Physics of Condensed Matter I

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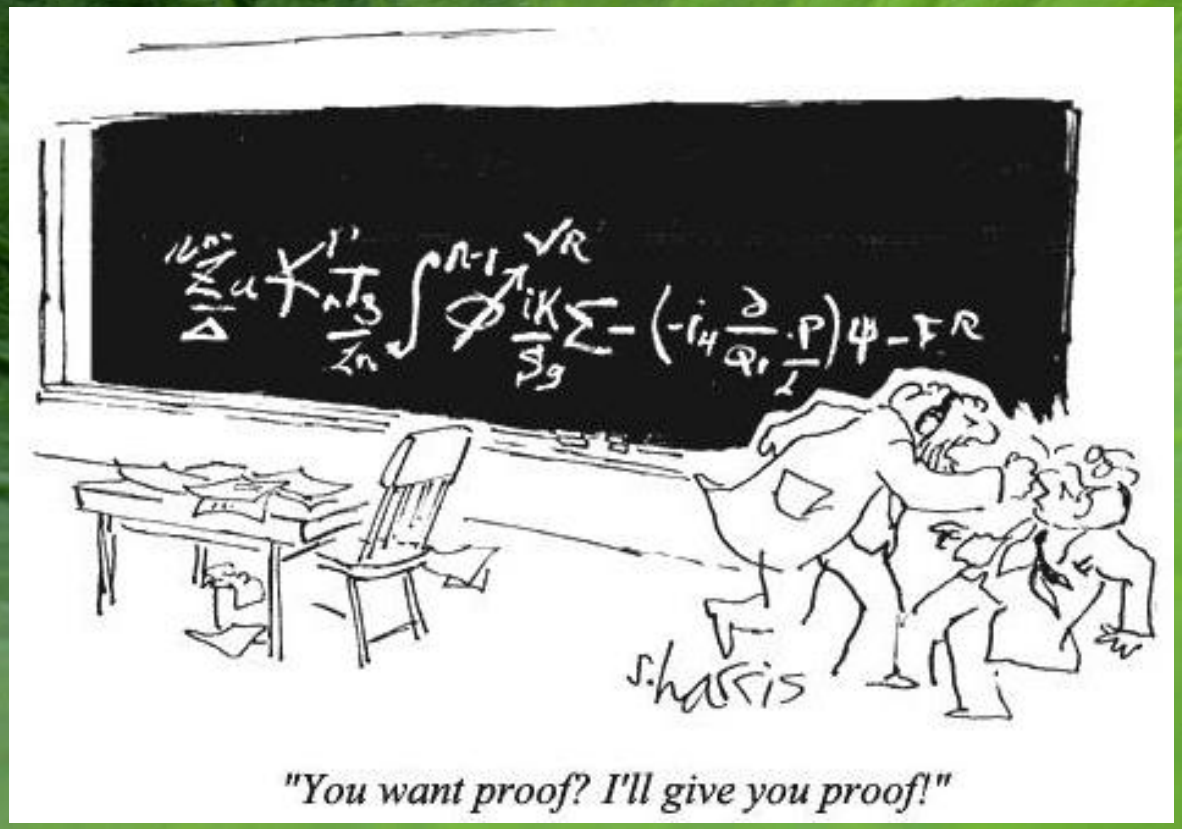


"You want proof? I'll give you proof!"

Molecules 3

Faculty of Physics UW

Jacek.Szczytko@fuw.edu.pl

inżynieria nanostruktur

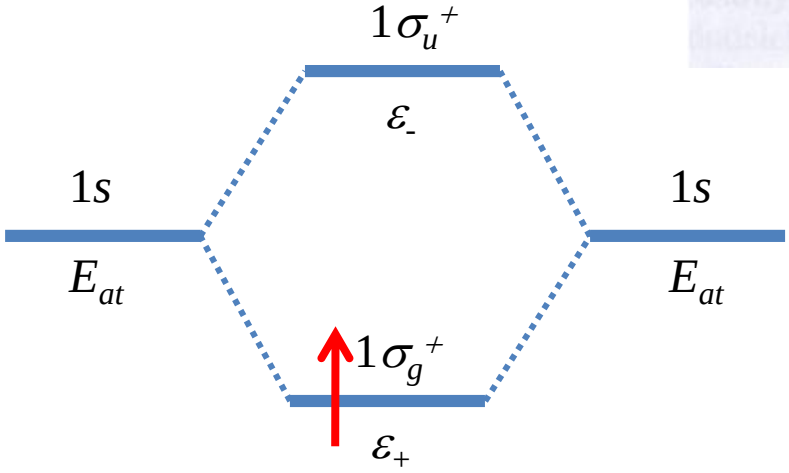
Molecules

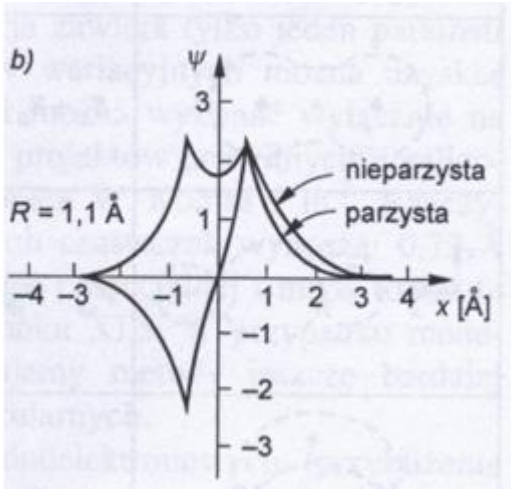
H_2^+ ion

Trial functions of the hydrogen atom (variational method)

$$\Psi_+ = N_+(1s_A + 1s_B)$$

$$\Psi_- = N_-(1s_A - 1s_B)$$





P. Atkins

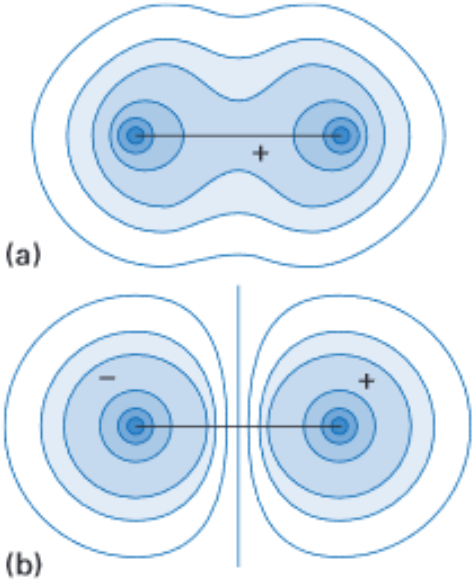


Fig. 8.6 Contour diagrams of the (a) bonding and (b) antibonding orbitals (1σ and 2σ, respectively) of the hydrogen molecule–ion in the LCAO approximation.

Atkins, Fridman *Molecular QM*

Molecules

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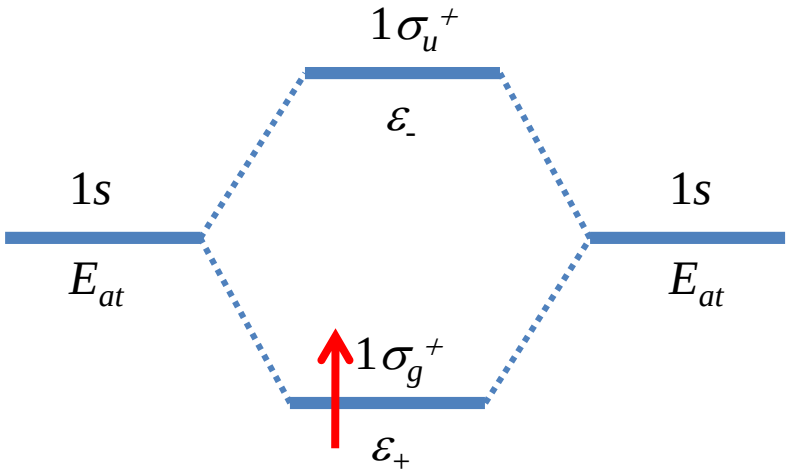


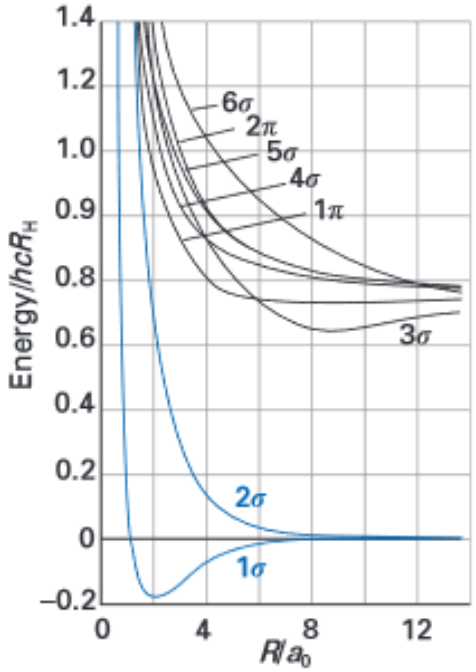
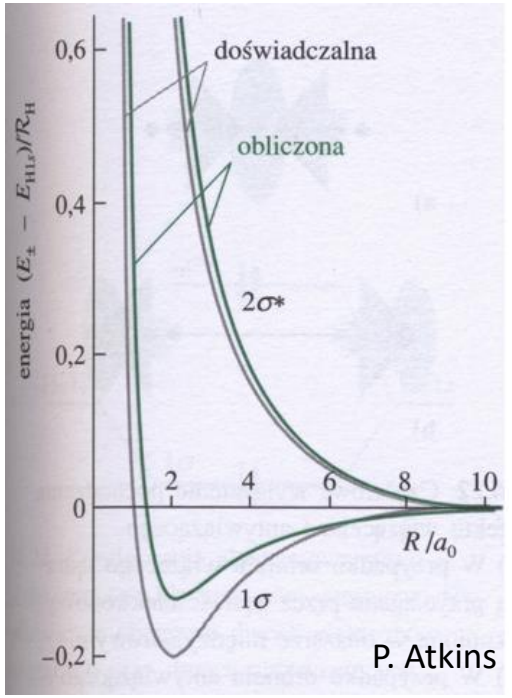


Fig. 8.5 The molecular potential energy curves for the hydrogen molecule–ion.



