Physics of carbon nanostructures

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- Brief historical review
- Defects and some interesting experiments
- Theoretical models and results
- Nanotechnologies
- Conclusion

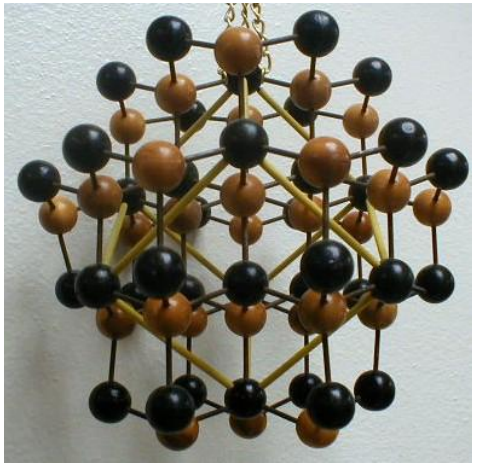
Part 1

Brief historical review

Carbon lattices

Sp3

Tetrahedral network



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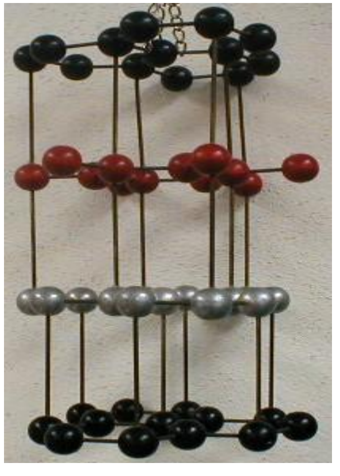
strong bonds

Sp2

Hexagonal layers



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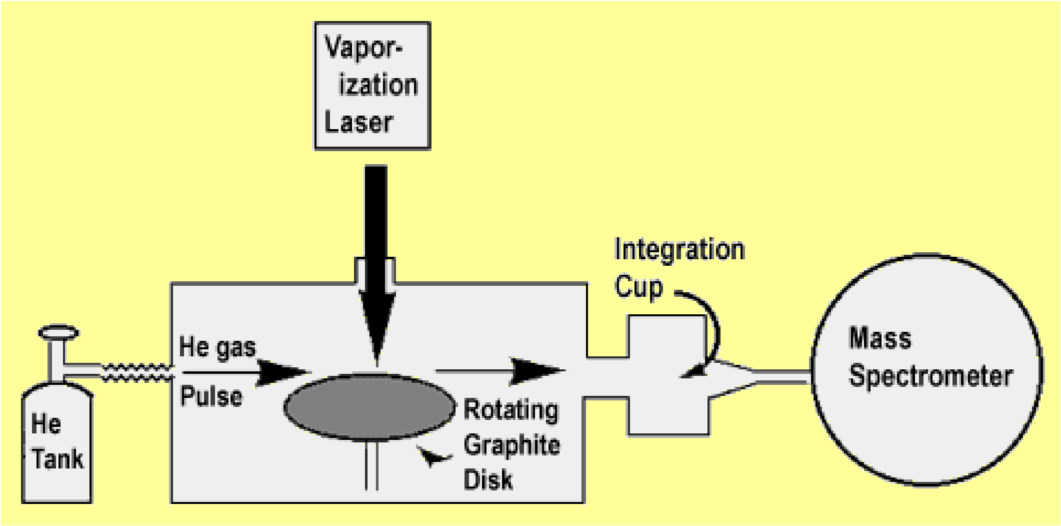
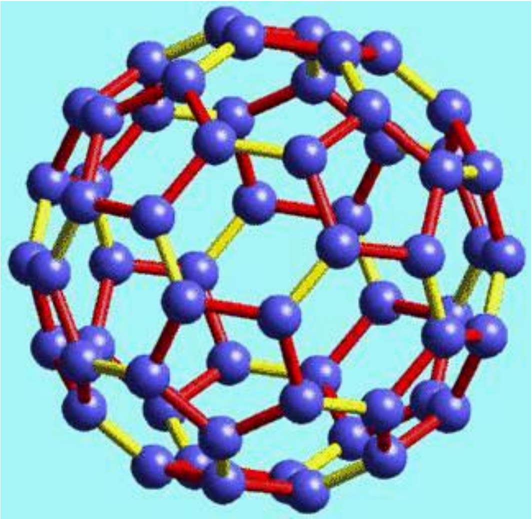
weak VDW forces between the layers

Ideas

- 1970 Osawa: a molecule made up of sp^2 hybridized carbons could have a soccer structure
- 1973 Bochvar and Gal'pern: proposed C_{60} and C_{20} structures and some their properties
- 1985 Kroto: an idea of the experiment with vaporized carbon

Third form of carbon (1985)

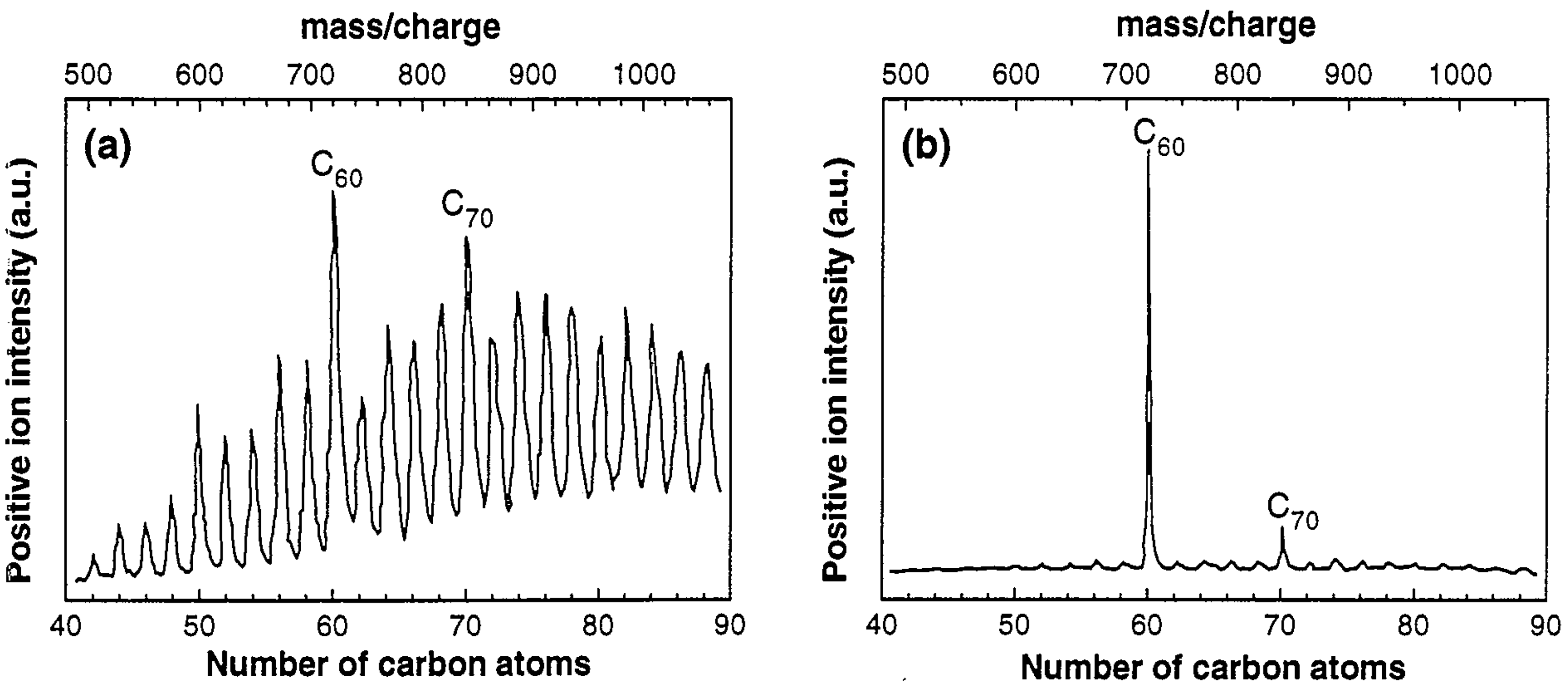




Smalley's graphite vaporization apparatus allows to produce fullerenes by vaporization of graphite in a helium environment: from metal clusters to carbon clusters

