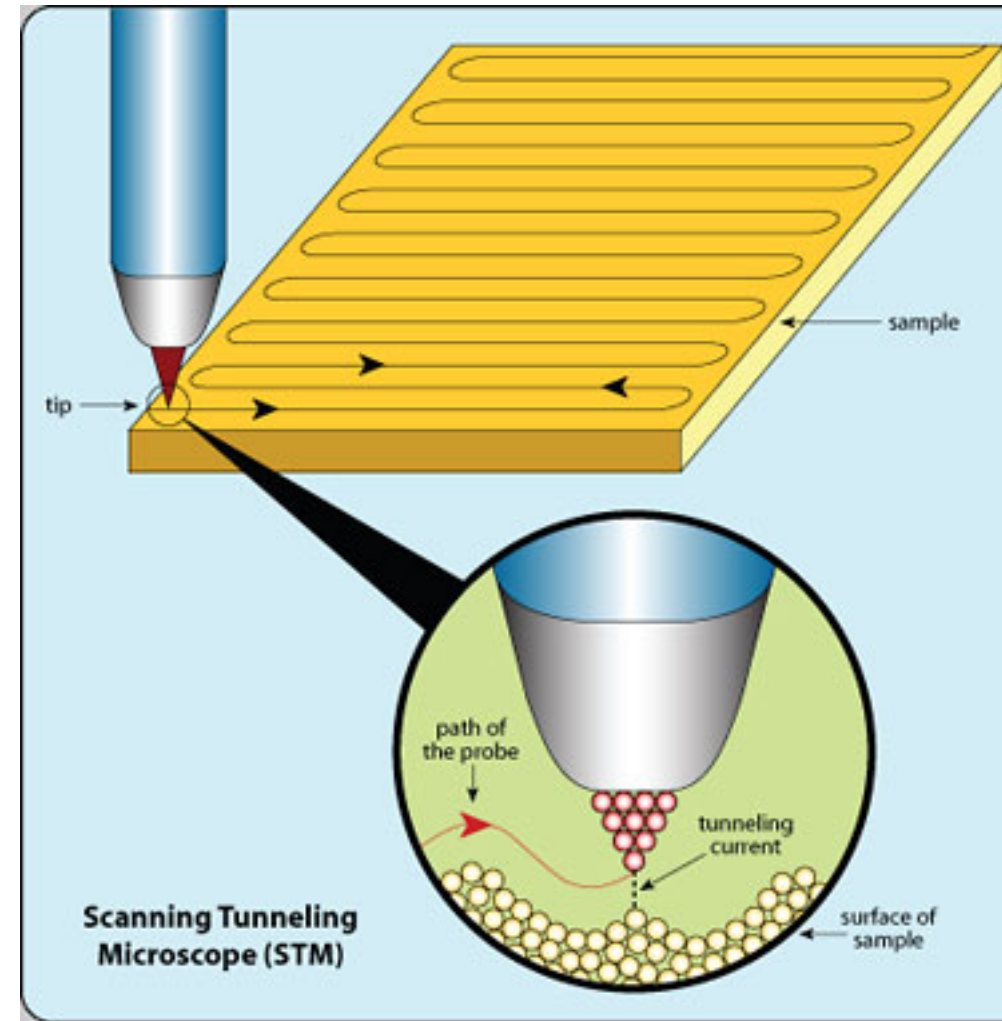
- If we are to manipulate atoms we have to control and know their positions in space! **SEE THEM!**
- can we see atoms with microscope?
 - Using visible light?
 - NO, best resolution with visible light, 200 nm (atom ~ 1 nm)
 - Using electrons?:
 - Yes easy to have electrons with shorter wavelength than light (up to Atomic resolution!!!)

Start of Nanotechnology

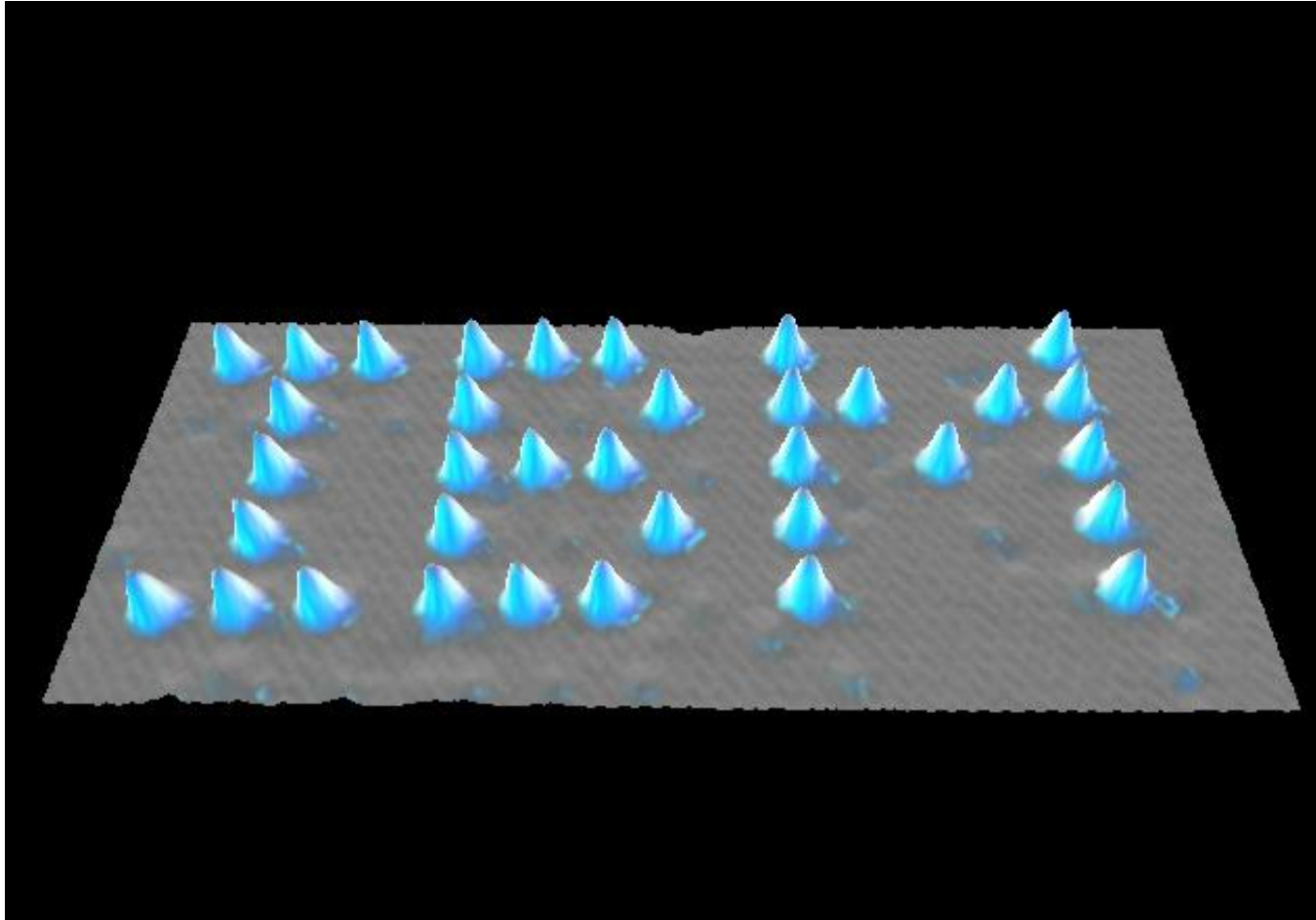
- In 1986 single atoms could be directly *imaged* for the first time with Scanning Tunneling Microscopy (**STM**)
- **MAJOR BREAKTHROUGH:** [Gerd Binnig](#) and [Heinrich Rohrer](#), Nobel Prize of Physics **same year!**
- Description (STM FOR dummies): http://www.nobelprize.org/nobel_prizes/physics/laureates/1986/press.html

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.