Atkins, Fridman *Molecular QM*

Molecules

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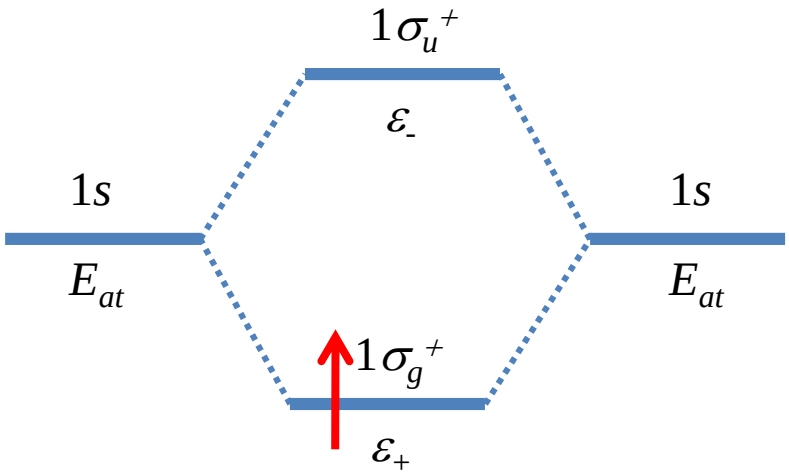

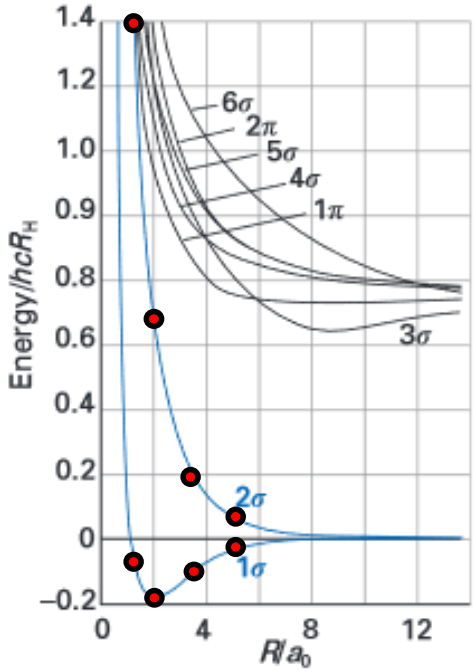

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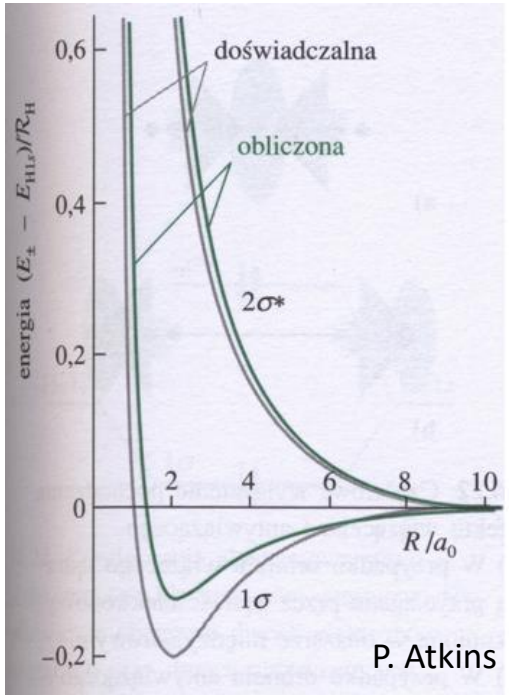


Atkins, Fridman *Molecular QM*

Electronic states

Electrons energy strongly depends on the distance between nuclei.

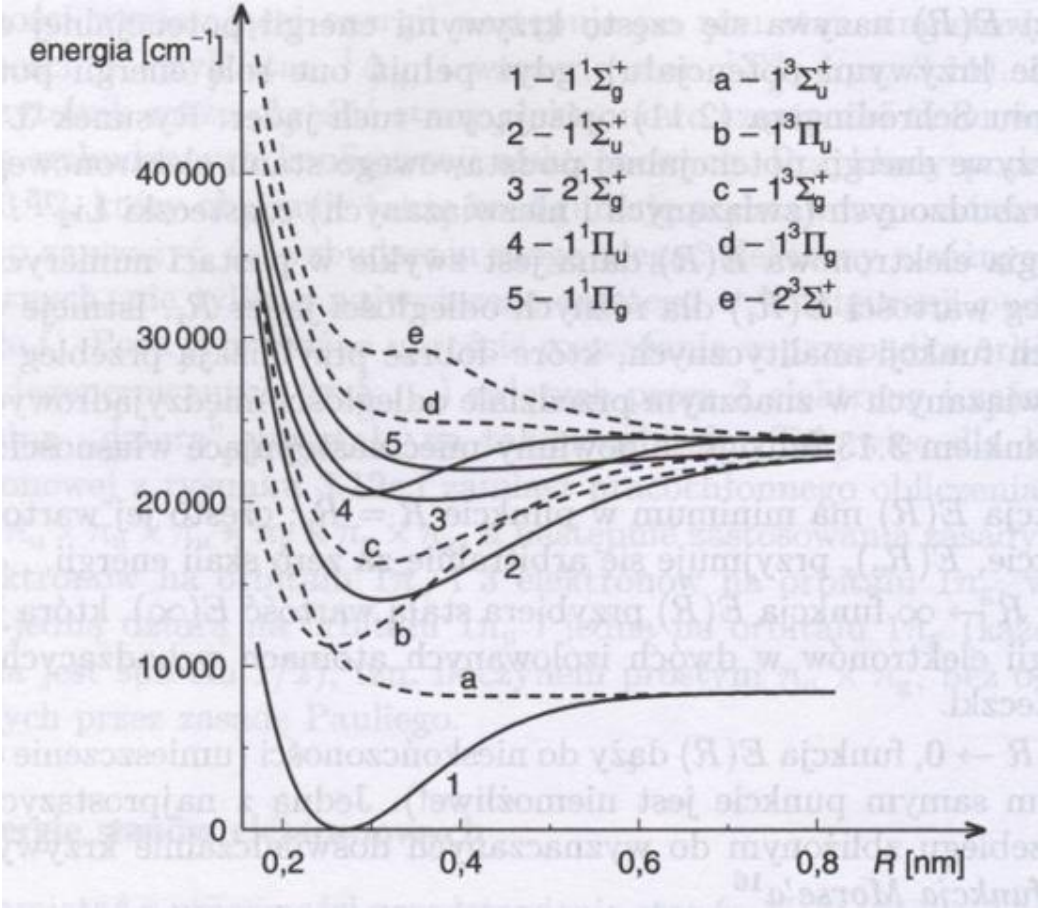
$E(R)$ - usually in numerical form.

Approximations: Morse potential
eg. Lithium

$$V(r) = D_e\left[1 - e^{-\alpha(r-r_0)}\right] + V(r_0)$$

Approximations: Lenard-Jones potential

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + V(r_0)$$



P. Kowalczyk

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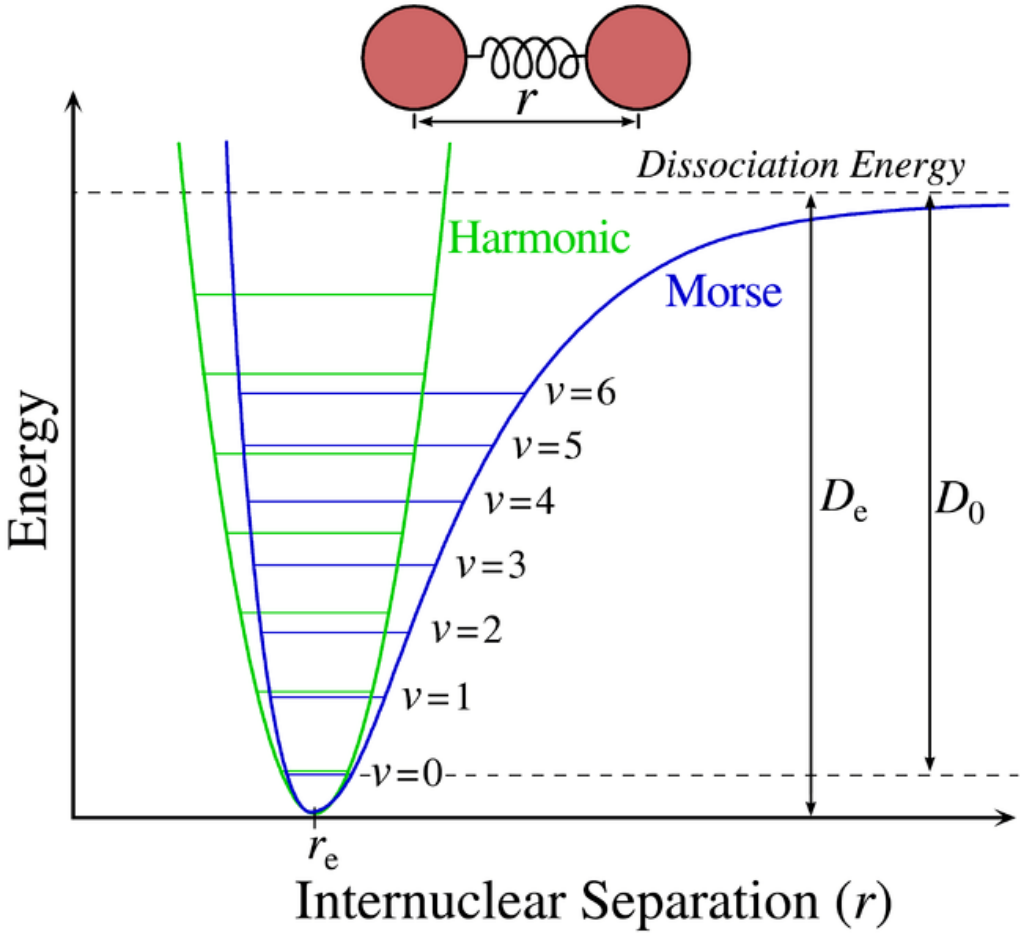

Wikipedia

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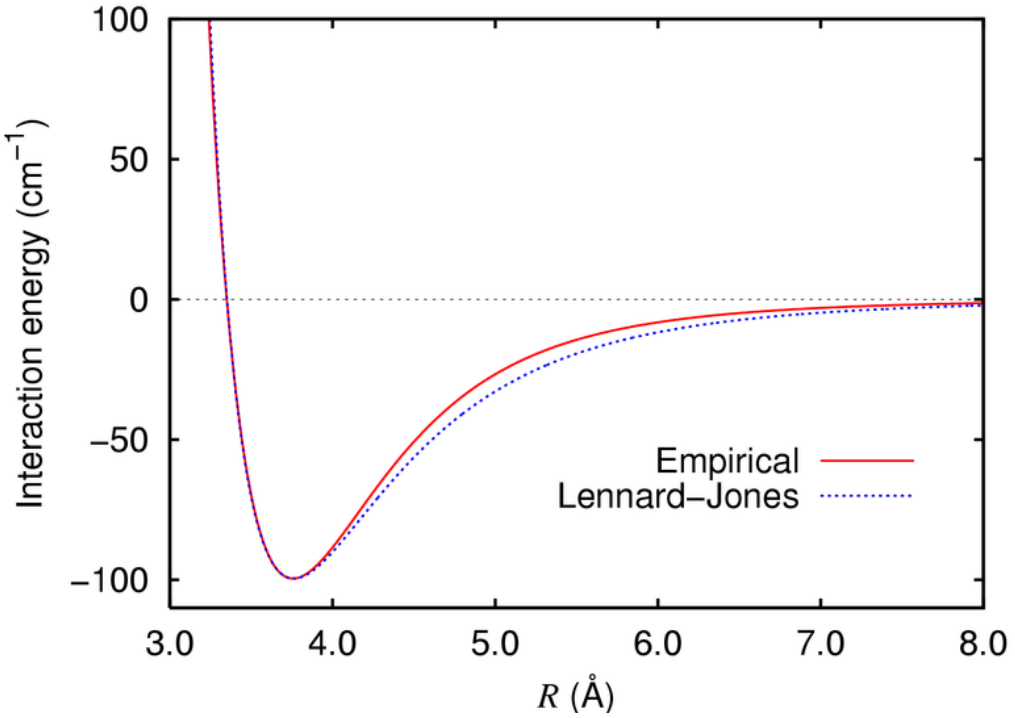