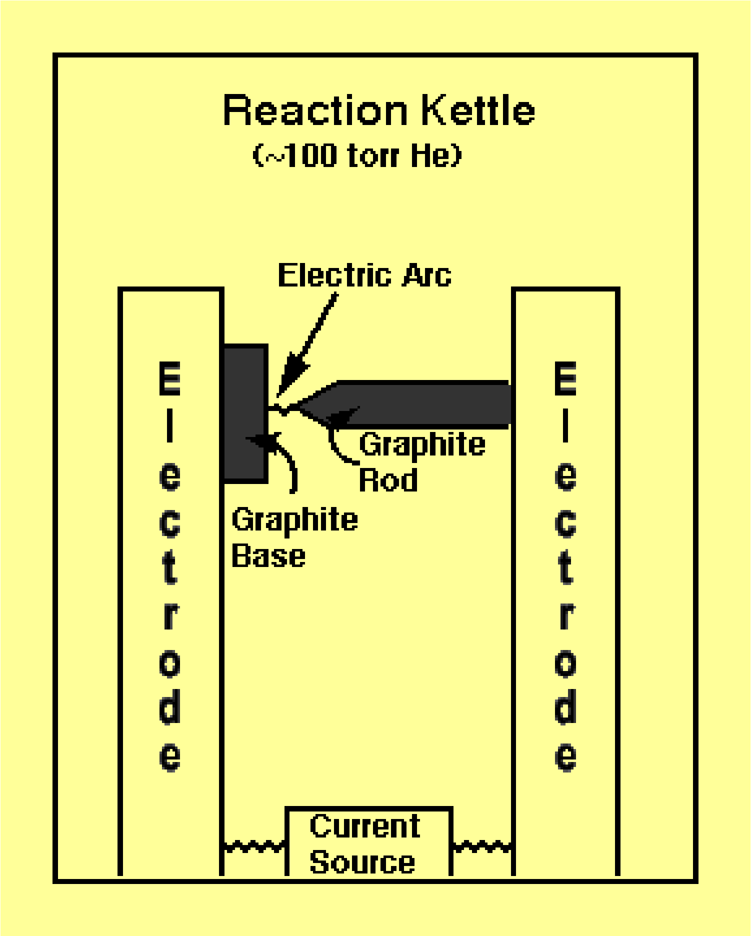
Mass spectrum of carbon clusters

H.W. Kroto, JR. Heath, S.C. O'Brien, R.F. Curl, R.E. Smalley, Nature 318 (1985) 162



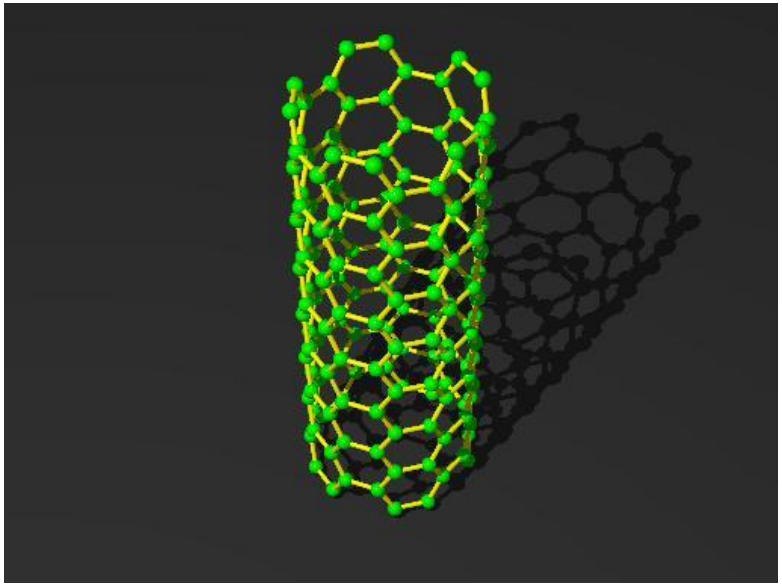
(a) At low He pressure (less than 10 Torr) a nearly uniform distribution of even-numbered clusters was obtained,
(b) Under certain (optimized) clustering conditions the relative abundance of C60 was greatly enhanced.

Kratschmer-Huffman graphite vaporization apparatus (1990)

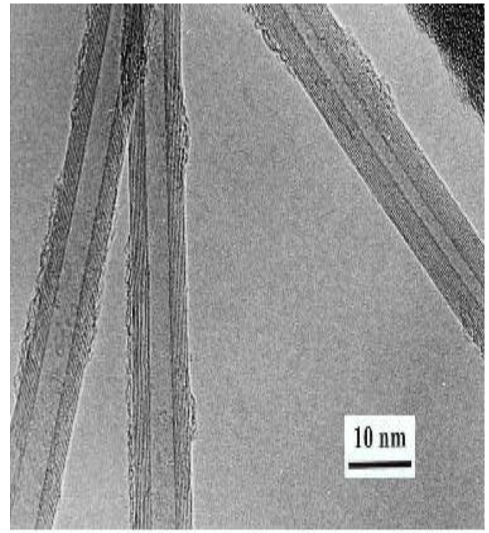


- A simple way to produce macroscopic quantities of solid fullerenes by arc-vaporization of graphite in a helium environment
- This made it possible to perform a more complete analysis of C_{60} properties.
- The analyses led to the first solid evidence that C_{60} was a closed sphere.

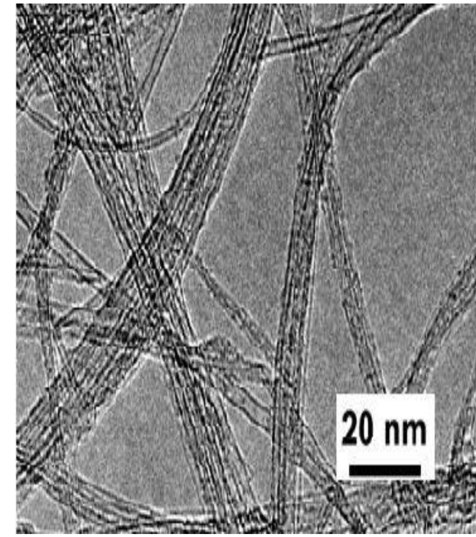
Carbon nanotubes (Iijima, 1991)