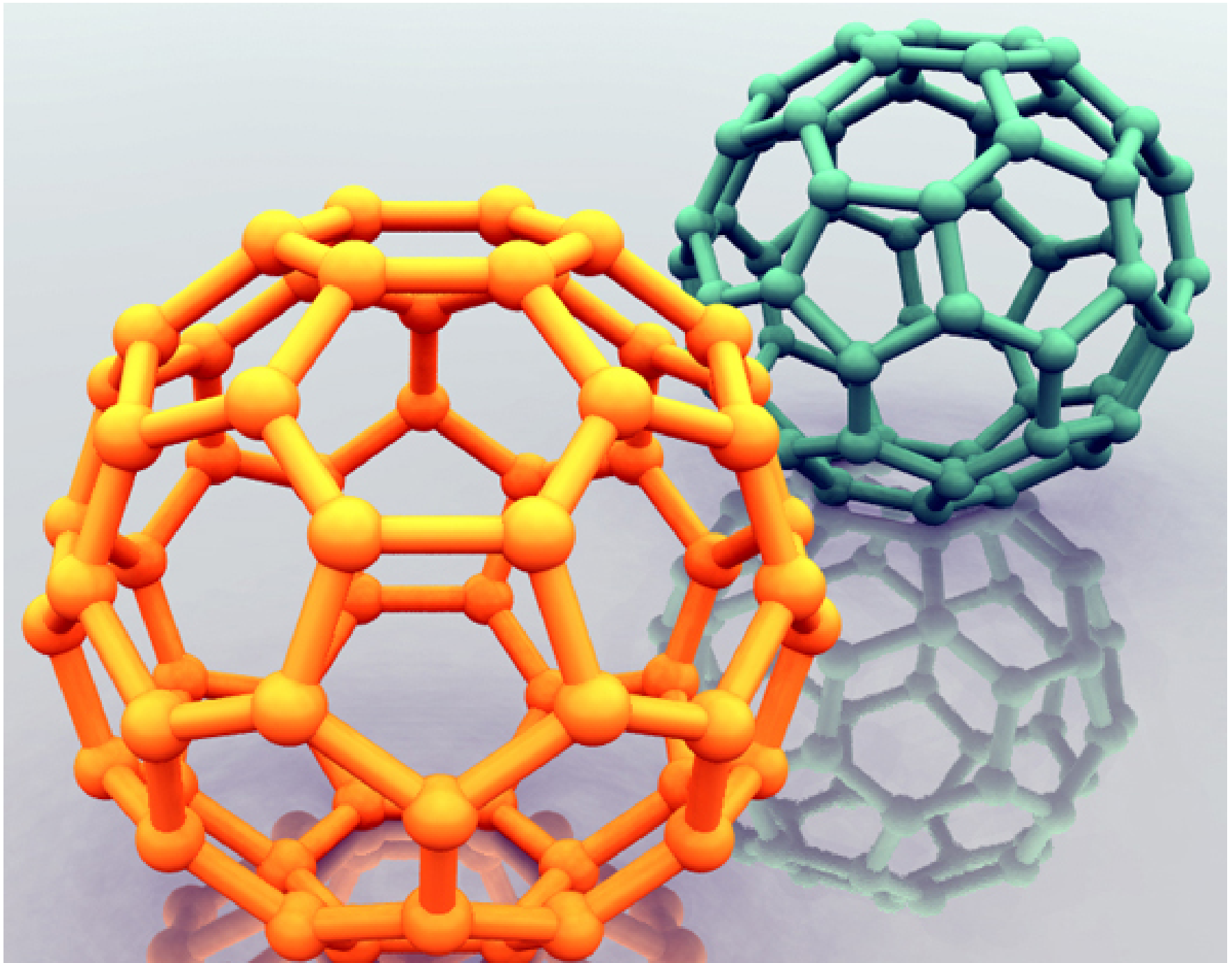
The world smallest corporate logol



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]

STM "images" grid data of the surface

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



Carbon Nanotechnology!

Carbon nanotechnology started in space!

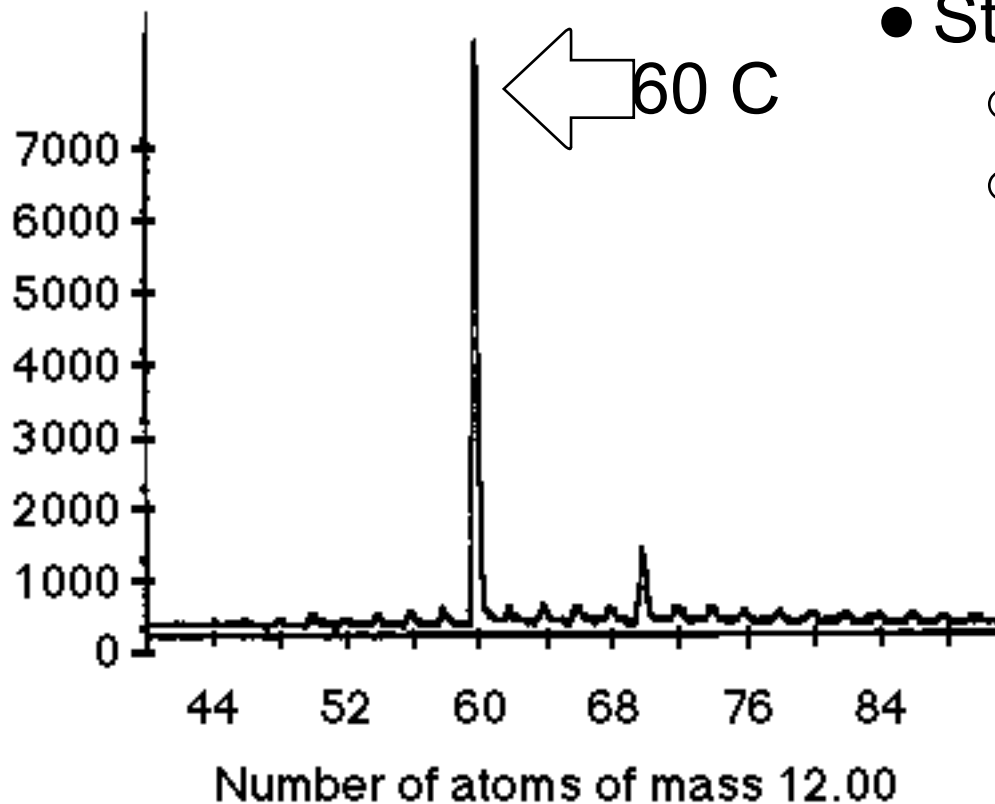
- In **1985**, British chemist Harry Kroto was puzzling over strange chains of **carbon atoms** that could be **detected billions of kilometres** away in space by **radiotelescopes**. He thought that these chains might form in conditions that are found **near red giant stars**. **[Science is AMAZING 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](#))

What was the molecular structure?