Wikipedia

Molecules

These were

Homonuclear diatomic molecules, eg. H_2, Li_2, N_2, O_2

The molecule is diatomic so we are looking for a combination of two orbitals φ_A and φ_B.

$$\Psi = c_A\varphi_A + c_B\varphi_B \qquad |c_A|^2 = |c_B|^2 \Rightarrow c_A = \pm c_B$$

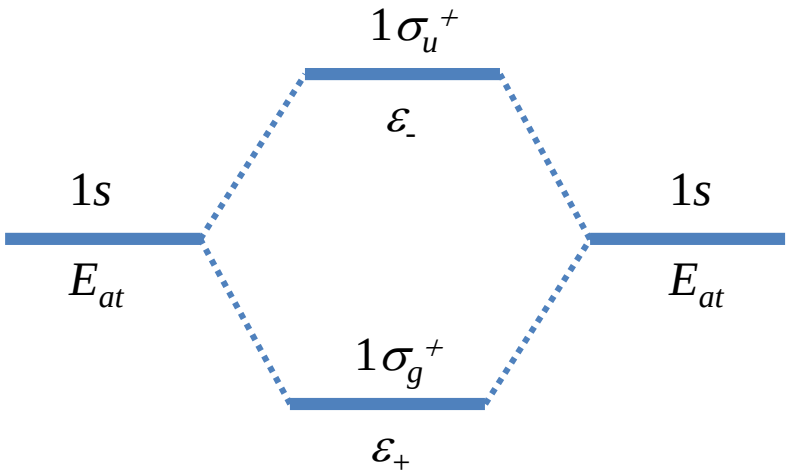
$$S = \int \varphi_A\varphi_B \, d\vec{r} > 0 \quad \text{overlap integral}$$

$$\varepsilon_{\pm} = \int \Psi_{\pm}^{*}\hat{H}^0\Psi_{\pm}d\vec{r}$$

$$N_+ = \frac{1}{\sqrt{2(1+S)}} \qquad N_- = \frac{1}{\sqrt{2(1-S)}}$$

$$\varepsilon_+ = \frac{E_{at} - |H_{AB}|}{1+S}$$ bonding orbital

$$\varepsilon_- = \frac{E_{at} + |H_{AB}|}{1-S}$$ antibonding orbital



$$H_{AA} = \int \varphi_A^{*}\hat{H}^0\varphi_A d\vec{r} = H_{BB} \approx E_{at}$$

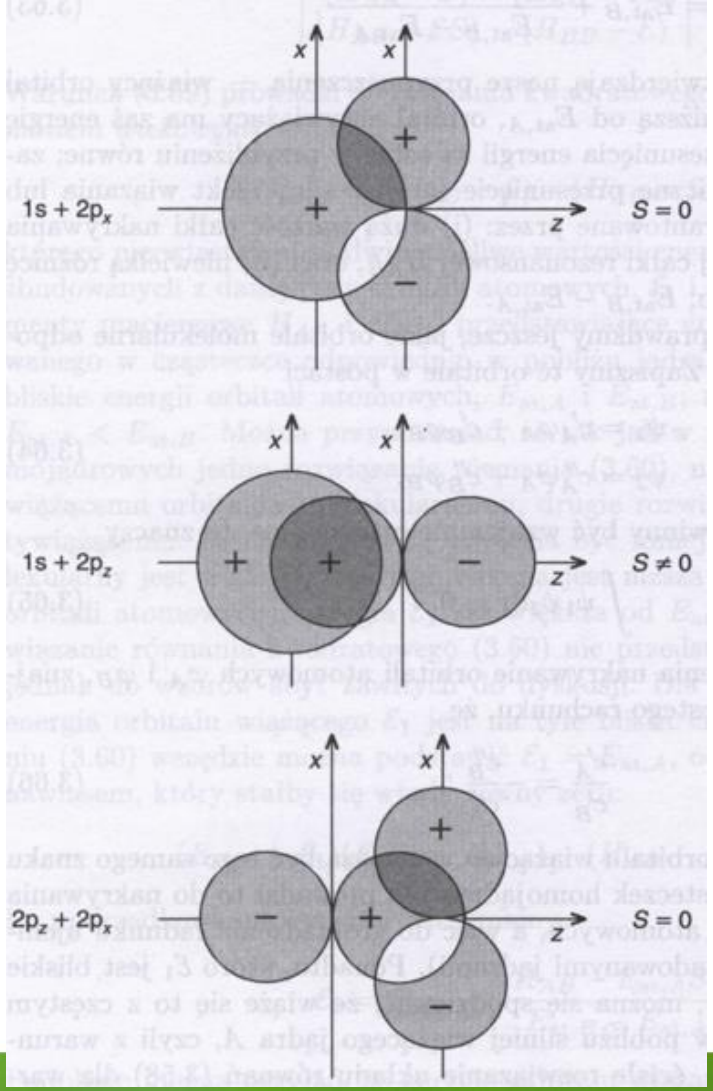
$$H_{AB} = \int \varphi_A^{*}\hat{H}^0\varphi_B d\vec{r} < 0$$

Molecules

Heteronuclear diatomic molecules, eg. **CO, NO, HCl, HF**

$\Psi = c_A\varphi_A + c_B\varphi_B$ $\quad |c_A|^2 = |c_B|^2 \Rightarrow c_A = \pm c_B$

$S = \int \varphi_A\varphi_B \, d\vec{r} > 0$ overlap integral



$E_{at,B}$

$E_{at,A}$

Molecules

Heteronuclear diatomic molecules, eg. **CO, NO, HCl, HF**

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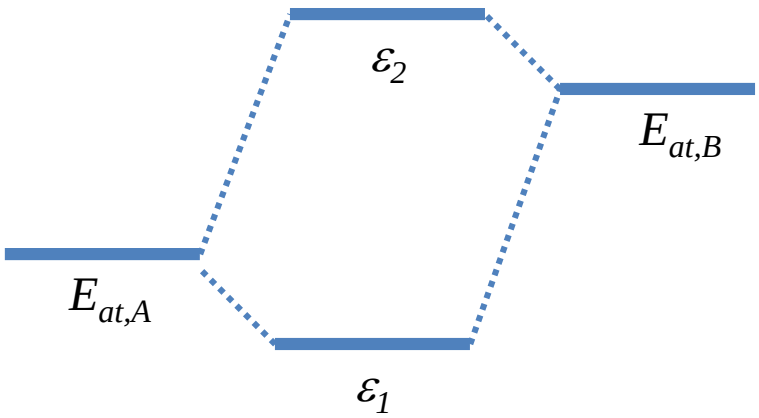
$$\Psi = c_A\varphi_A + c_B\varphi_B \qquad |c_A|^2 \neq |c_B|^2$$

$$S = \int \varphi_A\varphi_B \, d\vec{r} > 0$$

variational method $\varepsilon < \dfrac{\int \Psi_{\pm}^{*} \hat{H}^0 \Psi_{\pm} d\vec{r}}{\int \Psi_{\pm}^{*} \Psi_{\pm} d\vec{r}}$

$$\varepsilon(c_A^2 + c_B^2 + 2c_Ac_BS) = c_A^2H_{AA} + c_B^2H_{BB} + 2c_Ac_B\,H_{AB}$$

$$\frac{\partial\varepsilon}{\partial c_A} = \frac{\partial\varepsilon}{\partial c_B} = 0$$



$$\begin{bmatrix} H_{AA} - \varepsilon & H_{AB} - \varepsilon S \\ H_{AB} - \varepsilon S & H_{BB} - \varepsilon \end{bmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = 0$$

$$H_{AA} \approx E_{at,A}$$

$$H_{BB} \approx E_{at,B}$$

Let's assume that $E_{at,A} < E_{at,B}$

Molecules

Heteronuclear diatomic molecules, eg. **CO, NO, HCl, HF**

The molecule is diatomic so we are looking for a combination of two orbitals φ_A and φ_B.

$$\Psi = c_A\varphi_A + c_B\varphi_B \qquad |c_A|^2 \neq |c_B|^2$$

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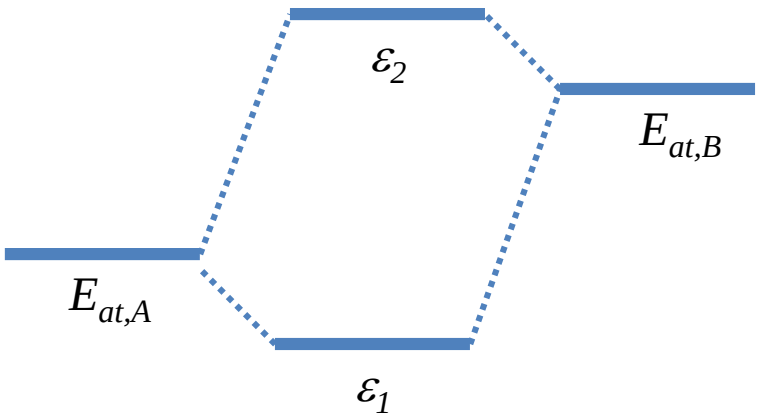


$$\begin{bmatrix} H_{AA} - \varepsilon & H_{AB} - \varepsilon S \\ H_{AB} - \varepsilon S & H_{BB} - \varepsilon \end{bmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = 0$$

$$\varepsilon_1 \approx E_{at,A} - \frac{\left(H_{AB} - E_{at,A}S\right)^2}{E_{at,B} - E_{at,A}}$$

$$\varepsilon_2 \approx E_{at,B} + \frac{\left(H_{AB} - E_{at,B}S\right)^2}{E_{at,B} - E_{at,A}}$$