source: Alexandre Mayer's gallery of carbon nanotubes

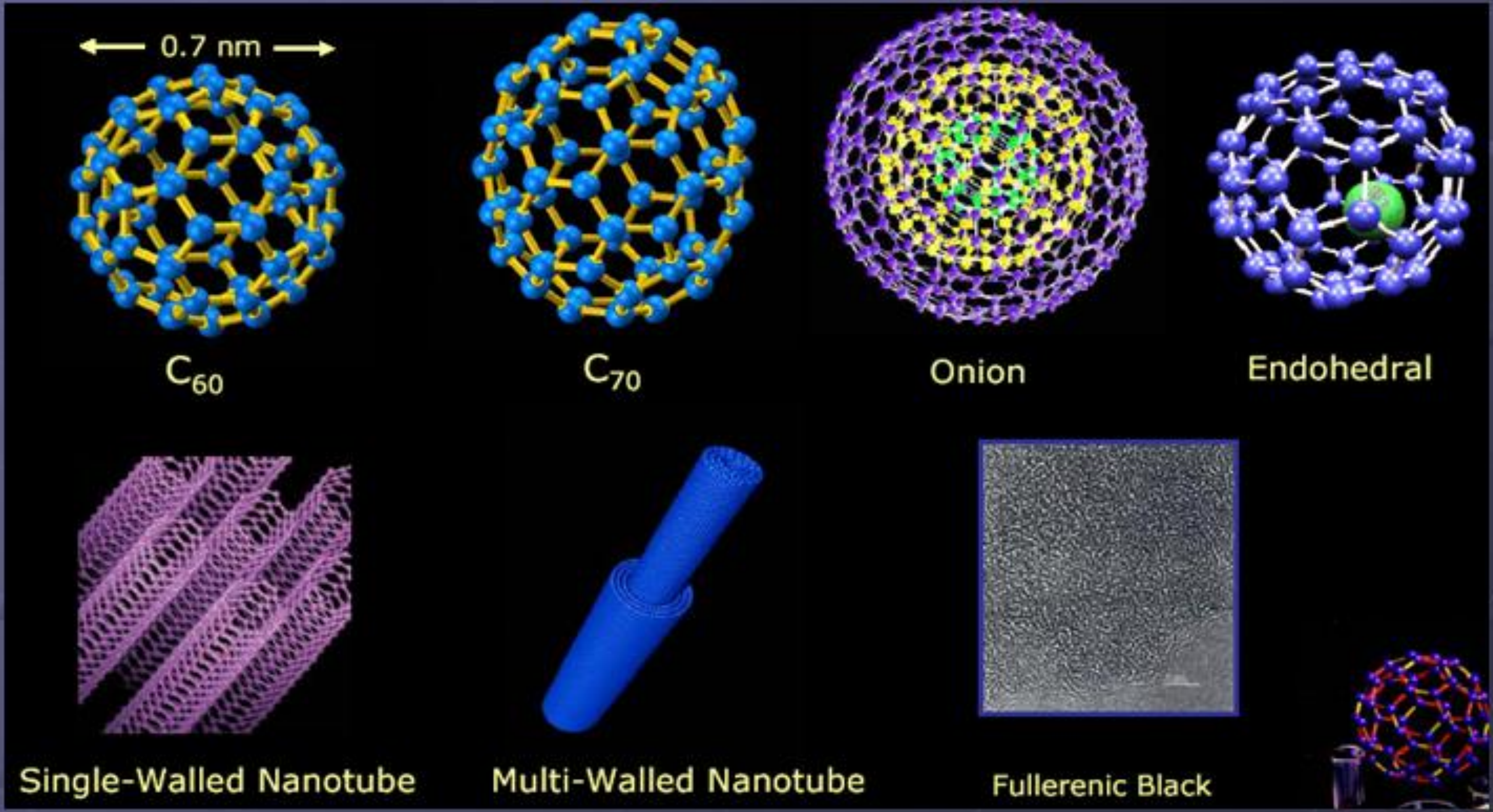


multi-walled

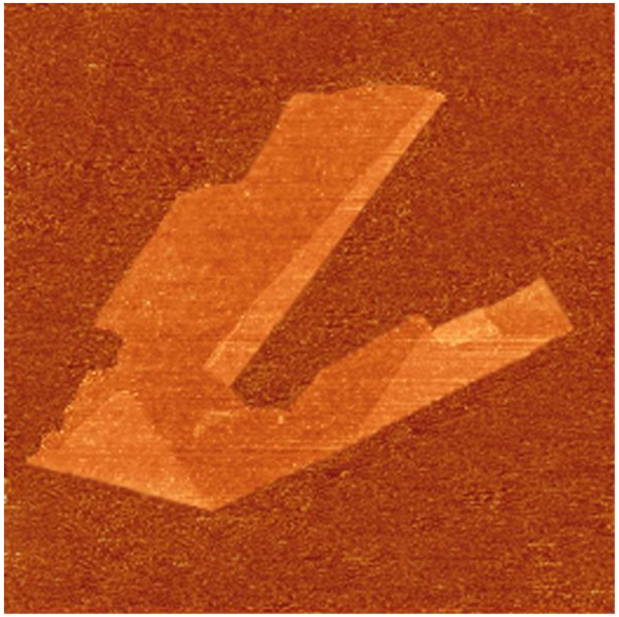


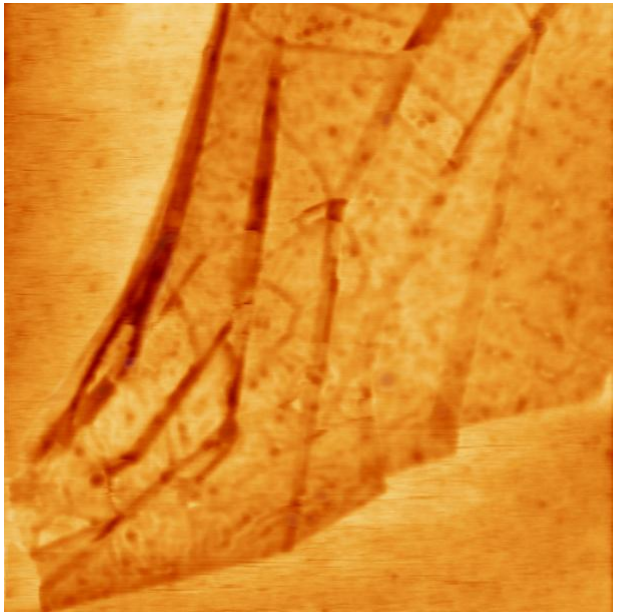
single-walled

Several Nanocarbon Structures



Graphene (2005)



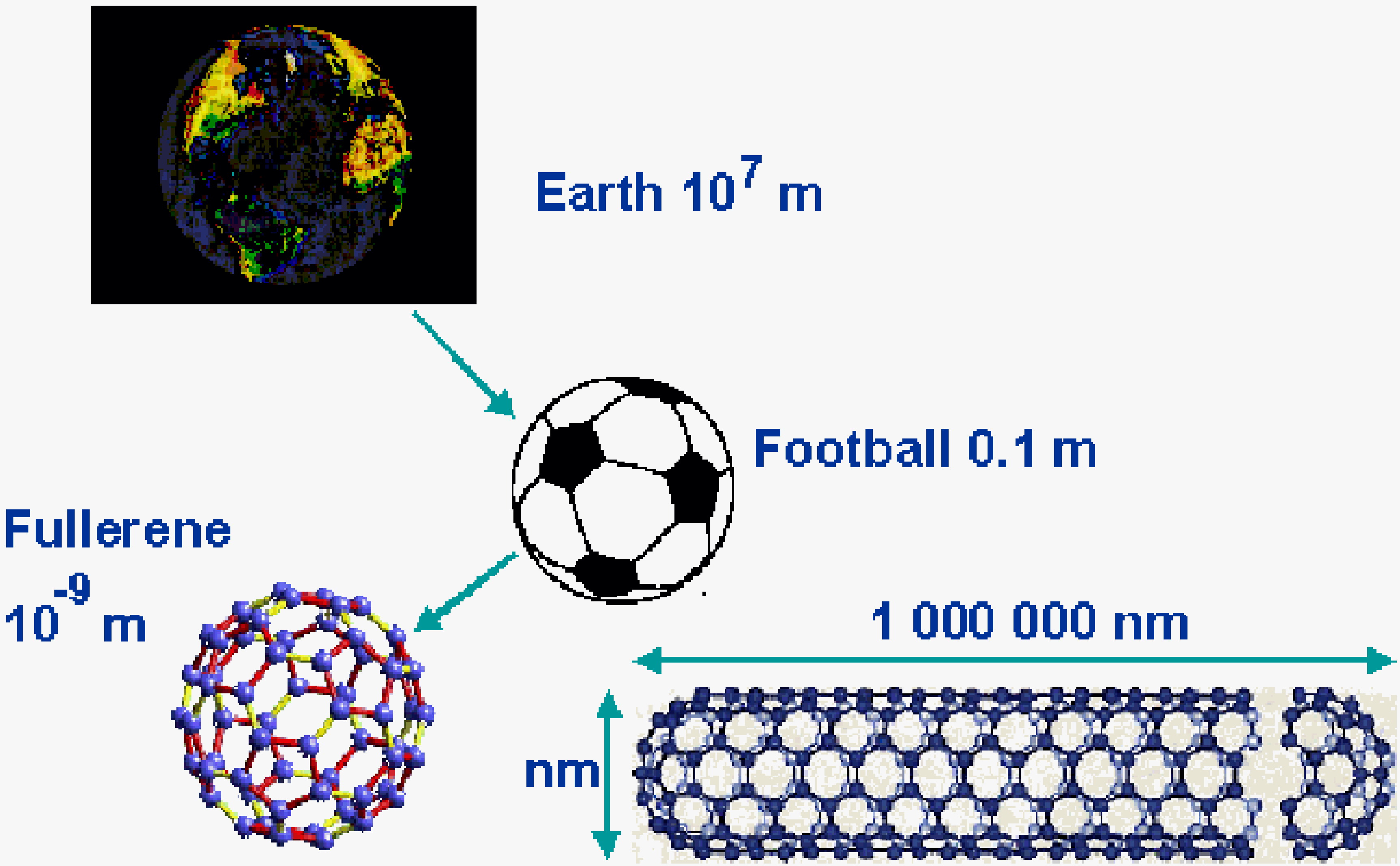


source: site of Mesoscopic Physics Group (Manchester University)

AFM images of: a graphene molecule (left). The window size is 10x10 micron (the graphene film is only one atom thick but approx. 100,000 atoms long in the two lateral directions;

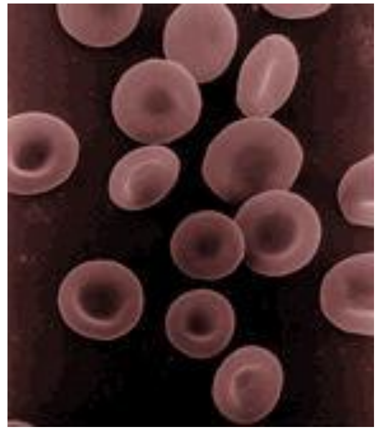
single-atom-thin carbon nanofabric (right) (3x3 micron in size). Graphene looks just like a silk tissue thrown on a surface: it is creased with many folds, pleats and wrinkles.