- Stable (observation)
 - Spherical (from chemistry)
 - Symmetrical (speculation)



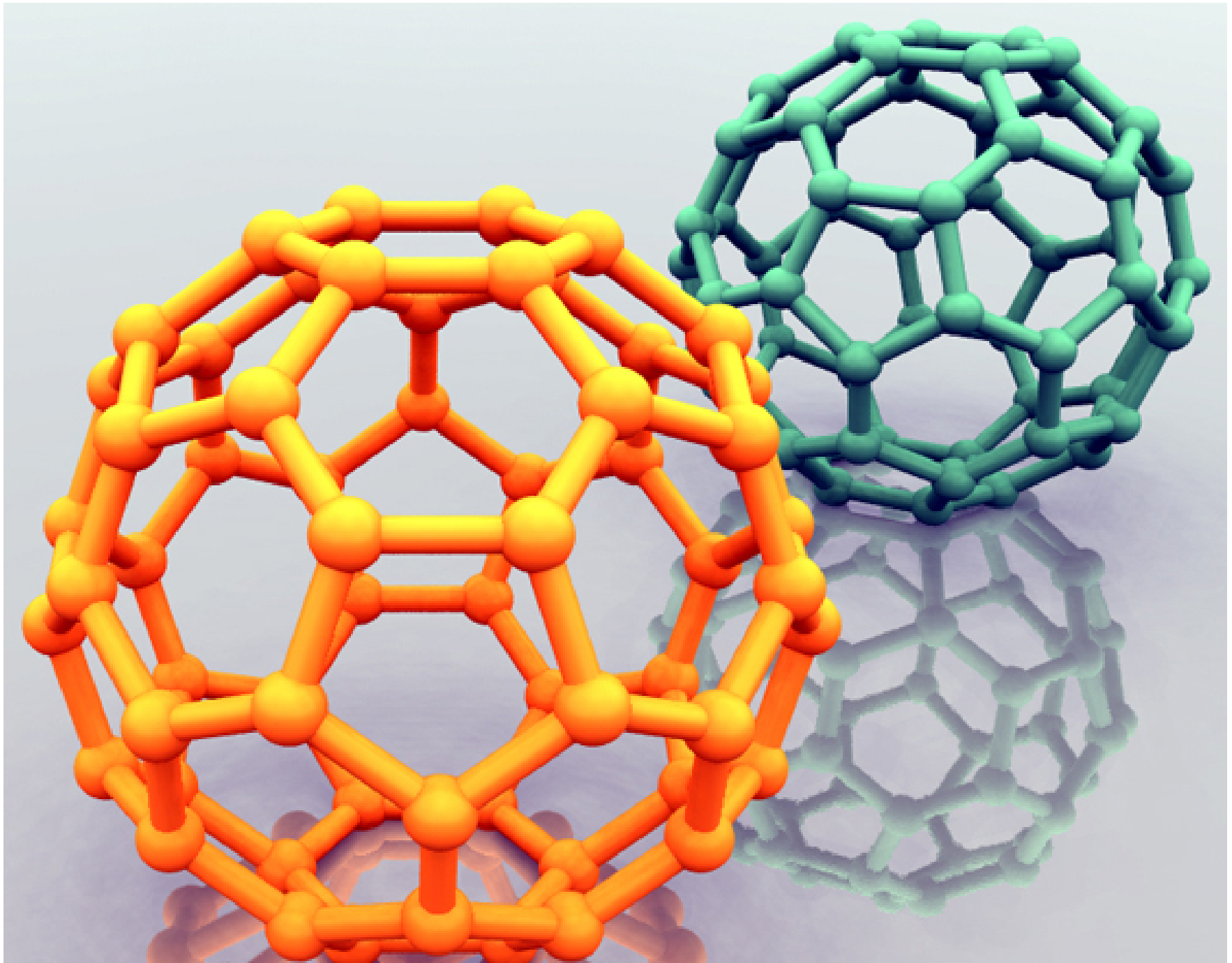
Finding the structure?

What was the structure?

Very difficult, as last resort **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 actually 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: graph theory gives another 1811 possibilities. But C_{60} is the most symmetrical one!



Fullerene C₆₀ 1nm Diameter spherical molecule

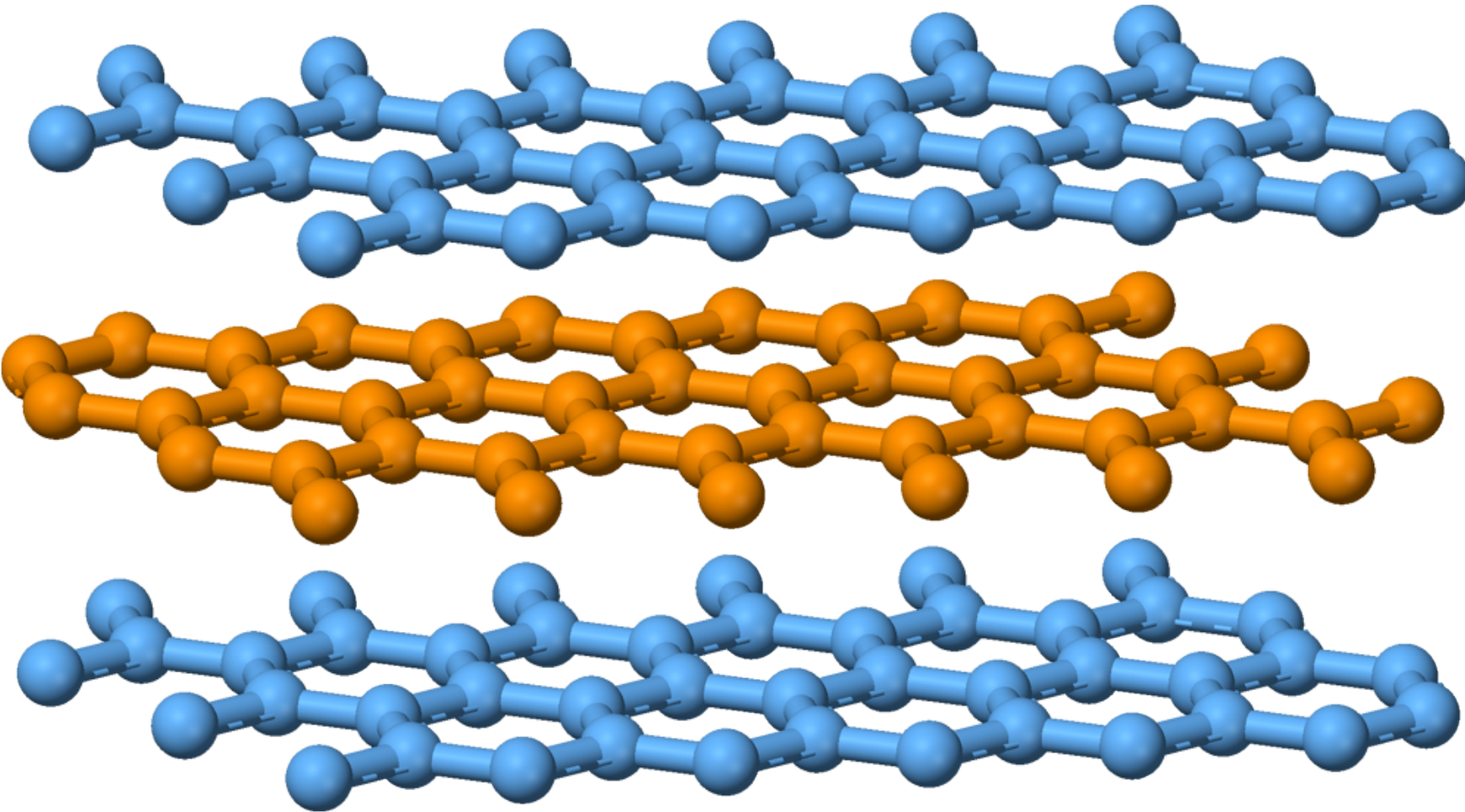
Graphite

- THE Mineral made of carbon
- So, found in large quantities in natural form
- Thermodynamically **the most stable form of carbon** (wait long enough all diamond will turn into graphite!)