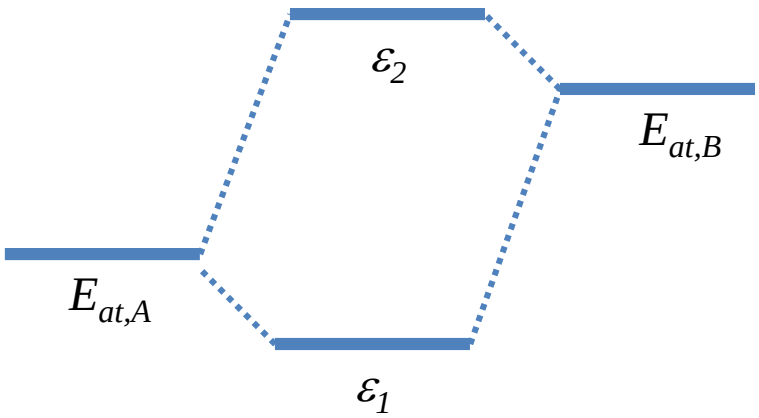
Molecules

The bonding is strong when:

The large value of the overlap integral S and proportional to it integral H_{AB}.
The small difference of the energy of atomic orbitals $E_{at,A}$, $E_{at,B}$.
Molecular orbitals **do not have to be** constructed with atomic orbitals of the same type ($s-s$ or $p-p$).

$$\varepsilon(c_A^2 + c_B^2 + 2c_A c_B S) = c_A^2 H_{AA} + c_B^2 H_{BB} + 2c_A c_B\, H_{AB}$$

$$\frac{\partial \varepsilon}{\partial c_A} = \frac{\partial \varepsilon}{\partial c_B} = 0$$



$$\begin{bmatrix} H_{AA} - \varepsilon & H_{AB} - \varepsilon S \\ H_{AB} - \varepsilon S & H_{BB} - \varepsilon \end{bmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = 0$$

$$\varepsilon_1 \approx E_{at,A} - \frac{\left(H_{AB} - E_{at,A} S\right)^2}{E_{at,B} - E_{at,A}}$$

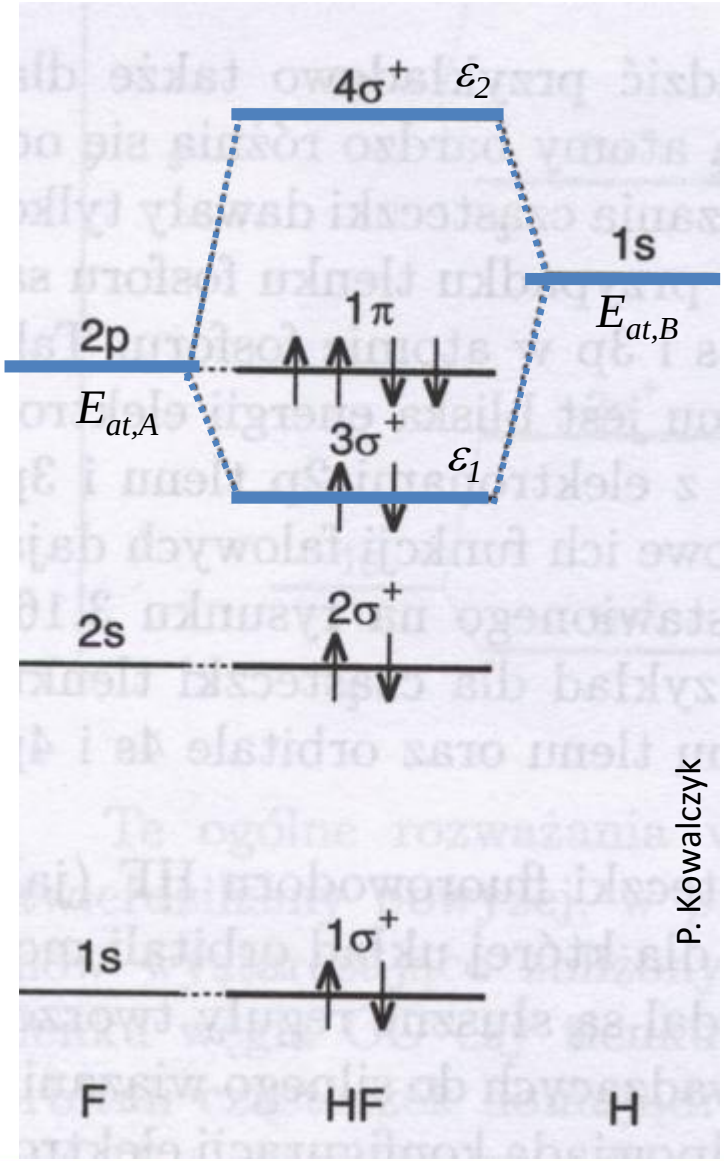
$$\varepsilon_2 \approx E_{at,B} + \frac{\left(H_{AB} - E_{at,B} S\right)^2}{E_{at,B} - E_{at,A}}$$

Molecules

Example: HF molecule

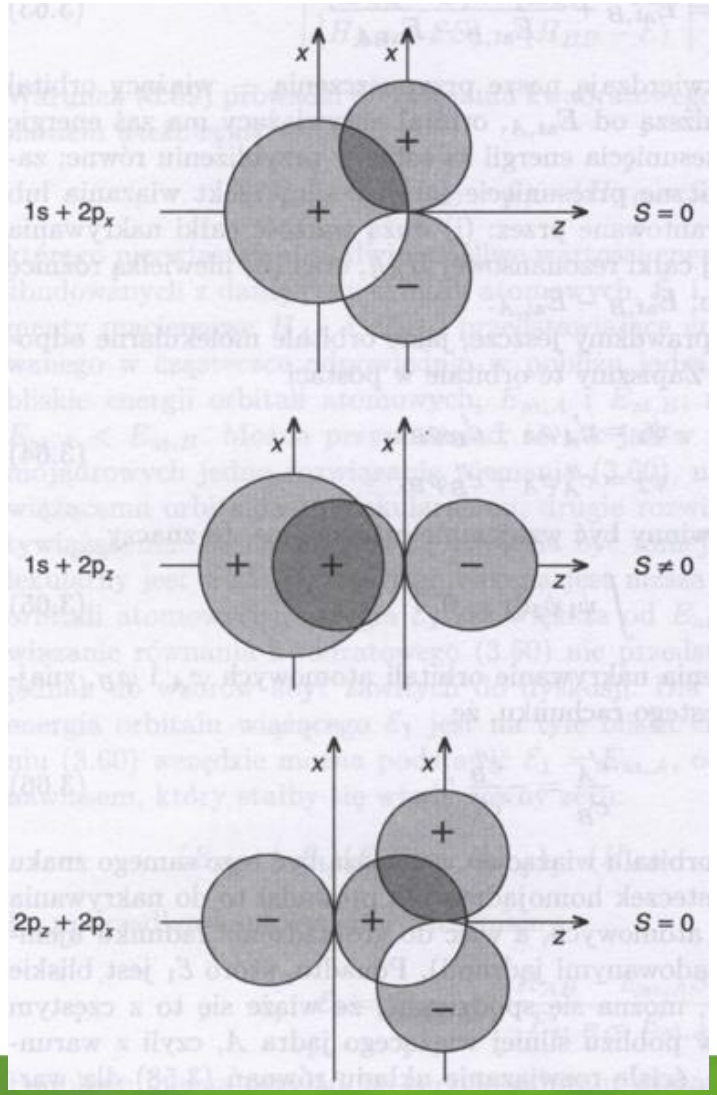
F: $(1s)^2(2s)^2(2p)^5$ H: $(1s)^1$

1. Similar energy values have $2p$ of F and $1s$ of H.
2. Only $2p_z$ orbital gives non-zero overlap integral with $1s$ (bonding orbital σ).
3. 2 Fluorine electrons $2p_x$ i 2 electrons $2p_y$ are not involved in the HF molecular bonding and are called **lone pair** (***wolna para elektronowa***)
4. Similarly fluorine 1s and 2s atomic orbitals do not form a bond with the 1s hydrogen electron because of the large energy difference
5. Ground state: $^1\Sigma^+$



Molecules

Hybridization and overlap integrals



P. Kowalczyk

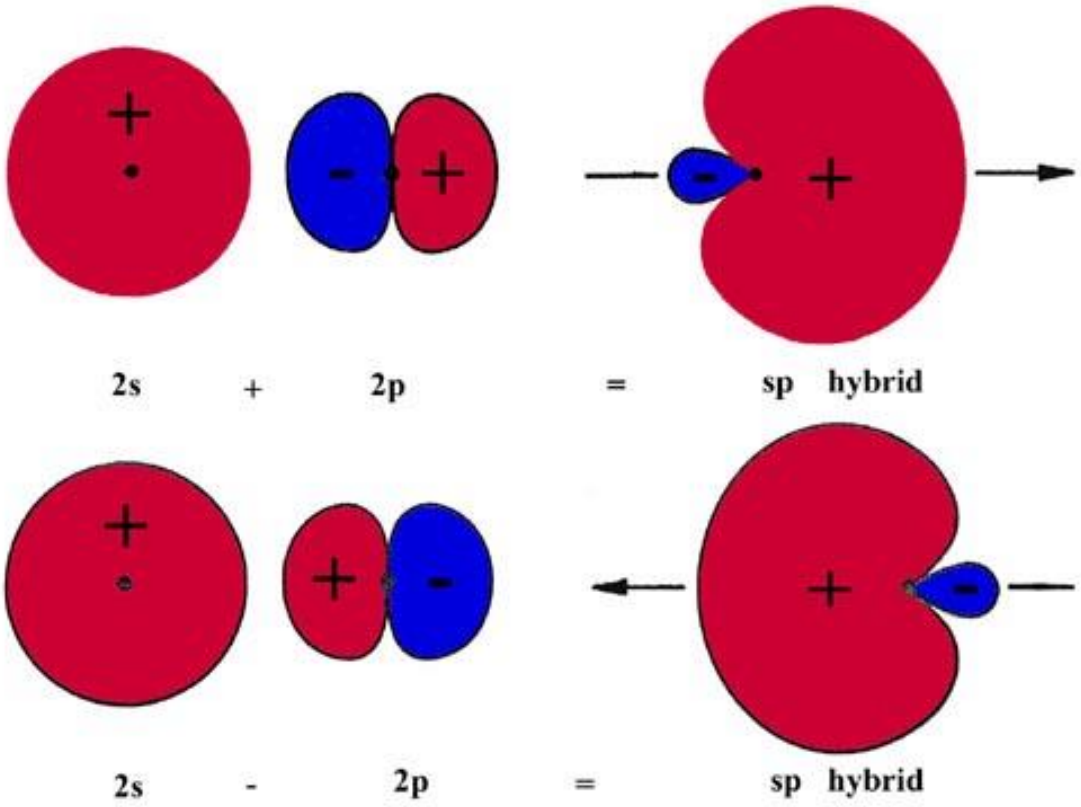
Atomic orbitals combined	Hybrid orbitals formed	Bonding electron pairs and lone pairs around central atom	VSEPR geometry
1 *s* orbital & 1 *p* orbital	sp hybrid (2 orbitals)	2	linear
1 *s* orbital & 2 *p* orbitals	sp^2 hybrid (3 orbitals)	3	trigonal planar
1 *s* orbital & 3 *p* orbitals	sp^3 hybrid (4 orbitals)	4	tetrahedral
1 *s* orbital & 3 *p* orbitals & 1 *d* orbital	dsp^3 hybrid (5 orbitals)	5	trigonal bipyramidal
1 *s* orbital & 3 *p* orbitals & 2 *d* orbitals	d^{2}sp^3 hybrid (6 orbitals)	6	octahedral