Size Comparison

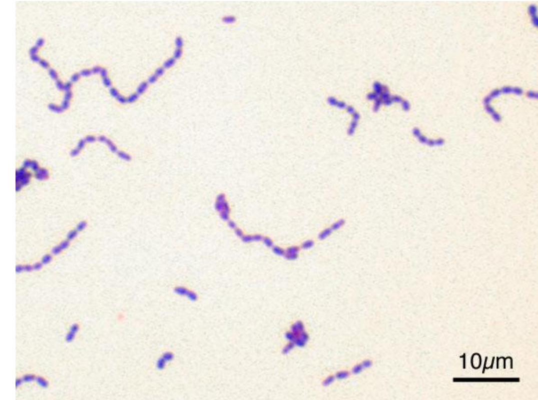


Living matter

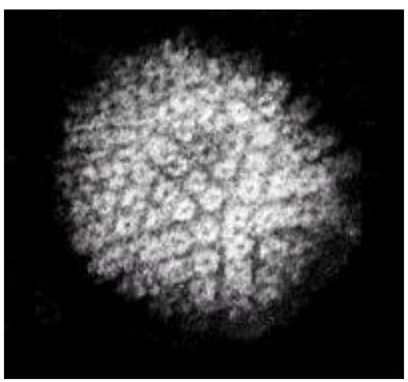
Width of hair:
50,000 nm



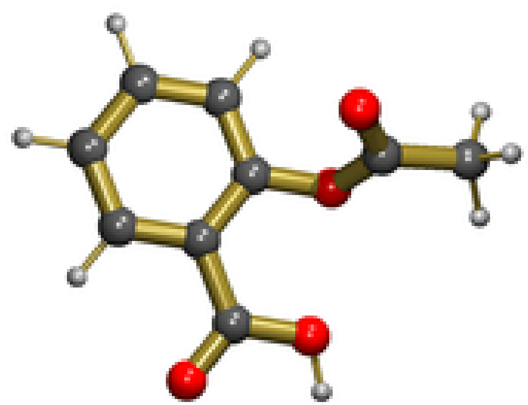
Red blood cell:
7,000 nm



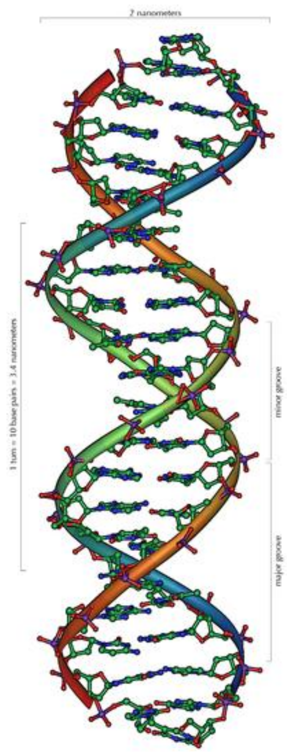
Streptococcus bacterium:
1,000 nm



Herpes virus:
100 nm



Aspirin molecule ($C_9H_8O_4$):
1 nm

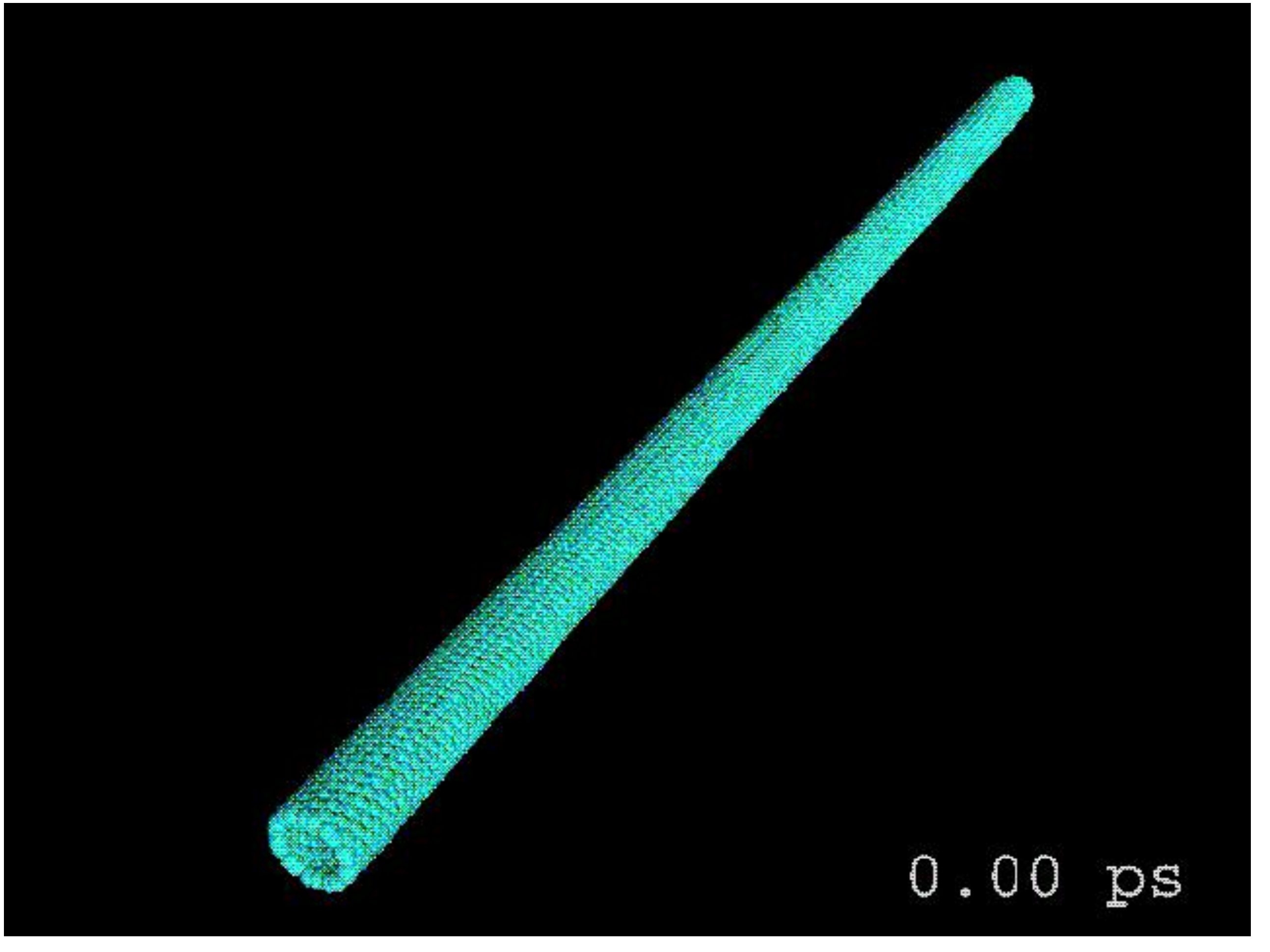


Width of DNA: 2.5 nm

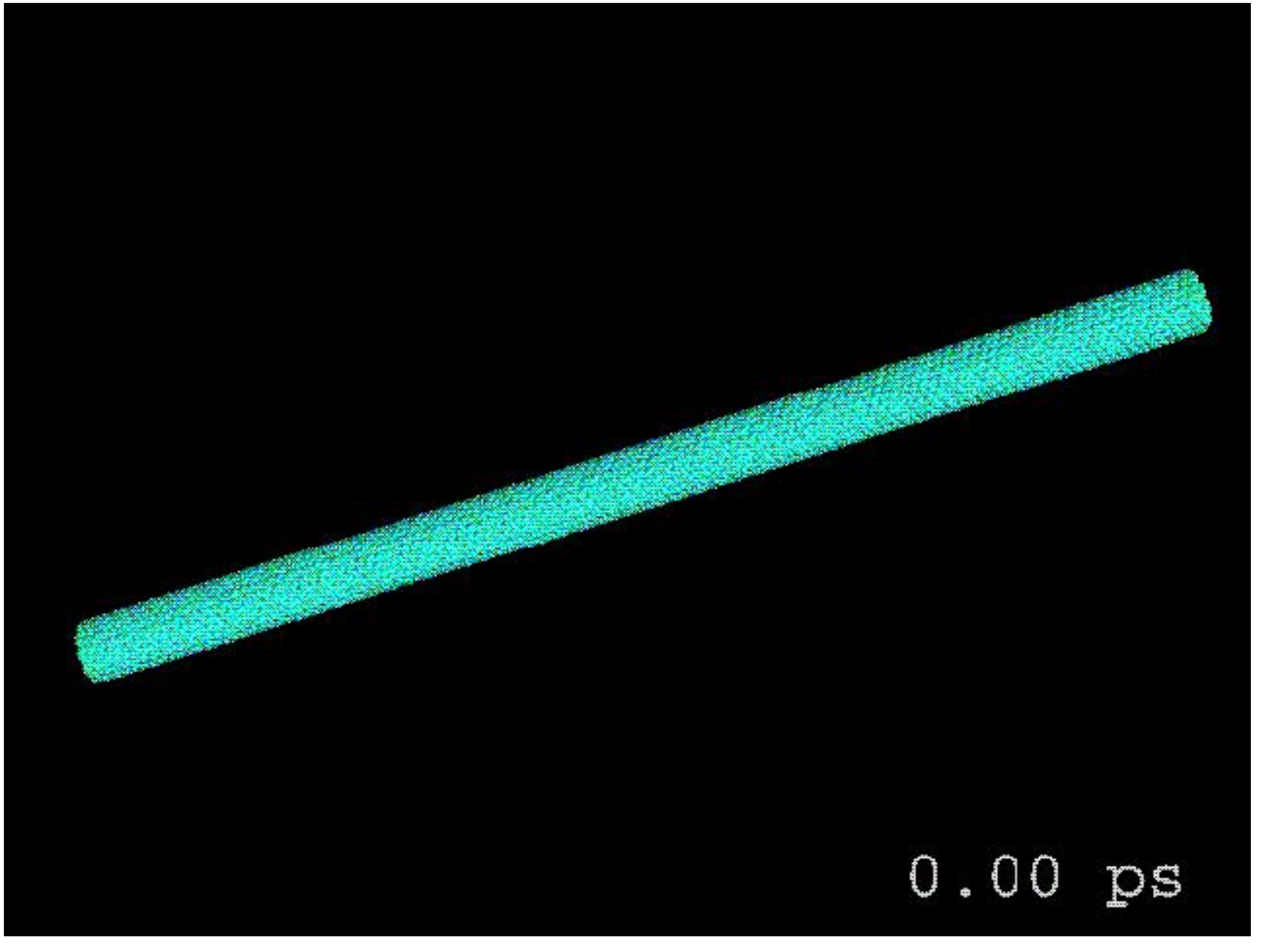
Important properties

- the high flexibility of carbon (variously shaped carbon nanoparticles: nanotubes, fullerenes, cones, toroids, graphitic onions, nanohorns, etc.)
- mechanical stress greater than that of Fe; density lower than that of Al; thermal stability at 1400C in a vacuum
- emit electrons from their tips at low electric field (application in flat-panel displays)
- large gas-adsorption capacities (other atoms can be placed inside “cage”, using in fuel cells).
- superconductivity