Many historical and contemporary technological applications:

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

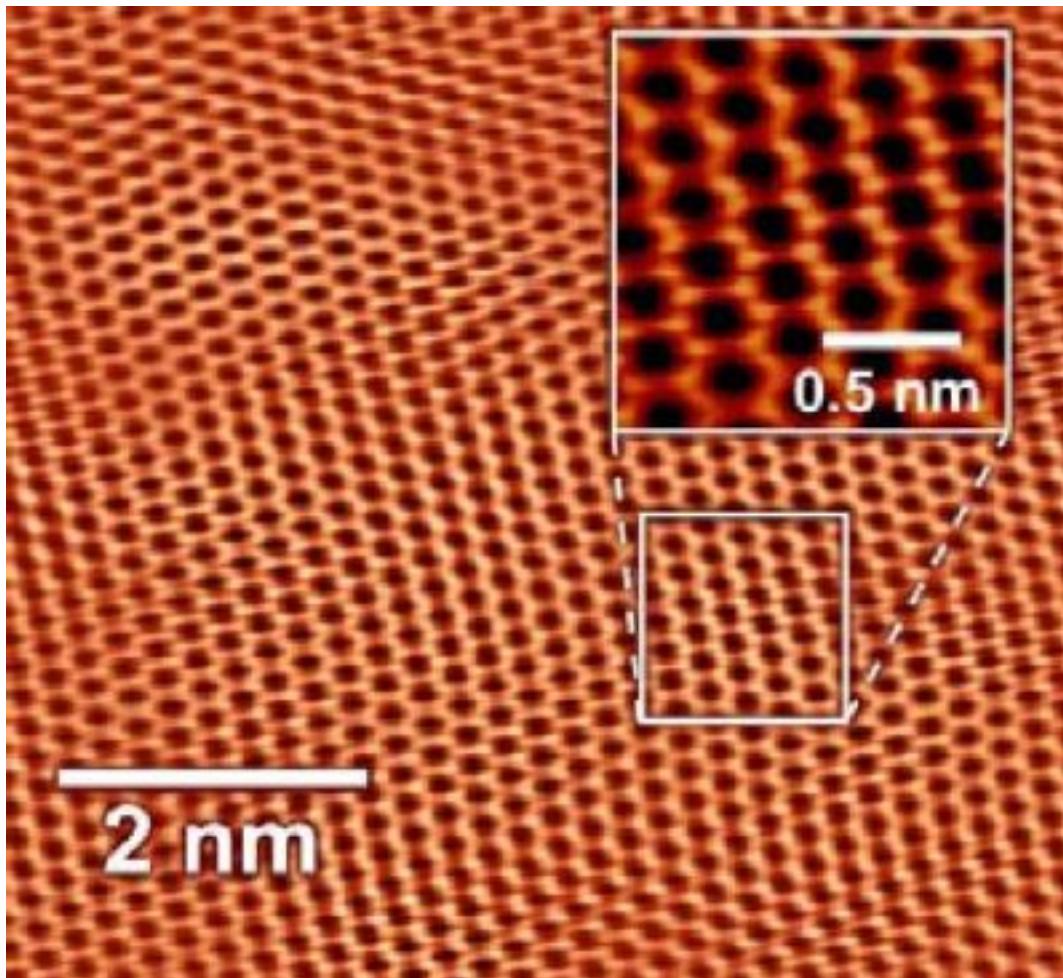
Graphite Structure



Layered structure, carbon (sp^2) layers 0.35 nm apart
The most stable form of carbon (diamond goes to graphite with time!!!)

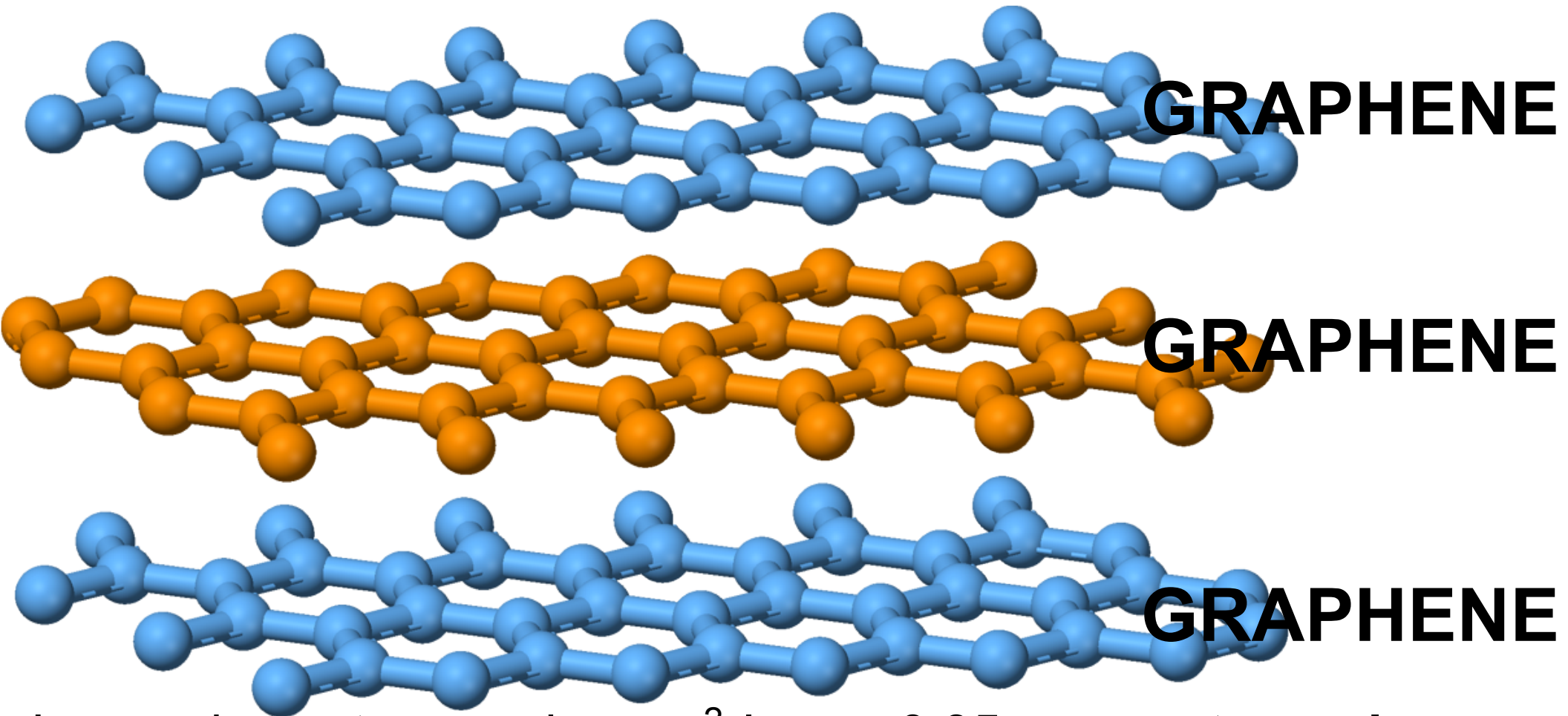
Graphite surface

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



- Electron Microscopy great BREAKTHROUGH 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?