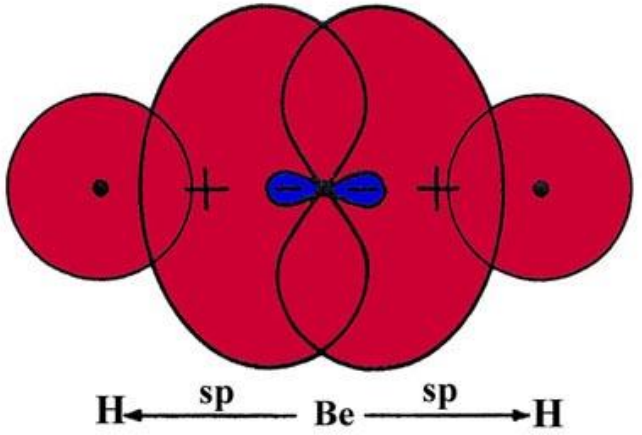
http://sparkcharts.sparknotes.com/chemistry/organicchemistry1/section2.php

Molecules

Hybridization sp, eg. BeH_2

The angle between the bonds is 180˚.





$$h_1 = \frac{1}{\sqrt{2}}s - \frac{1}{\sqrt{2}}p_x$$

$$h_2 = \frac{1}{\sqrt{2}}s + \frac{1}{\sqrt{2}}p_x$$

Molecules

Hybridization sp^2, eg. C_2H_4

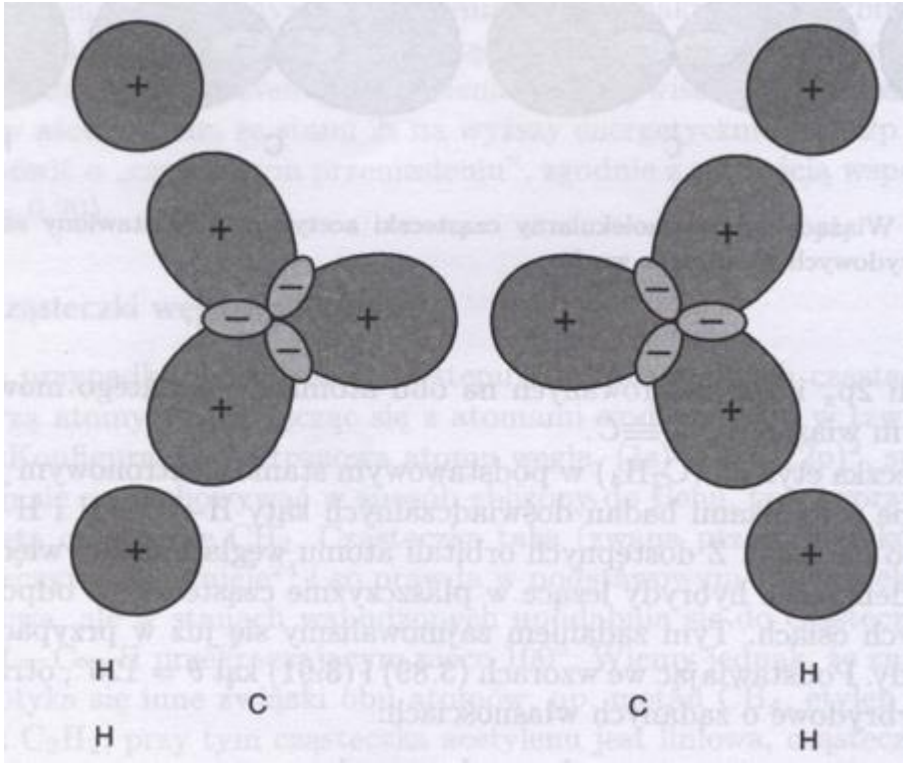
The angle between the bonds is 120˚.

Ethylene C_2H_4

$$h_1 = \frac{1}{\sqrt{3}}s - \frac{1}{\sqrt{2}}p_x - \frac{1}{\sqrt{6}}p_z$$

$$h_2 = \frac{1}{\sqrt{3}}s + \frac{1}{\sqrt{2}}p_x - \frac{1}{\sqrt{6}}p_z$$

$$h_3 = \frac{1}{\sqrt{3}}s + \frac{1}{\sqrt{2}}p_z$$



P. Kowalczyk

Molecules

Hybridization sp^3, eg. CH_4

Methane CH_4

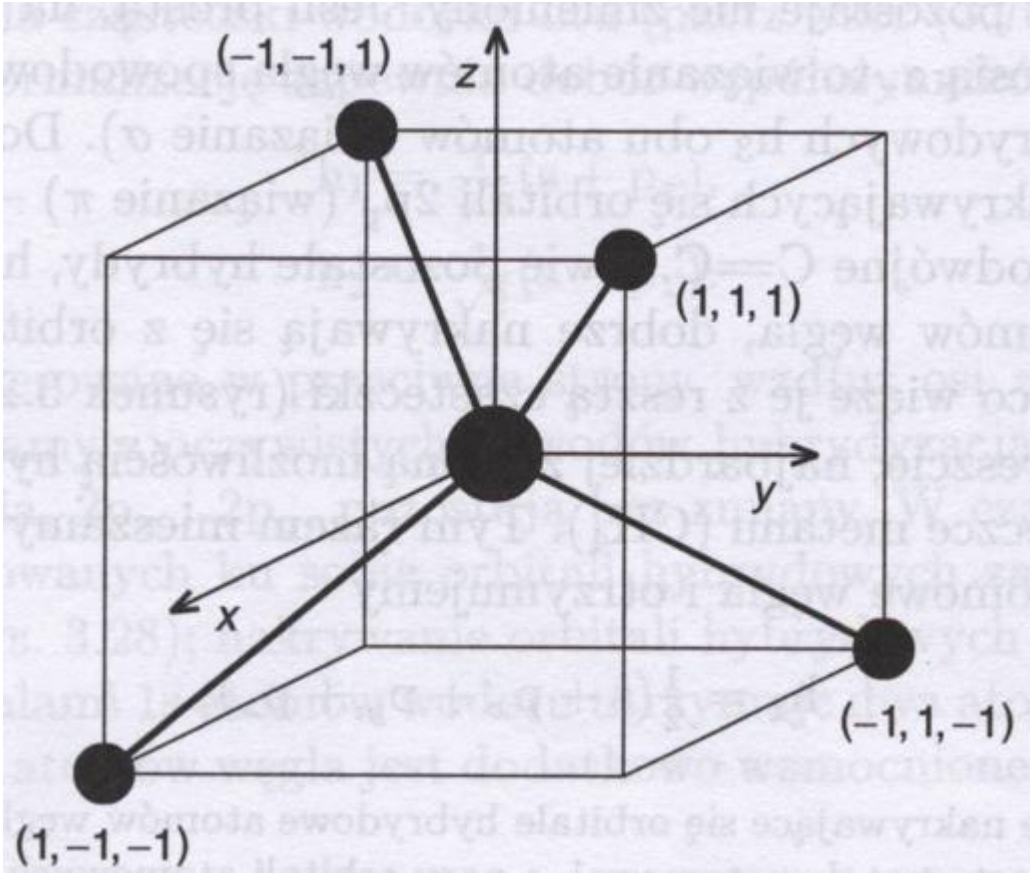
The angle between the bonds is 109,5˚.

$$h_1 = \frac{1}{2}(s + p_x + p_y + p_z)$$

$$h_2 = \frac{1}{2}(s + p_x - p_y - p_z)$$

$$h_3 = \frac{1}{2}(s - p_x + p_y - p_z)$$

$$h_4 = \frac{1}{2}(s - p_x - p_y + p_z)$$



P. Kowalczyk

Molecules

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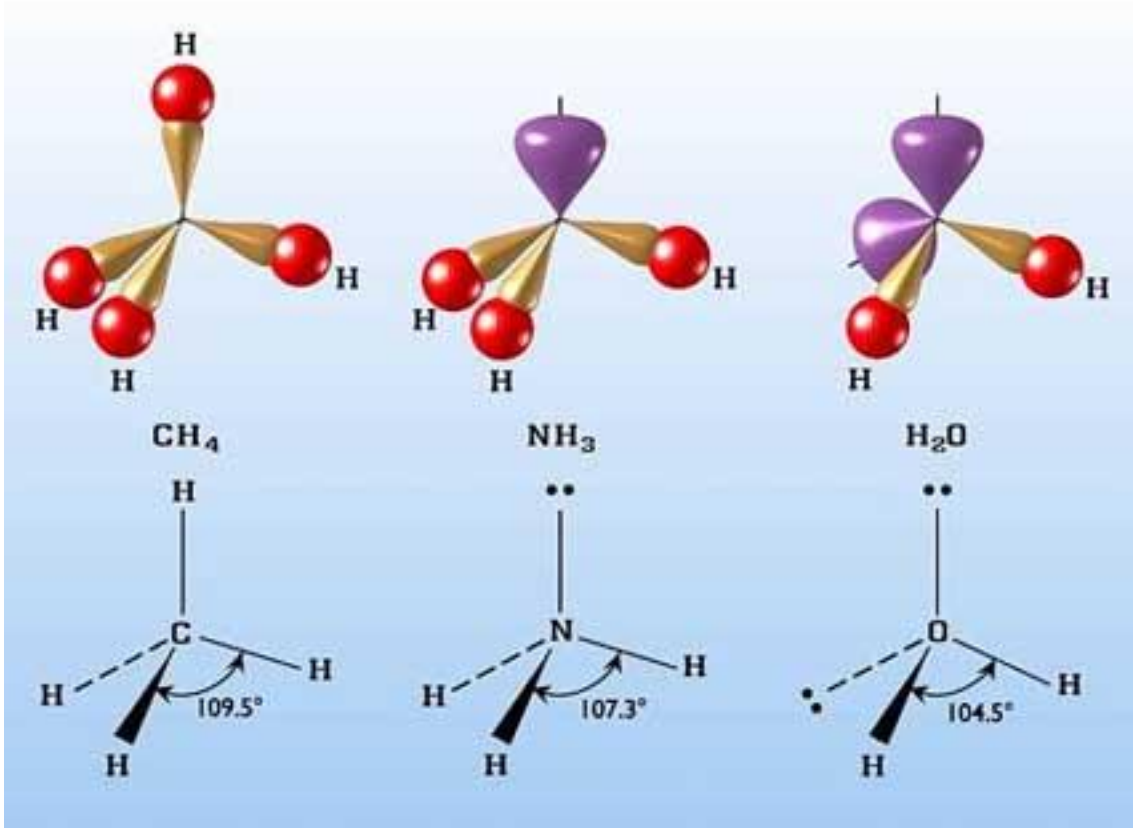
Methane CH_4 | **Ammonia NH_3** | **Water H_2O**



http://oen.dydaktyka.agh.edu.pl/dydaktyka/chemia/a_e_chemia/1_3_budowa_materii/01_04_03_2b.htm