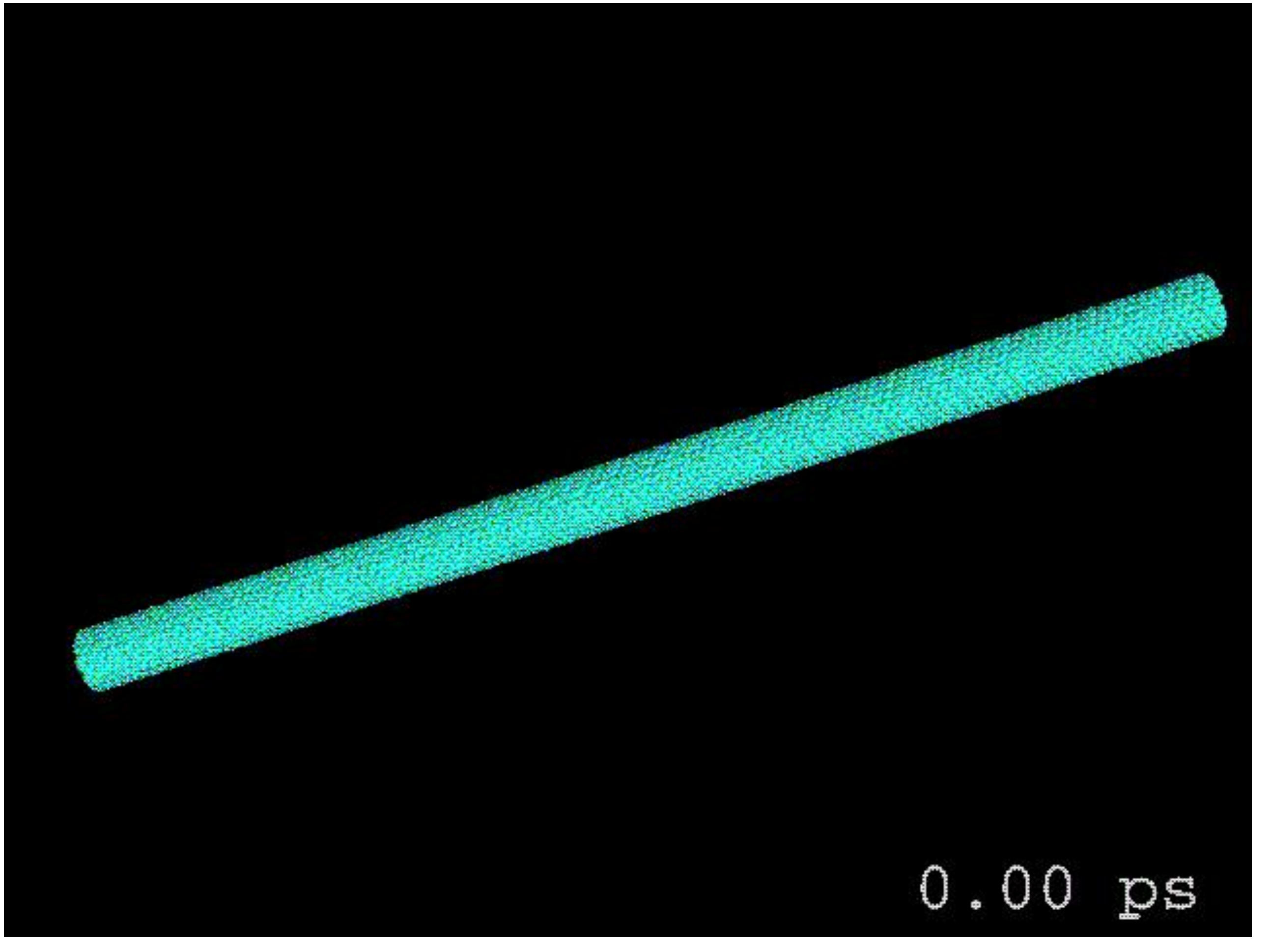
Compress



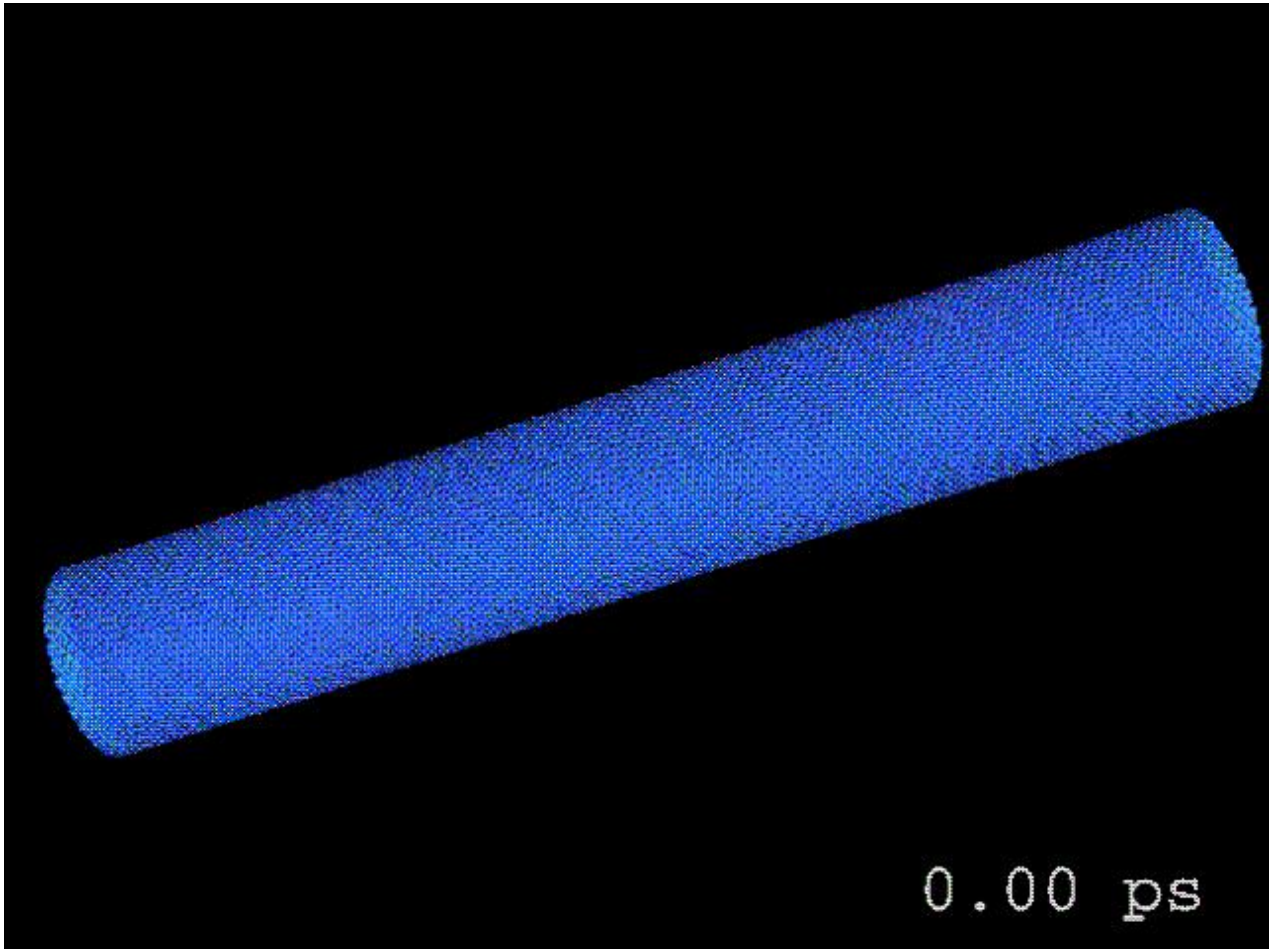
Bend



Twist



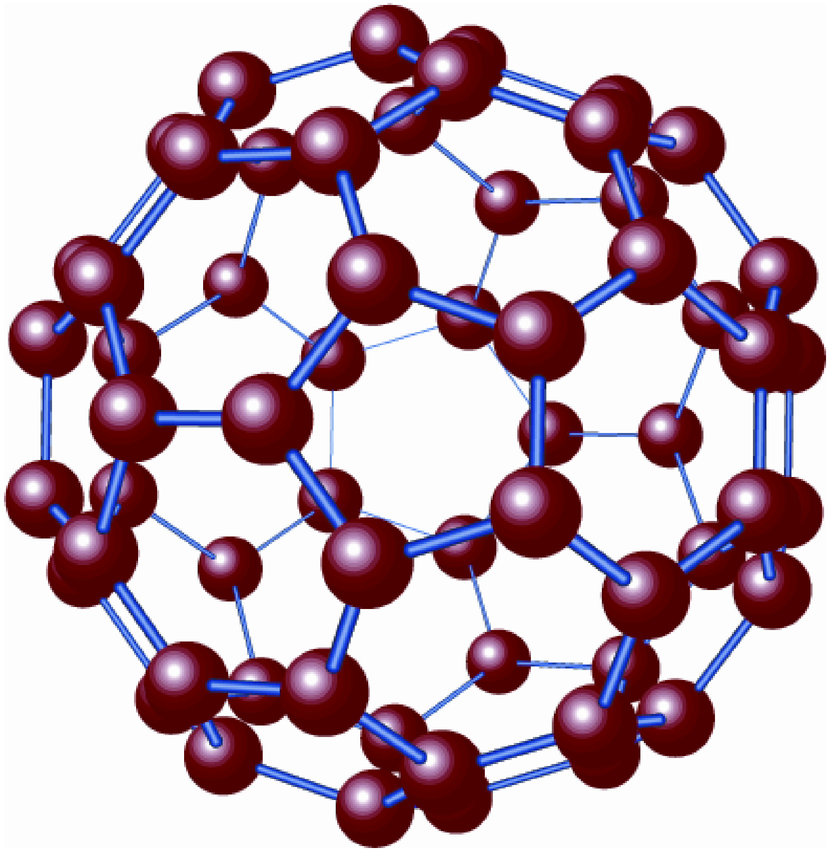
Bend multi-walled nanotube



Part 2

Defects, geometry and some interesting experiments

Pentagons (why twelve?)