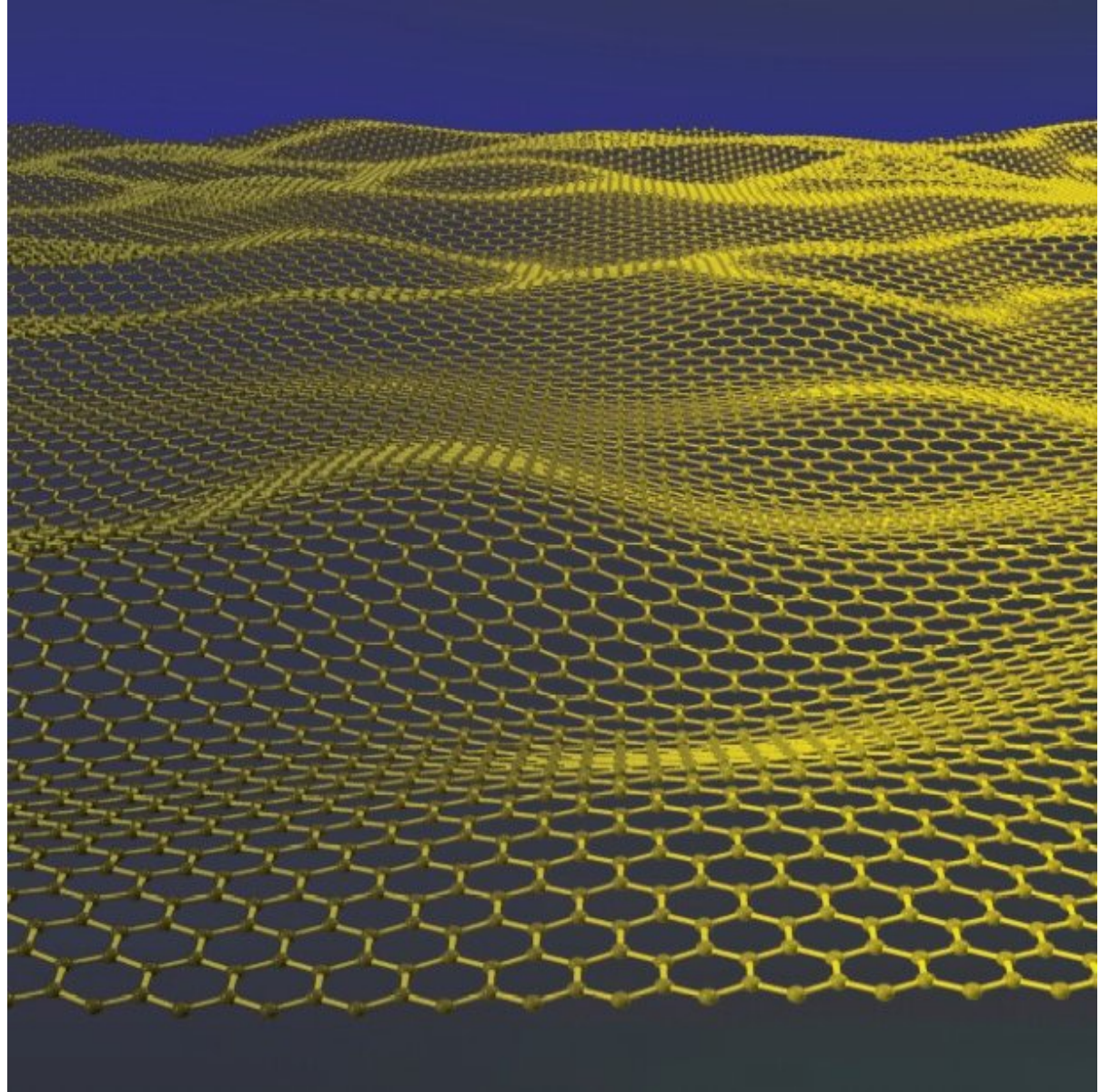
- **Perfect two-dimensional crystals cannot exist in the free state!**

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

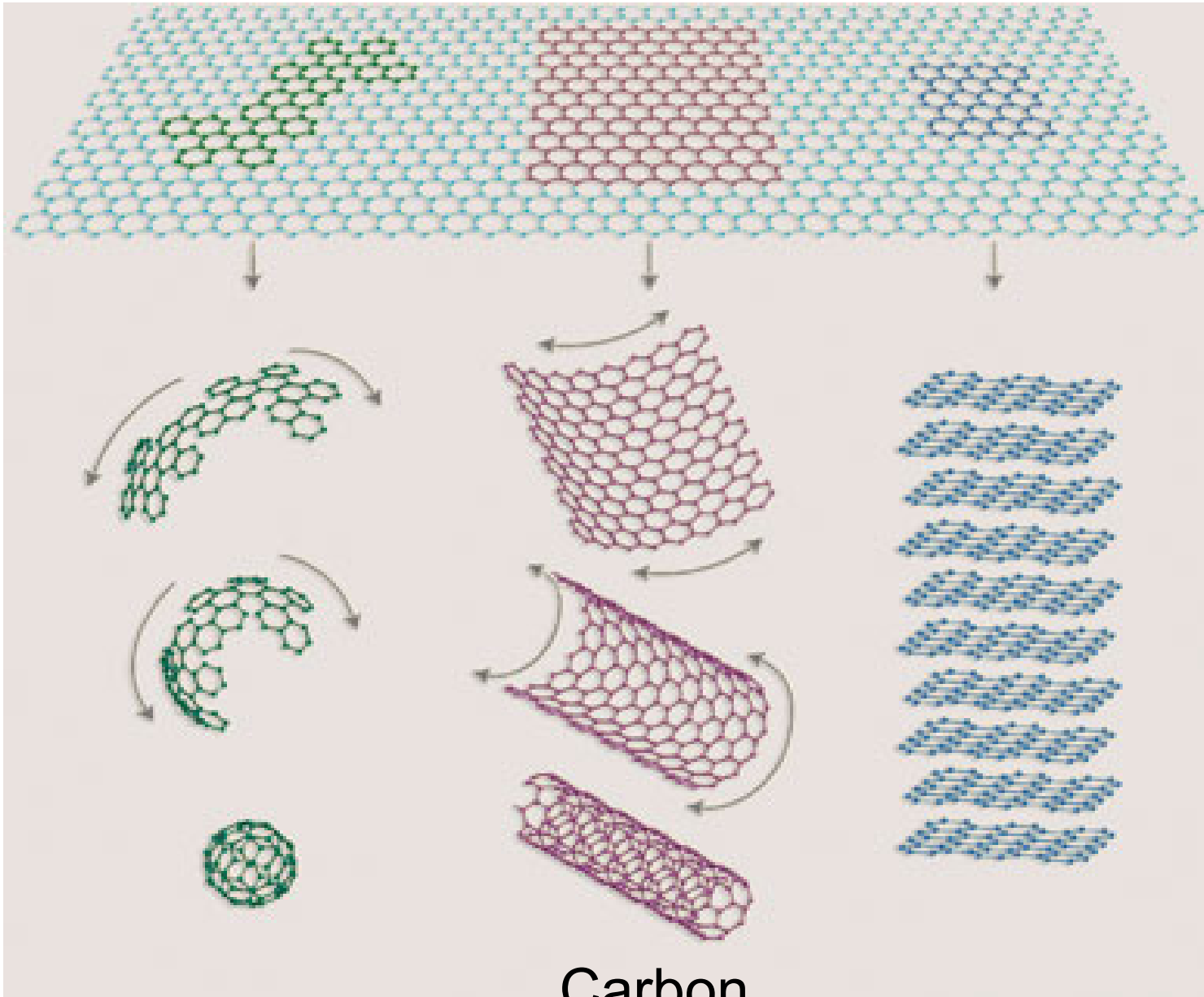
HOW?

graphene structure

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



Carbon nanomaterials



Buckyball

Carbon
Nanotube

Graphite

Graphene!

**Common
chemical
bricks
(Csp2!)**

**They all exist
and are
routinely
synthesized!**

Research in carbon **nanomaterials**

- 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, crucial 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 Zettl 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?