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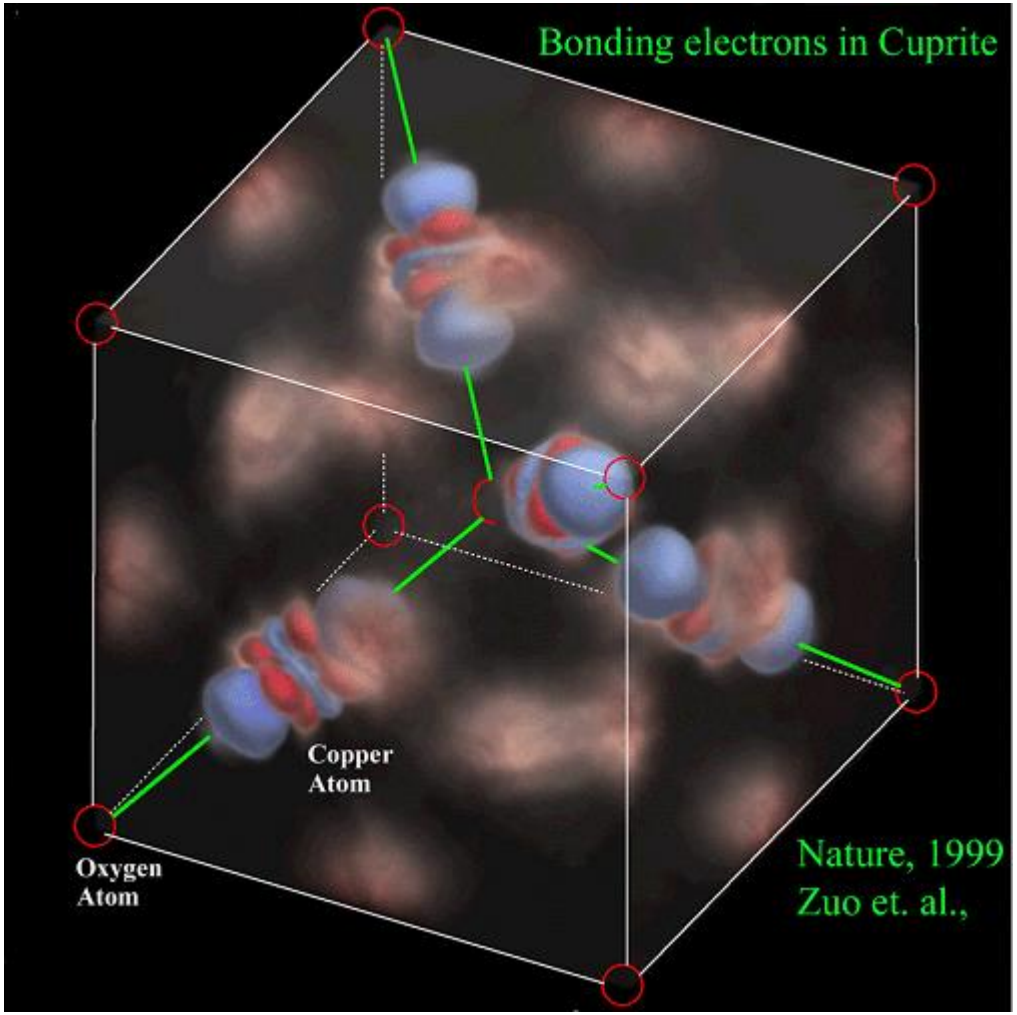


Molecules

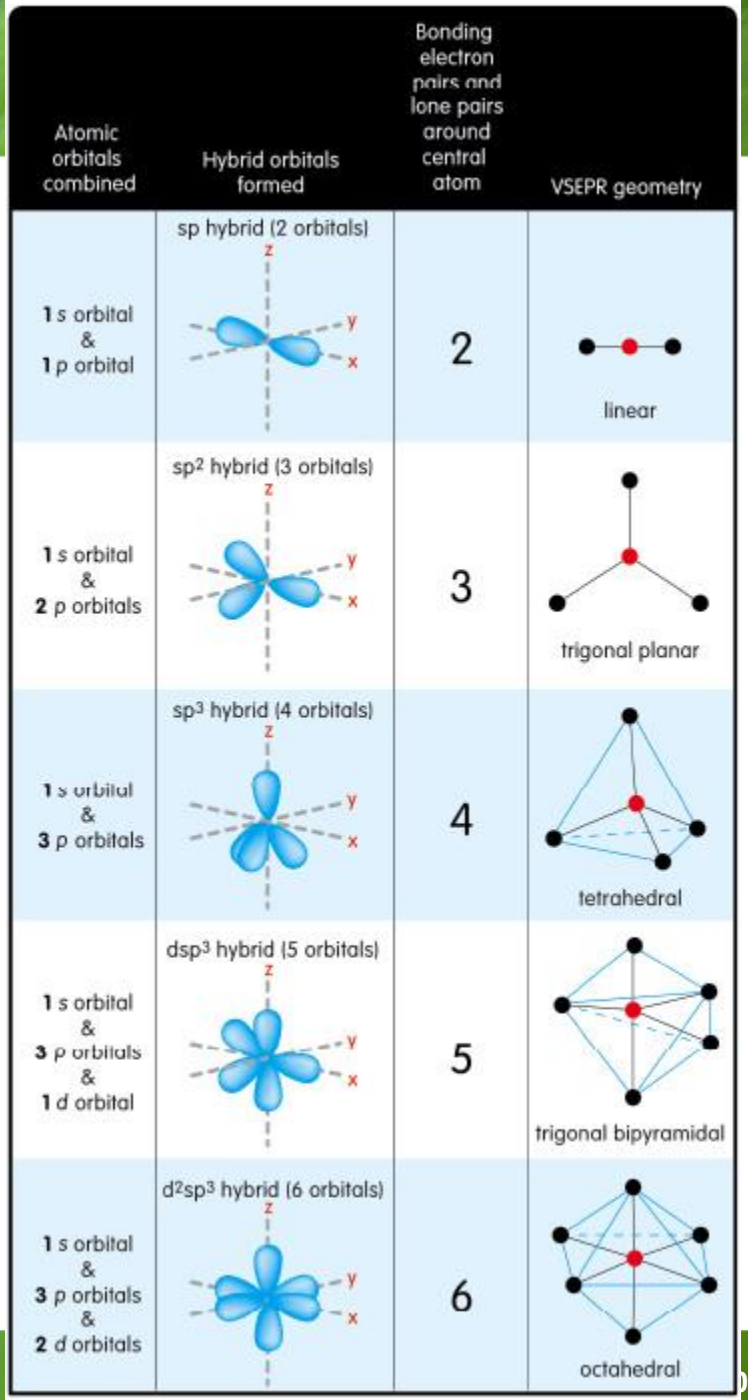
Hybridization

A summary of hybrid orbitals, valence bond theory, VSEPR, resonance structures, and octet rule.

Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
sp	sp^2	sp^3	dsp^3	d^2sp^3
BeH_2	BH_3	CH_4	PF_5	SF_6
BeF_2	BF_3	CF_4	PCl_5	IOF_5
CO_2	CH_2O	CCl_4	$PFCl_4$	PF_6^-
HCN	(>C=O)	CH_3Cl	$:SF_4$	SiF_6^{2-}
HC°CH	>C=C<	NH_4^+	$:TeF_4$	$:BrF_5$
	CO_3^{2-}	$:NH_3$	$::ClF_3$	$:IF_5$
	benzene	$:PF_3$	$::BrF_3$	$::XeF_4$
	graphite	$:SOF_2$	$:::XeF_2$	
	fullerenes	$::OH_2$	$:::I_3^-$	
	$\bullet NO_2$	$::SF_2$	$(:::I\ I_2^-)$	
	N_3^-		$:::ICl_2^-$	
	$:OO_2\ (O_3)$	SiO_4^{4-}		
	$:SO_2$	PO_4^{3-}		
	SO_3	SO_4^{2-}		
		ClO_4^-		

• a lone odd electron : a lone electron pair

http://www.science.uwaterloo.ca/~cchieh/cact/c120/hybrid.html



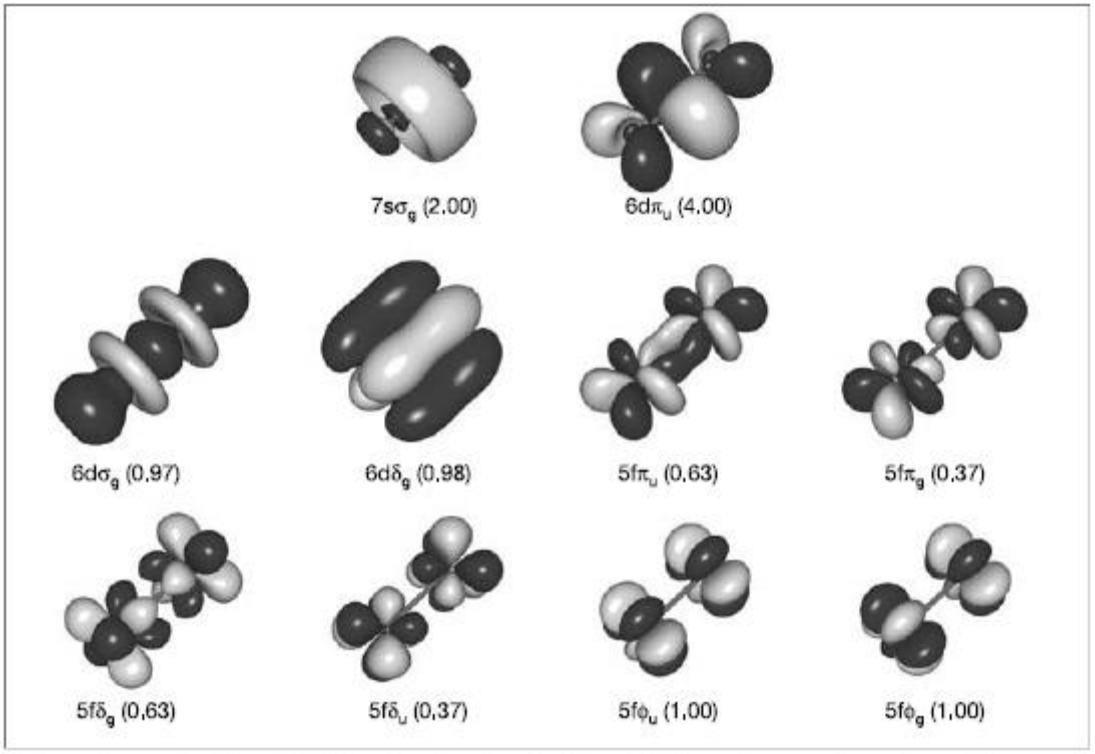
http://sparkcharts.sparknotes.com/chemistry/organicchemistry1/section2.php

Molecules

Hybridization

Uranium, a member of the actinide group of elements, can form molecules with five covalent bonds.
Each uranium atom has a total of 16 atomic orbitals that are available for bond formation. Gagliardi and Roos used an approach called CASSCF/CASPT2 to model how all the valence orbitals in one atom merge with those in the other atom to form the most stable chemical bond -- that is, the one with minimum energy.