$$\Sigma(6-x)n_x=12(1-g)$$

Euler’s theorem

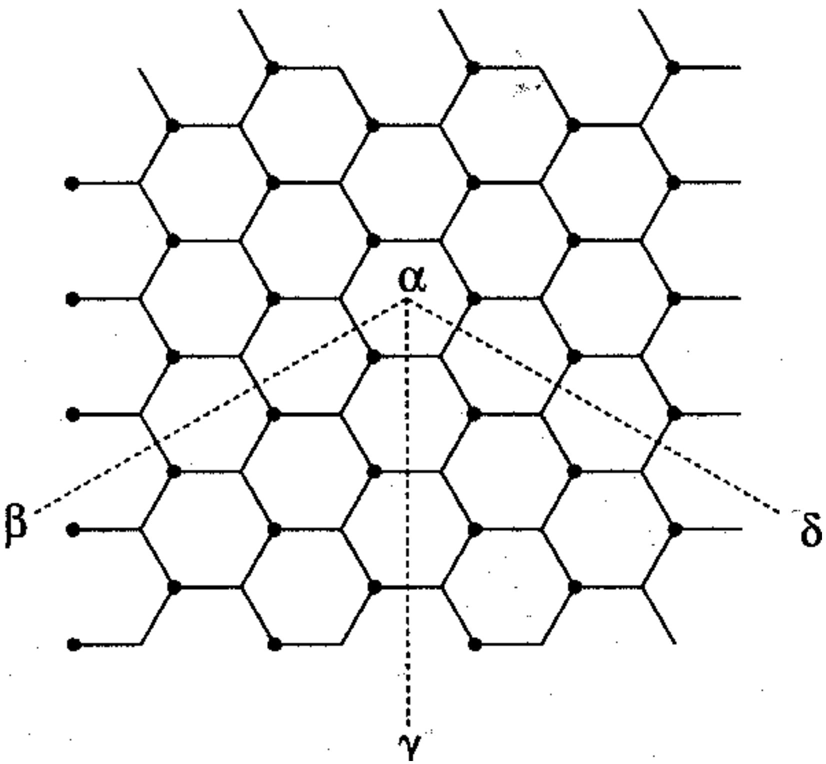
Euler's theorem relates the number of vertices, edges and faces of an object

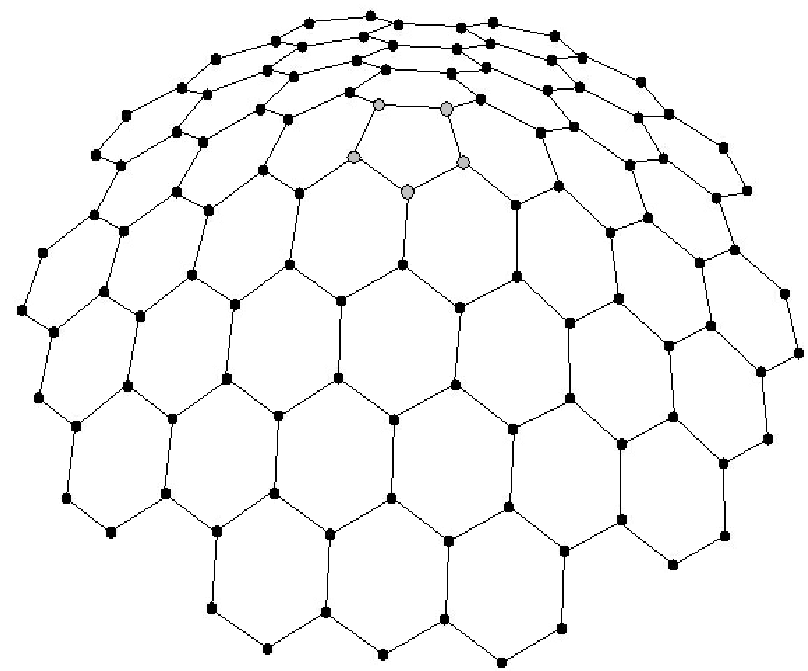
$$\mathbf{...2n_4+n_5-n_7-2n_8... = \sum(6\text{-}x)n_x = 12(1\text{-}g)}$$

n_x is the number of polygons having x sides, g is the genus. For sphere g=0, n_5=12. Thus, these microcrystals can only be formed by having a total disclination of 4π. According to the geometry of the hexagonal network this means the presence of twelve pentagons (60º disclinations) on the closed hexatic surface.

Important: Disclinations are generic defects in closed carbon structures

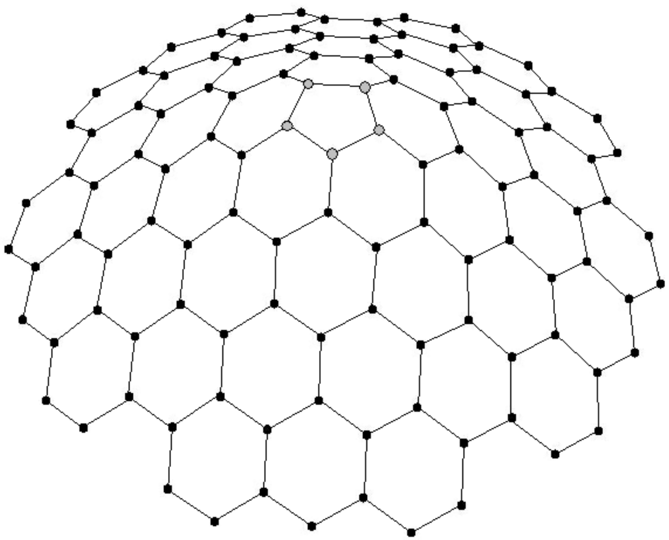
Pentagons and disclination buckling transition

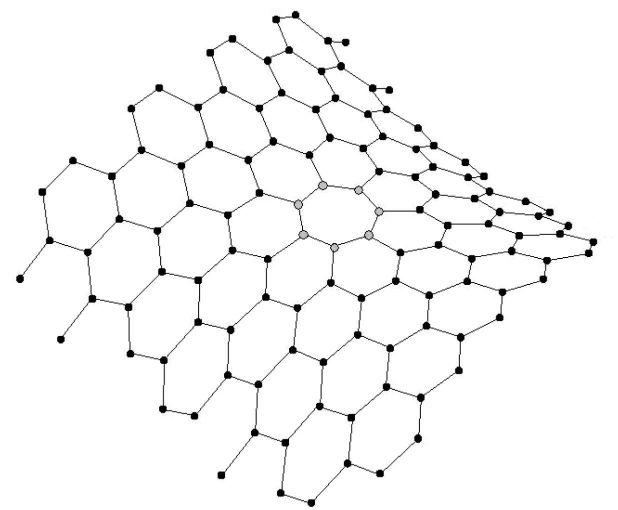




By its nature, the pentagon in a graphite sheet is a topological defect. Actually, fivefold coordinated particles (pentagons) are orientational disclination defects in the otherwise sixfold coordinated triangular lattice.