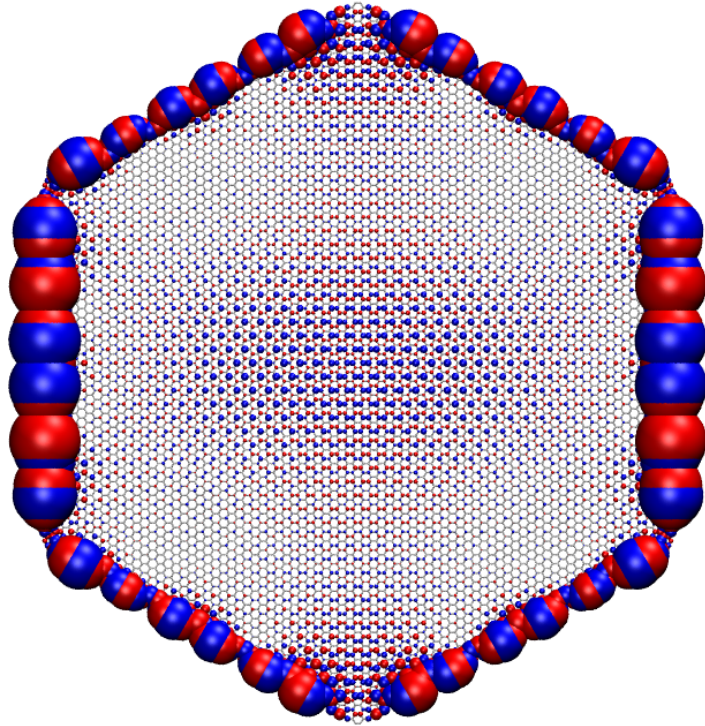
- **Carbon nanotechnology is very difficult:**
 - polydispersity (intrinsic):
 - all materials made with same building blocks (Csp²):
 - difficult to produce controlled materials
 - characterization problems
 - product separation problems
- No solution yet!!!!
- It needs complex **JOINT experimental and theoretical techniques** and analysis **GOOD FOR ME!**

**Computer models aid
COMPLEX experiments (I)
Electronic properties of carbon
nanomaterials!**

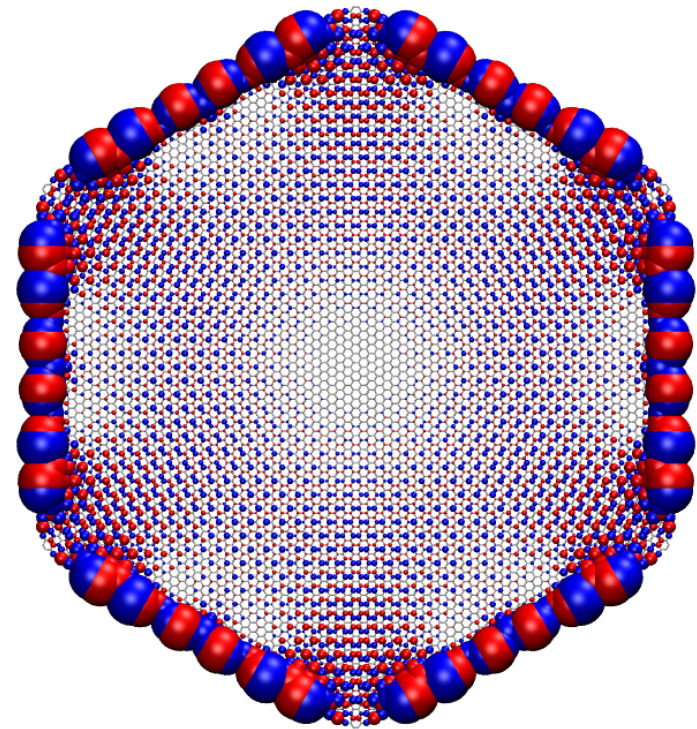
Developing QM software for carbon

- 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 (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 (indirect methods, distributed memory)

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 SOFTWARE**

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

3D structure of Graphene

- From results of 2011 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 ($5 * 10^{**4}$ atoms 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 extremely difficult impossible experimentally and see what happens

Very challenging: how to asses the quality of models without experiment?

Research III Virtual/in silico experiment

Nanonozzles (MD!!! what you study in this course!)

Ejection Dynamics of a Simple Liquid from Individual Carbon Nanotube Nozzles

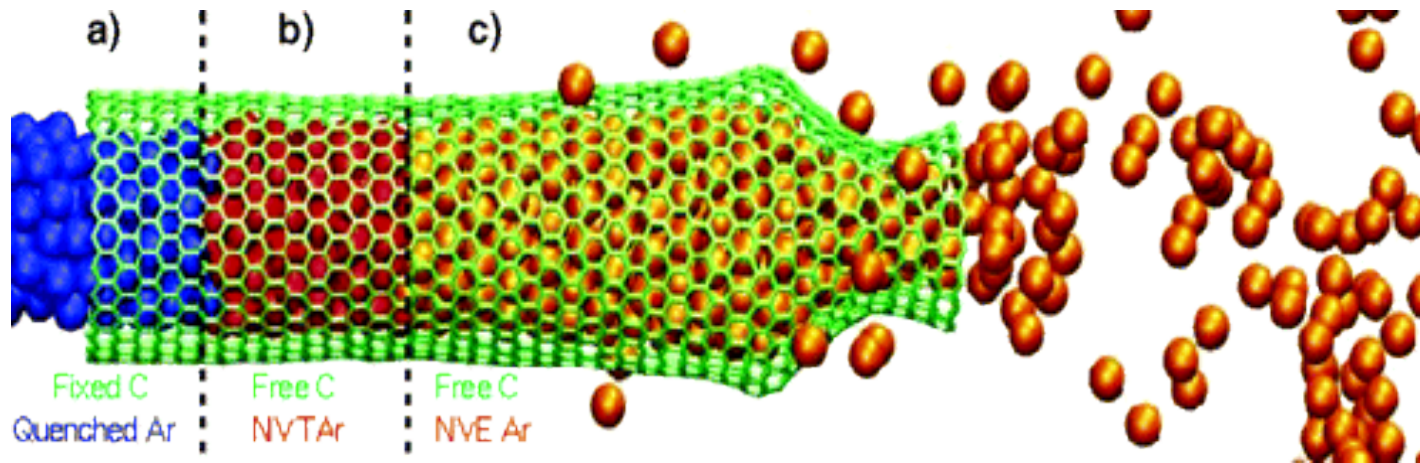
Manuel Melle-Franco^{*†‡} and Francesco Zerbetto^{*†‡}-Nano Lett., **2006**, 6 (5), pp 969–972

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.

Nanonozzles Virtual Experiments

Liquid Argon at high pressure trough carbon nanotube nozzle, **NANO-FLUIDICS!**

- 2 years programming
- 2 weeks simulations



Specific MD software to do this, very challenging algorithms and physics. **VIDEO!**