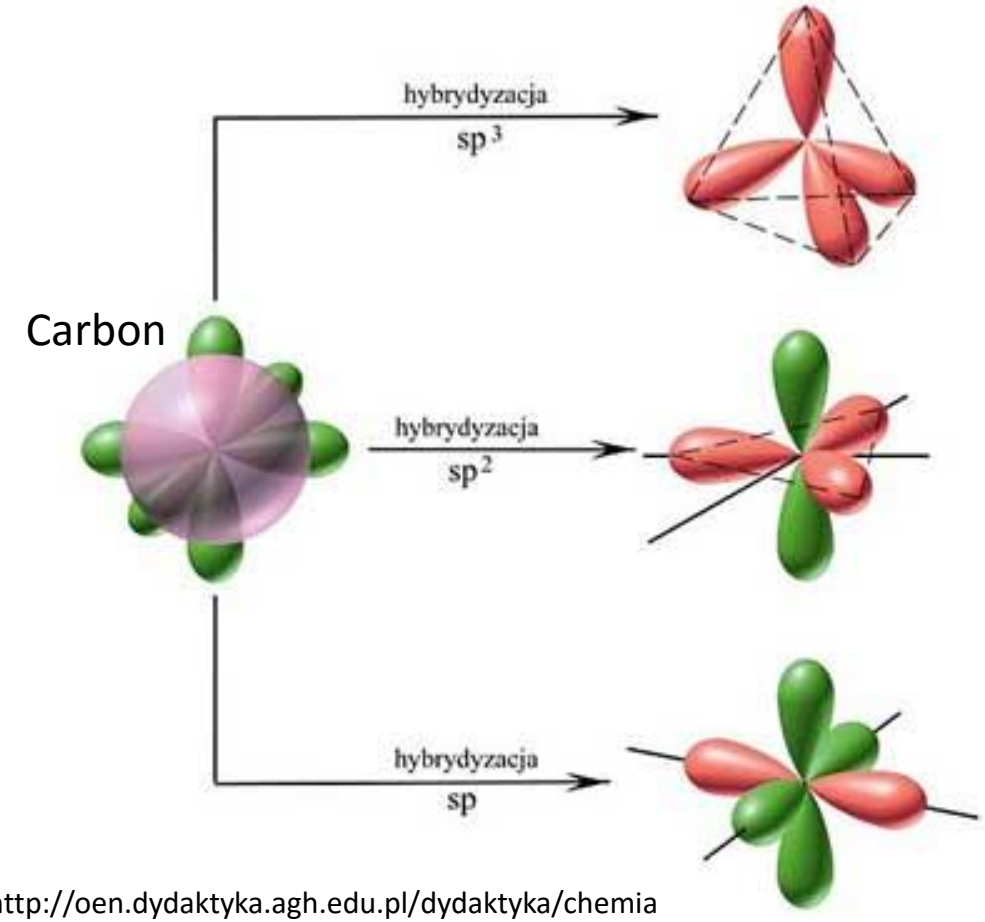
Gagliardi and Roos found that the uranium-uranium bond is more complex than any other known diatomic bond: it contains three normal electron-pair bonds and four weaker one-electron bonds. They also find evidence for ferromagnetic coupling between two electrons, each localized on one of the atoms. This means that all the known forms of covalent bonding are found in the molecule.



The active molecular orbitals forming the chemical bond between two uranium atoms. The orbital label is given below each orbital, together with the number of electrons occupying this orbital or pair of orbitals in the case of degeneracy (image courtesy: *Nature* **433** 848).

Molecules

Hybridization



Carbon

http://oen.dydaktyka.agh.edu.pl/dydaktyka/chemia

Atomic orbitals combined	Hybrid orbitals formed	Bonding electron pairs and lone pairs around central atom	VSEPR geometry
1 *s* orbital & 1 *p* orbital	sp hybrid (2 orbitals)	2	linear
1 *s* orbital & 2 *p* orbitals	sp^2 hybrid (3 orbitals)	3	trigonal planar
1 *s* orbital & 3 *p* orbitals	sp^3 hybrid (4 orbitals)	4	tetrahedral
1 *s* orbital & 3 *p* orbitals & 1 *d* orbital	dsp^3 hybrid (5 orbitals)	5	trigonal bipyramidal
1 *s* orbital & 3 *p* orbitals & 2 *d* orbitals	d^2sp^3 hybrid (6 orbitals)	6	octahedral

http://sparkcharts.sparknotes.com/chemistry/organicchemistry1/section2.php

Molecules

Benzene molecule

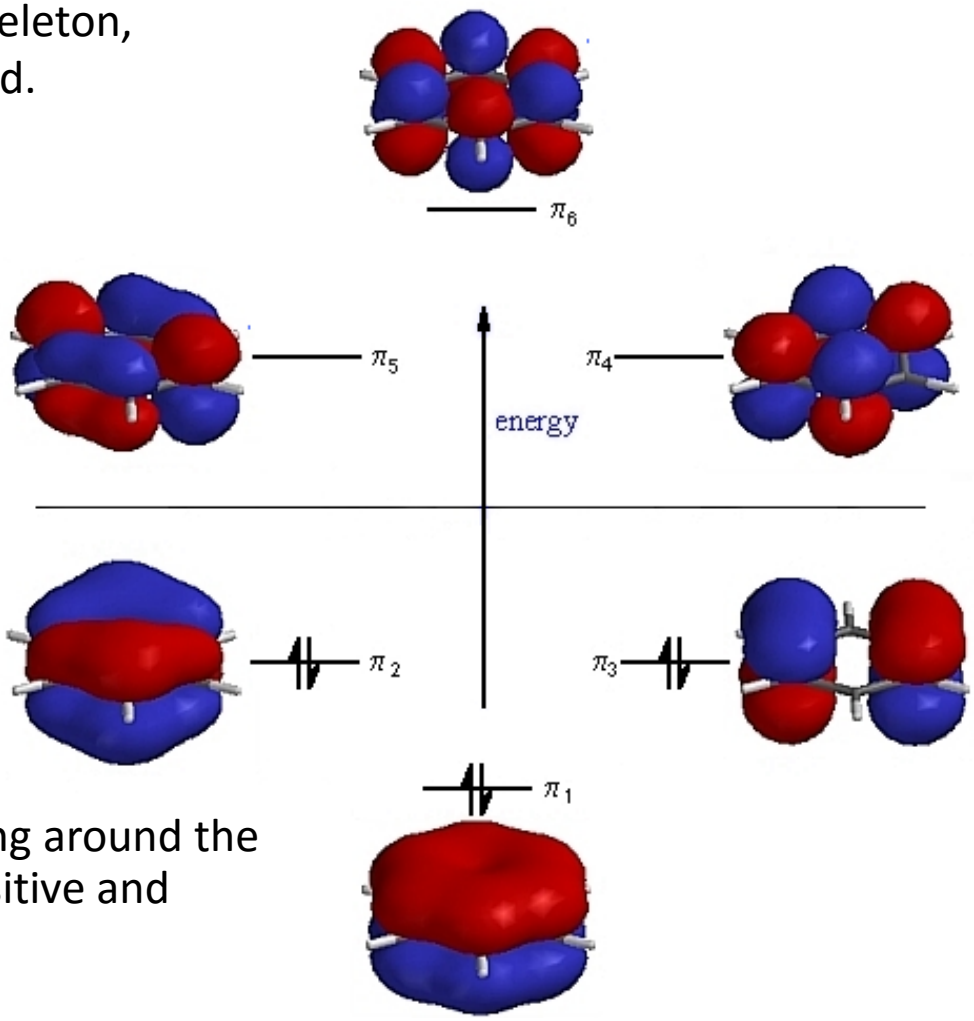
Benzene

σ-bonds (sp^2) are "localized" and form a rigid skeleton, while π-electrons forming a bond are delocalized.

$$\Psi_k = \frac{1}{\sqrt{6}} \sum_{n=1}^{6} e^{\frac{2\pi i}{6} kn} p_{z,n}$$

$$E_k = \alpha + 2\beta \cos\left(\frac{2\pi i}{6} k\right)$$

$$k = 0, \pm 1, \pm 2, 3$$



Six of atomic orbitals $2p_z$ gives an equal contribution to all of the molecular orbitals.