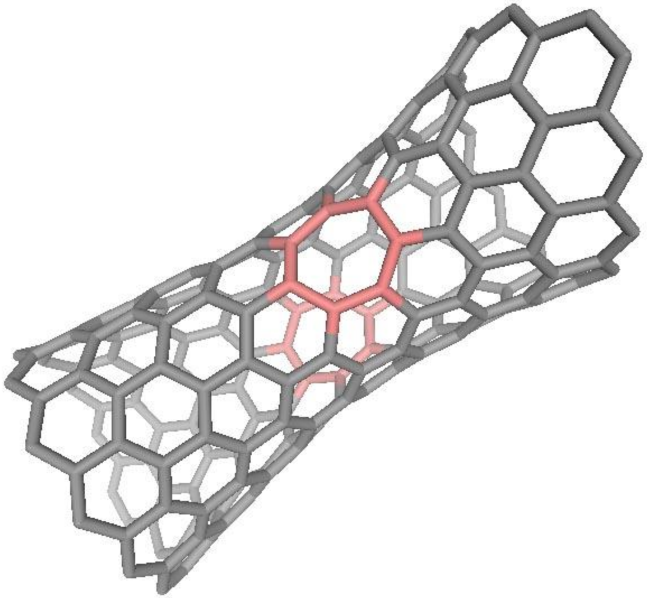
Defects, Curvature



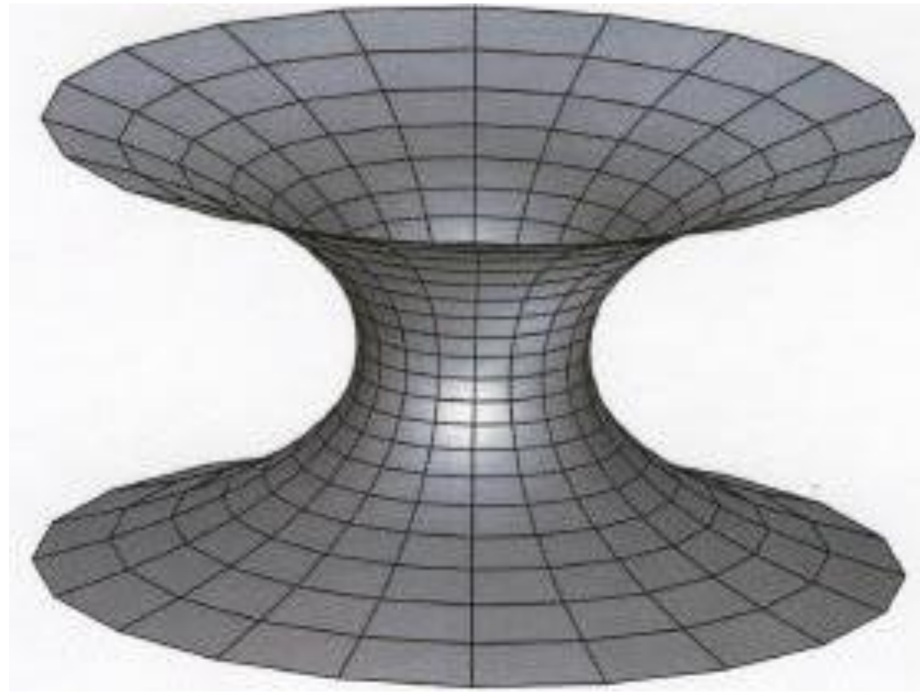


The pentagon (positive curvature) and the heptagon (negative curvature) in the hexagonal graphite lattice

Heptagons

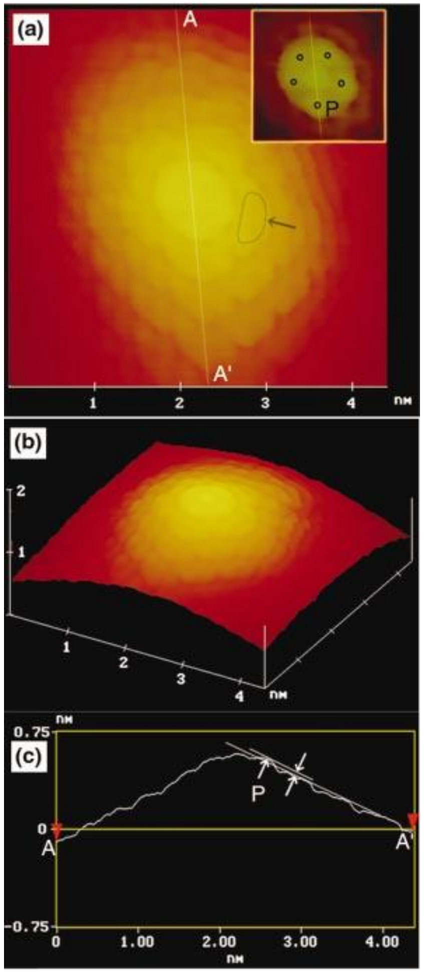


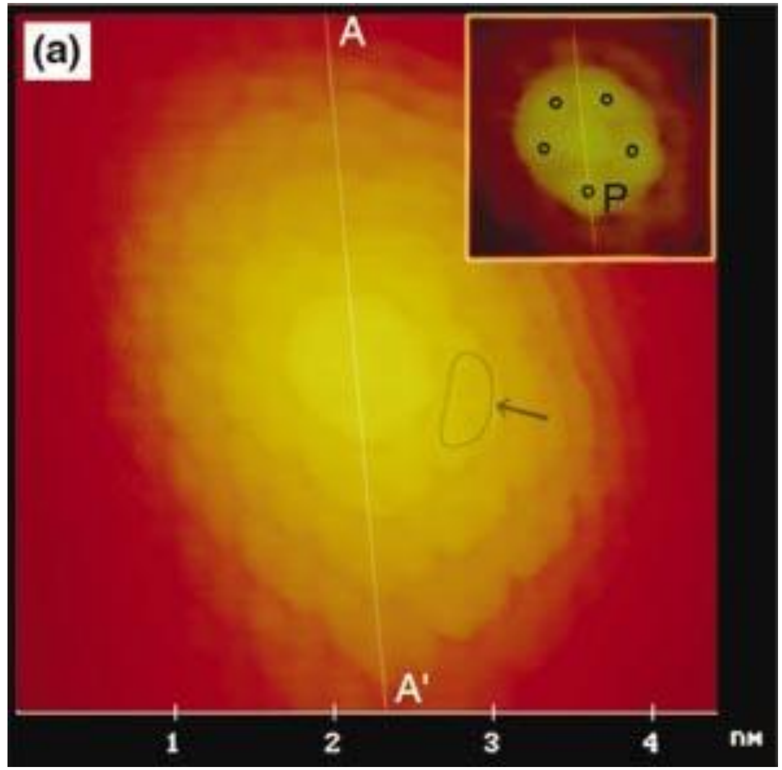
Two heptagons are inserted into graphite nanotube

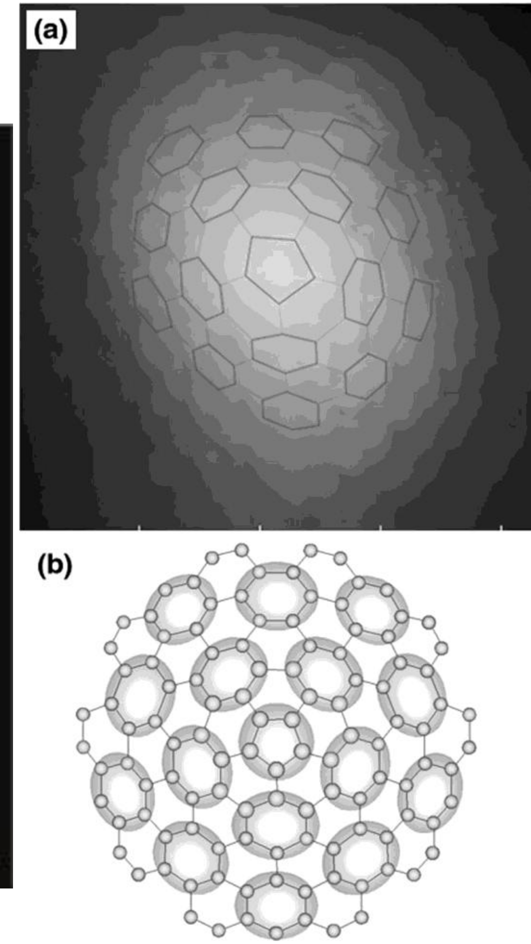


A ring of heptagons results in one-sheet hyperboloid

Experimental observation of the pentagon by STM (scanning tunneling microscopy)



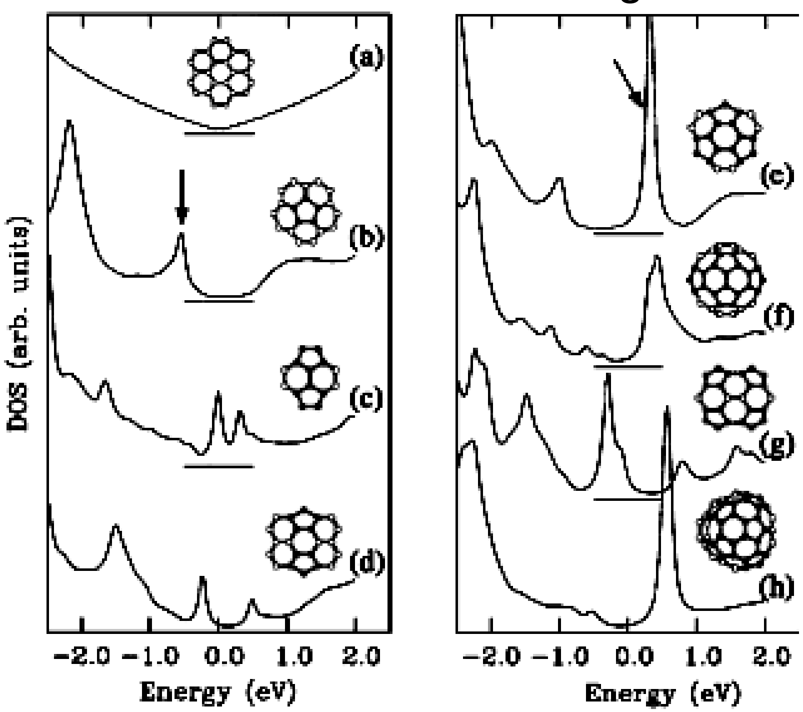




B.An et.al, Appl.Phys.Lett. 78, 3696 (2001): the enhanced charge density localized at each carbon atom in the pentagon was experimentally clarified. Typical images of the conical protuberance by STM: (a) Top view of the apex, (b) Bird's-eye view, (c) Cross section along line AA'. Five bright spots are clearly seen.