Research IV Virtual/in silico experiments

BIO-nanotechnology

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

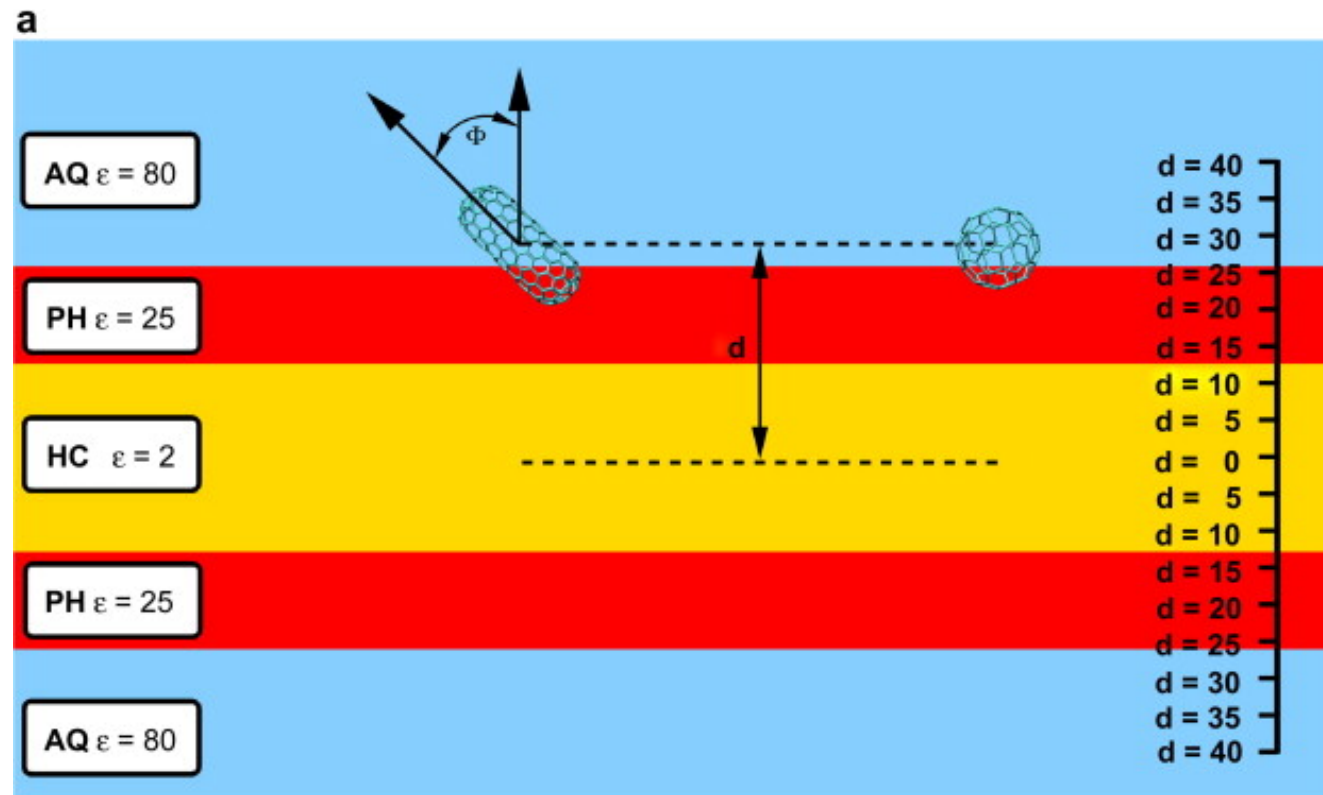
[Biomaterials](#) [Volume 32, Issue 29](#), October 2011, Pages 7079-7085

Siegfried Höfner^{a, b, , ,}, Manuel Melle-Franco^c, Tommaso Gallo^a, Andrea Cantelli^a, Matteo Calvaresi^a, José A.N. F. Gomes^c, Francesco Zerbetto^a

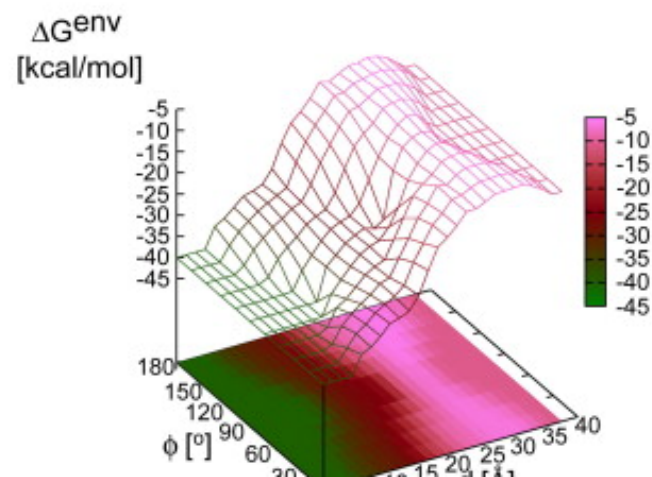
Carbon nanotubes have been proposed to serve as nano-vehicles to deliver genetic or therapeutic material into the interior of cells because of their capacity to cross the cell membrane. A detailed picture of the molecular mode of action of such a delivery is, however, difficult to obtain because of the 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.

Nanocarbon and membranes

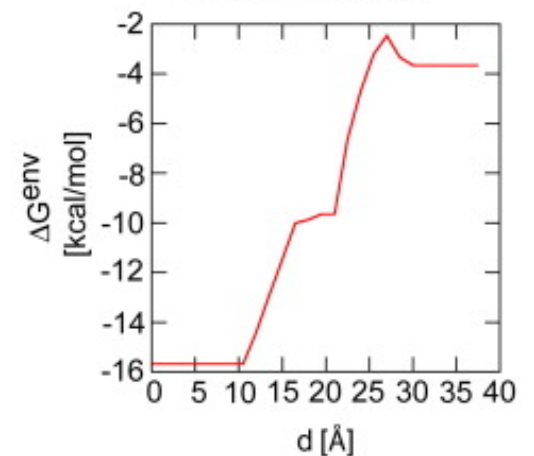
- Membrane (Spanish flag)
- Energetics for a C_{60} and small nanotubes entering the membrane (yellow apolar part: MORE STABLE than outside)



b Membrane Insertion Profile for a Small NT (21Å x 8Å)



c Membrane Insertion Profile for C60 Fullerene



Nanotoxicity

- Nanotoxicity is fundamental issue in nanotechnology!!!!
- Exp. PURE fullerenes and nanotubes are VERY TOXIC for cells!!!
 - High cytotoxicity -> 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 of nanomaterials
- Very complex problems need specific software and approaches
- Needed to complement / explain / justify experimental results of nanomaterials
- 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!!!

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:



Compressed sensing

Compressed sensing used for DSP and image processing:

- Fourier transforms 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!

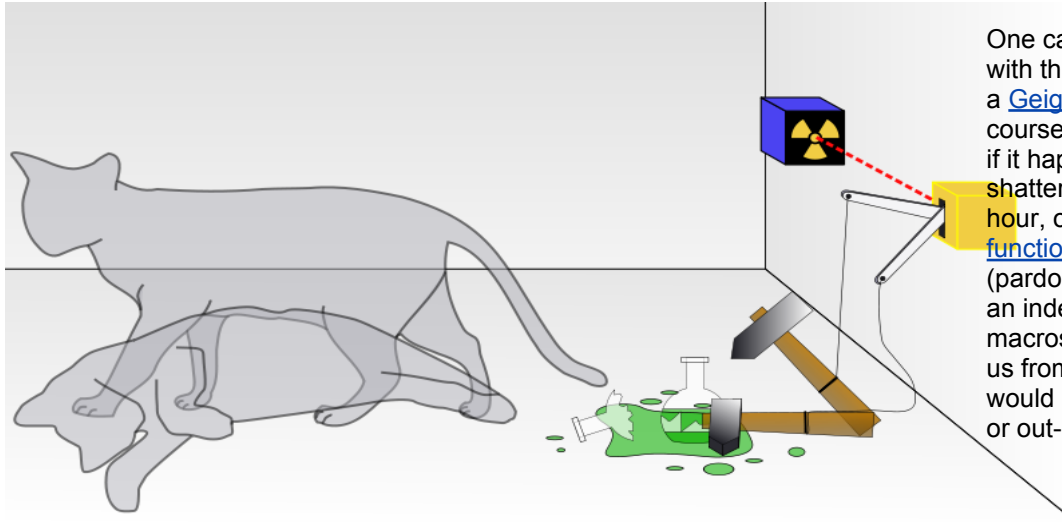
Final Comments

Short snapshots of what we do, we do many other things.

Work with chemists, physicists, biologists, mathematicians, and, now, directly with computer scientists!

I am an **active researcher**, I also direct, supervise and coordinate but most of my time **I DO RESEARCH myself, I am very curious and is FUN, that is why I do it!**

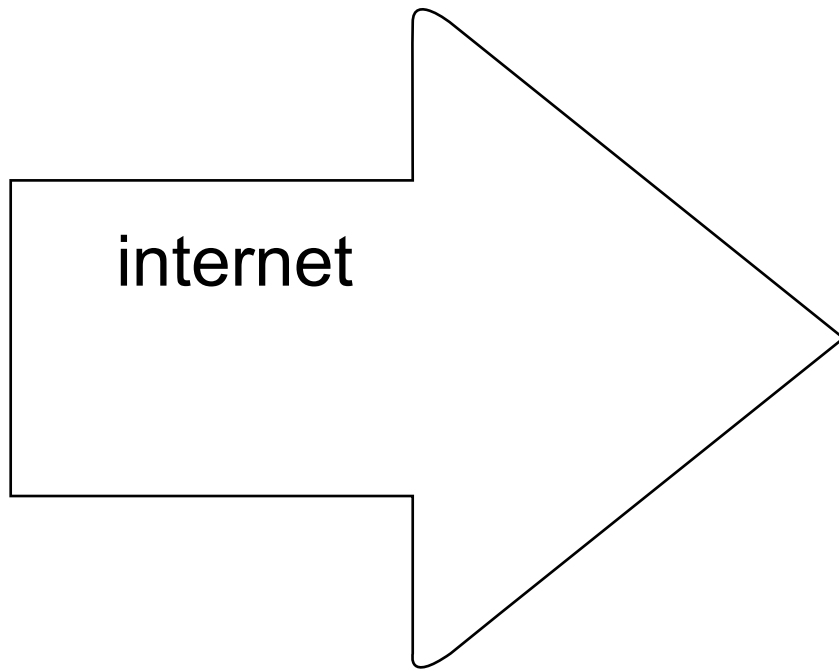
Schrödinger's cat in box



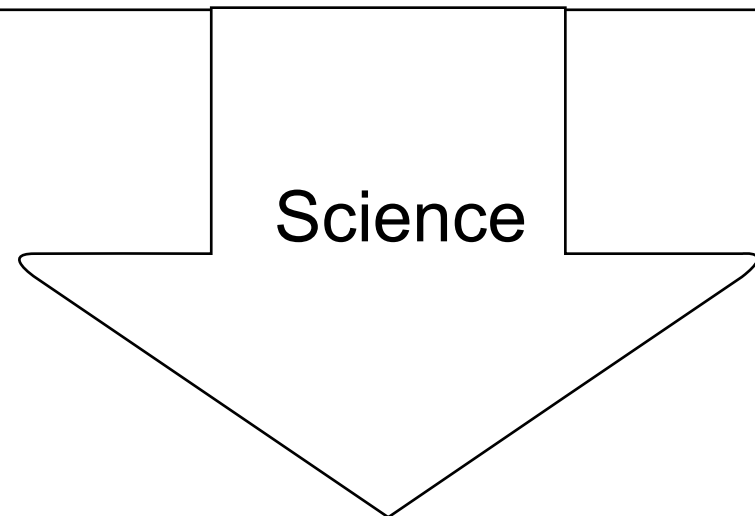
One can even set up quite ridiculous cases. A [cat](#) is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a [Geiger counter](#), there is a tiny bit of [radioactive](#) substance, so small that perhaps in the course of the 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 **SOMETIMES TOO!**



Feel free to contact me for any reason!

Room 3.21 in the DI

EMail/chat: manuelmelle@gmail.com

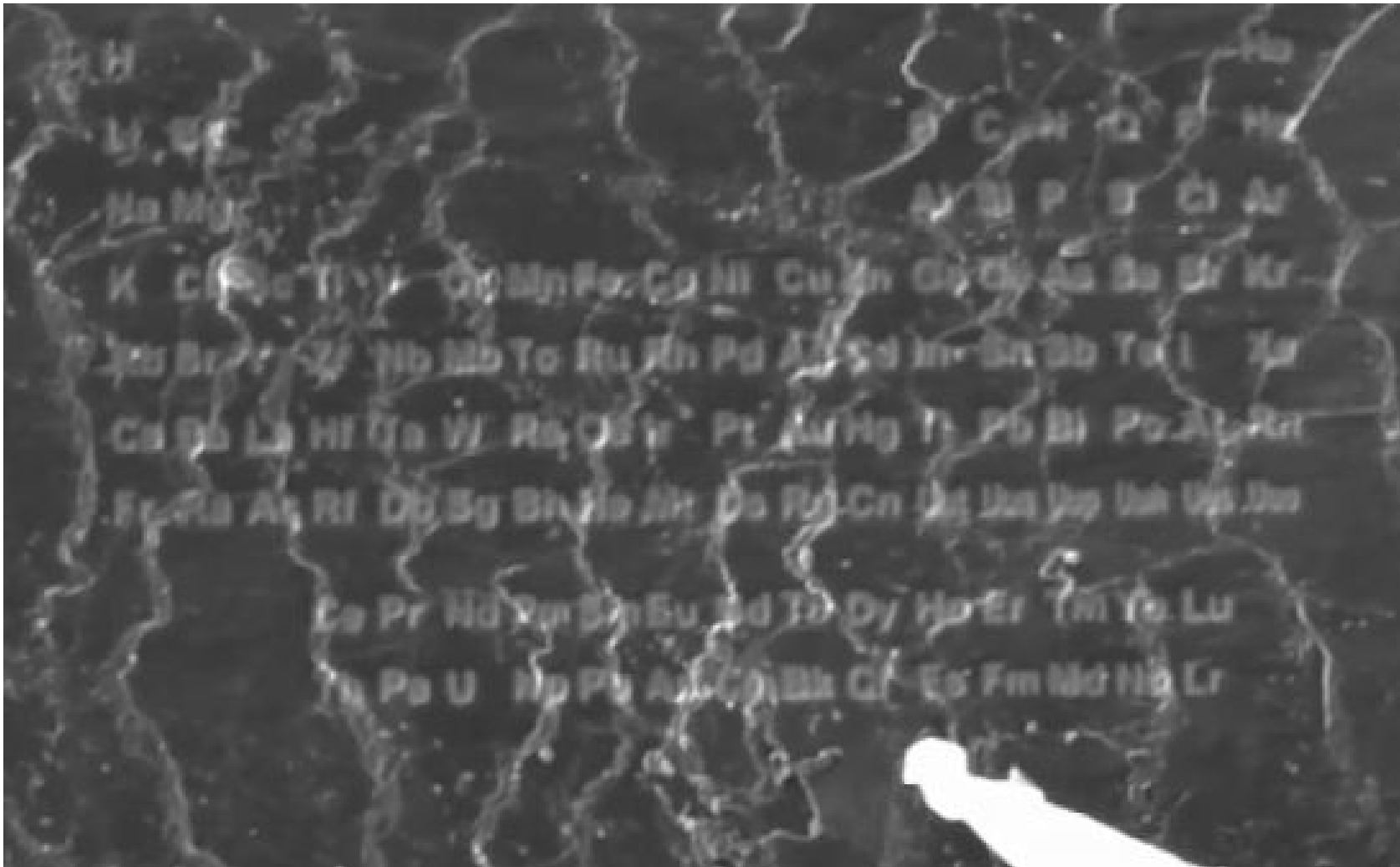
Email: manu@di.uminho.pt

Acknowledgements

- Funding: European Union, Portuguese government and Italian government
- Co-workers all over the world!
- **CCTC (DI UMINHO)** for hiring me to do more exciting science!!!

thank you for your time, :D
hope it was worth it!

Smallest Periodic table!!!!



0.046 mm

0.088 mm

On a human hair!!!