A presence of sharp resonant states in the region close to the Fermi energy

J.-C. Charlier and G.-M. Rignanese, Phys. Rev.Lett. 86, 5970 (2001)

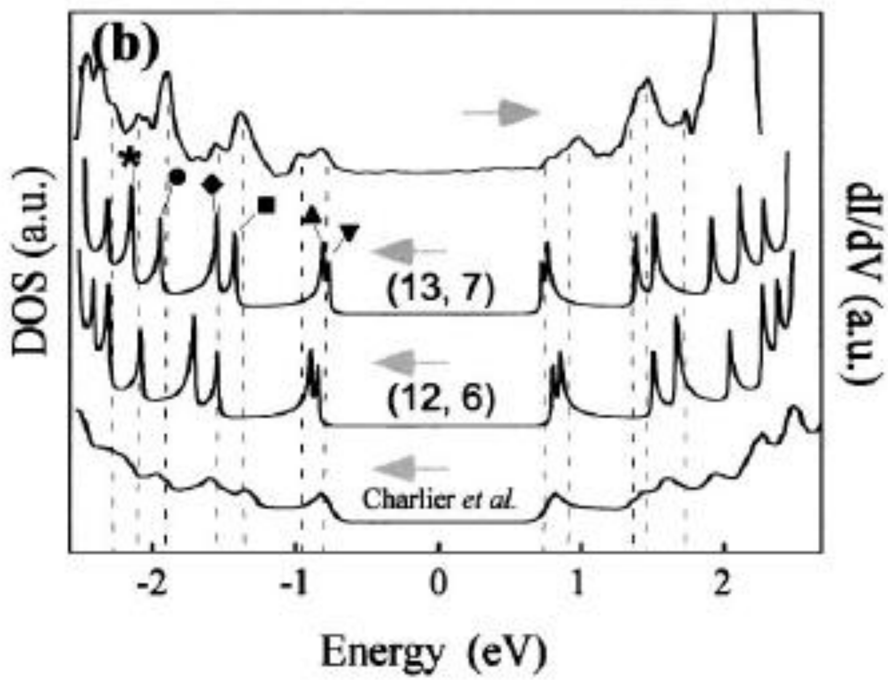


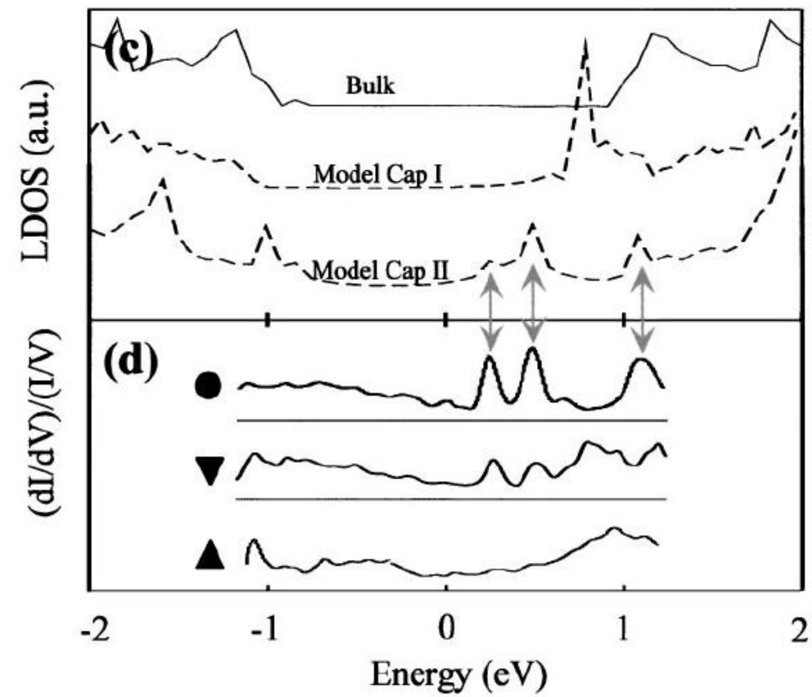
Computed tight-binding LDOS for a single graphene layer (a), and nanocones with one (b), two (c) and (d), three (e), four (f) and (g), and five (h) pentagons, respectively. The Fermi level is at zero energy.

The strength and the position of these states with respect to the Fermi level was found to depend sensitively on the number and the relative positions of the pentagons constituting the conical tip. In particular, a prominent peak which appears just above the Fermi level was found for the nanocone with three symmetrical pentagons (which corresponds to a 60˚ opening angle or, equivalently, to 180˚ disclination).

Electronic structure of SWNT

P. Kim et al., Phys.Rev.Lett. 82, 1225 (1999)



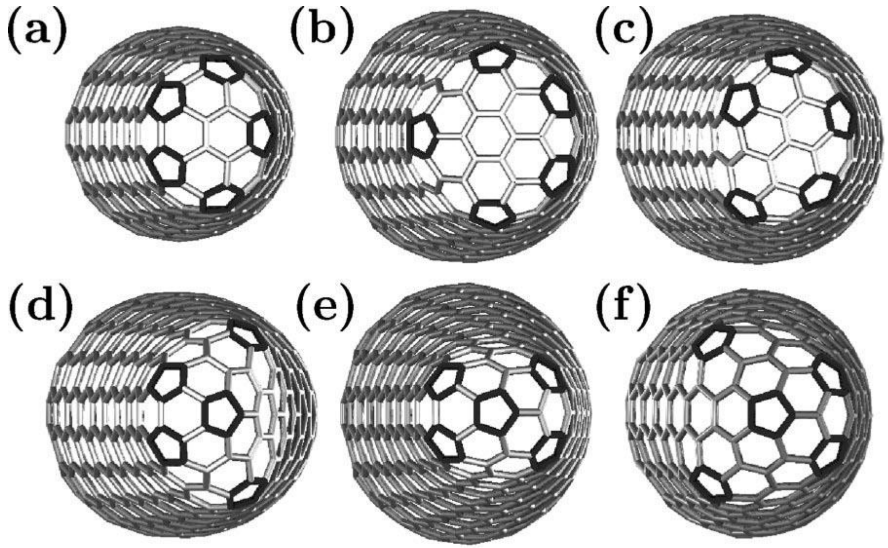


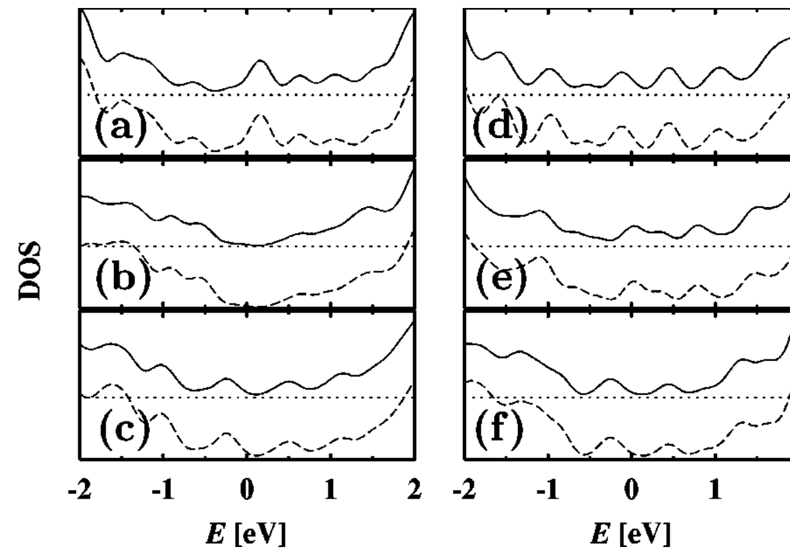
Comparison of the DOS obtained from experiment (upper curve) and a p-only tight-binding calculation for the (13, 7) SWNT (second curve from top)

A model (-13,2) SWNT with two different cap structures; (c) LDOS obtained from tight-binding calculations; (d) Experimental tunneling spectra from the end( ), near the end ( ), and far from the end ( )

Nanohorns

Source: S. Berber et al., Phys.Rev.B 62, R2291 (2000)





Carbon nanohorn structures with a total disclination angle of 5(π/3), containing five isolated pentagons at the terminating cap. Structures (a)–(c) contain all pentagons at the conical ‘‘shoulder,’’ whereas structures (d)–(f) contain a pentagon at the apex.

Main conclusions

- Pentagons are generic defects in closed carbon structures

- Pentagons/heptagons have a marked impact on the electronic structure of carbon nanoparticles.