These functions correspond to the waves running around the carbon atoms ring in opposite directions for positive and negative values of k

Molecules

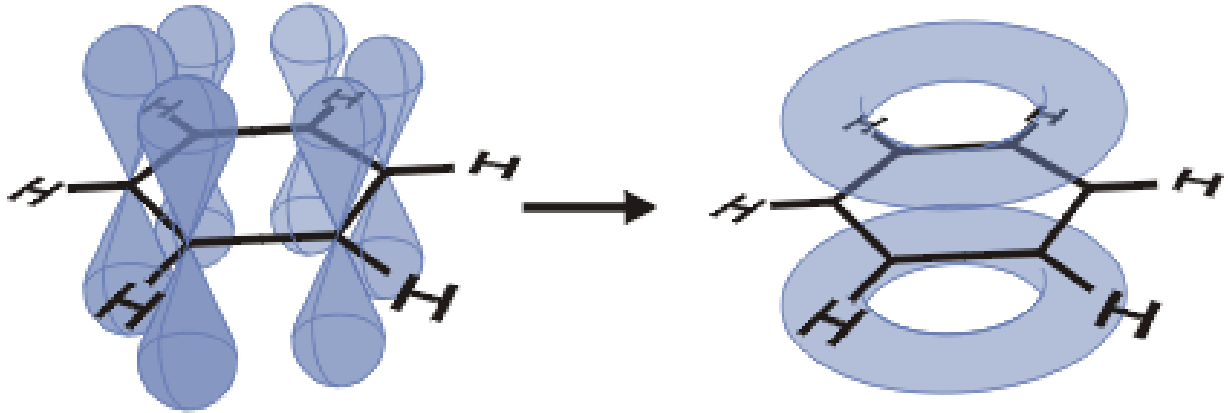
Benzene molecule

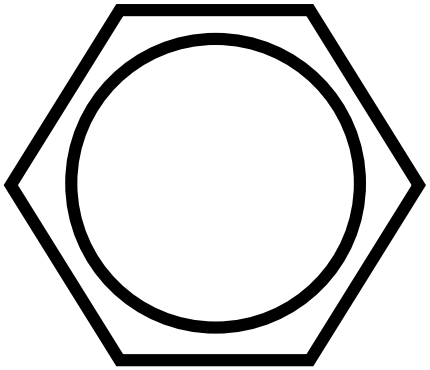
$$\Psi_{\mathrm{k}} = \frac{1}{\sqrt{6}} \sum_{n=1}^{6} e^{\frac{2\pi i}{6} kn} p_{z,n}$$

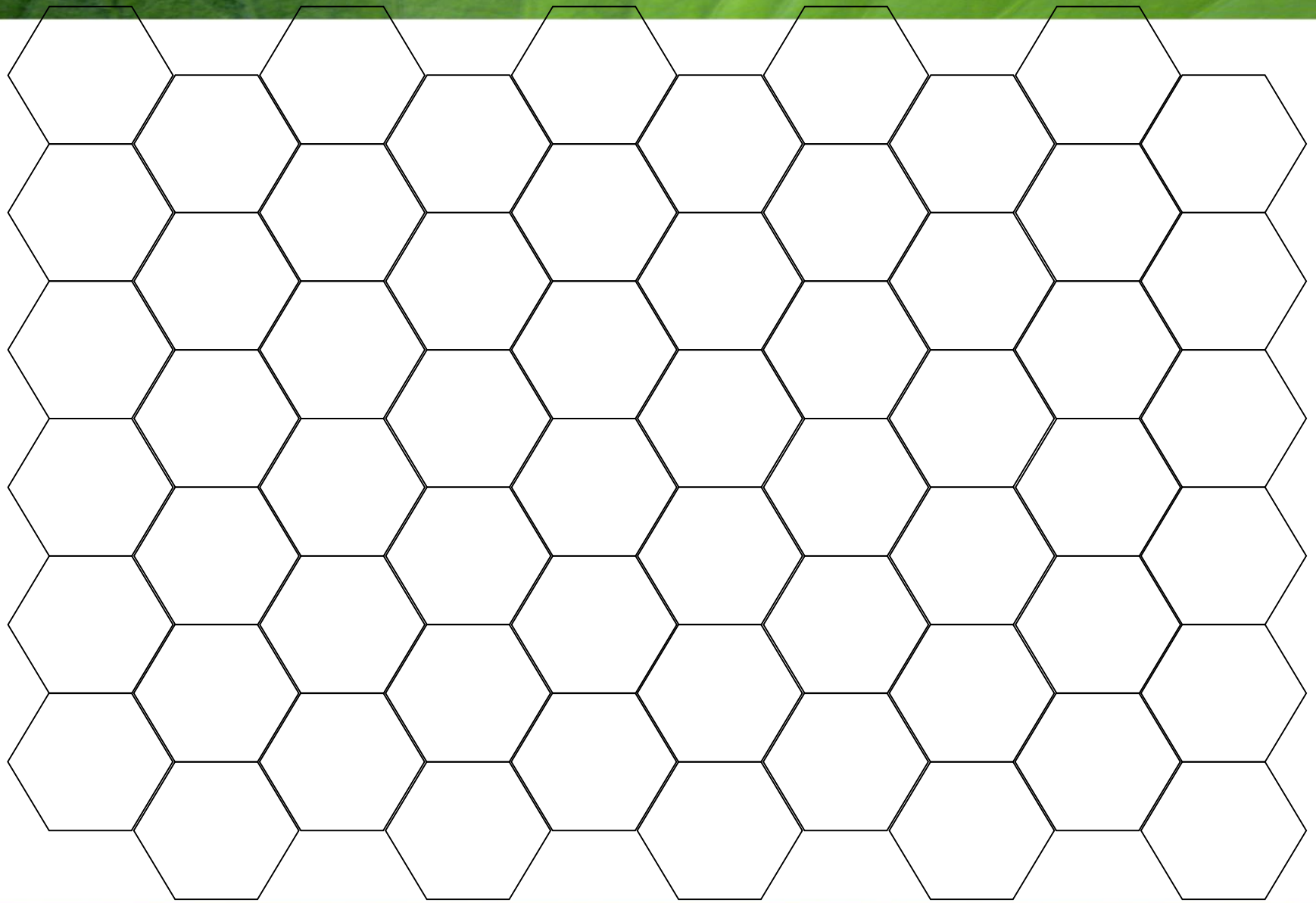
$$E_{\mathrm{k}} = \alpha + 2\beta \cos\left(\frac{2\pi i}{6}\ k\right)$$

$$k\ =\ 0, \pm 1, \pm 2, 3$$

Friedrich August Kekule 1829 - 1896

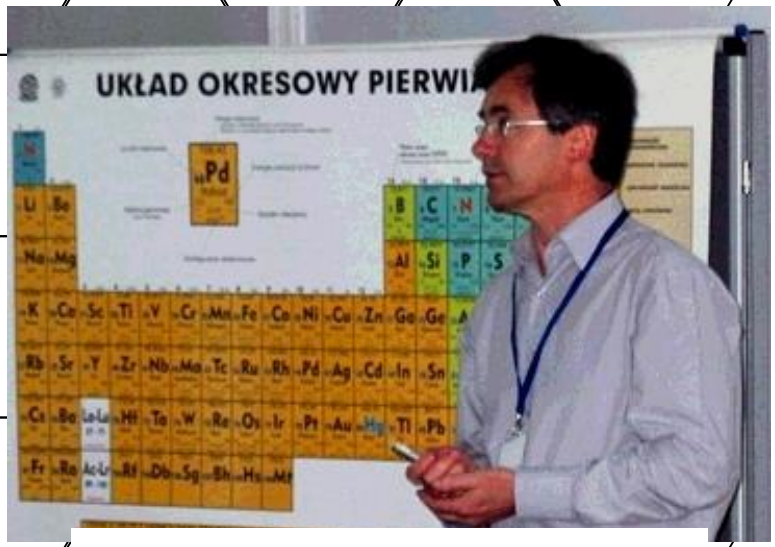






The Nobel Prize in Physics 2010

Andre Geim, Konstantin Novoselov



dr inż. Włodzimierz Strupiński,

dr hab. **Andrzej Wysmołek**

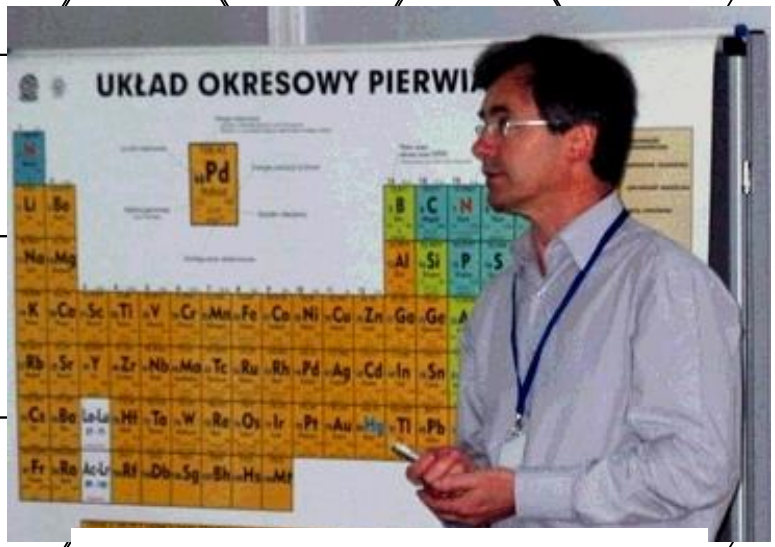
WYDZIAŁ FIZYKI

UNIWERSYTET WARSZAWSKI

ITME

The Nobel Prize in Physics 2010

Andre Geim, Konstantin Novoselov



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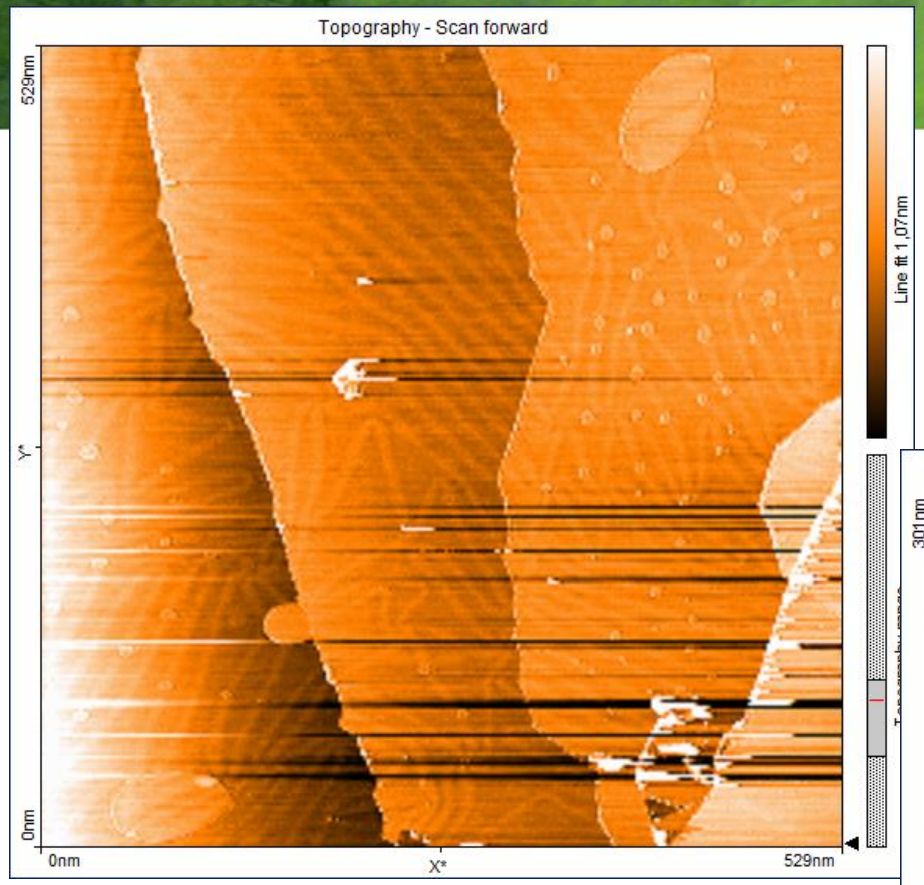
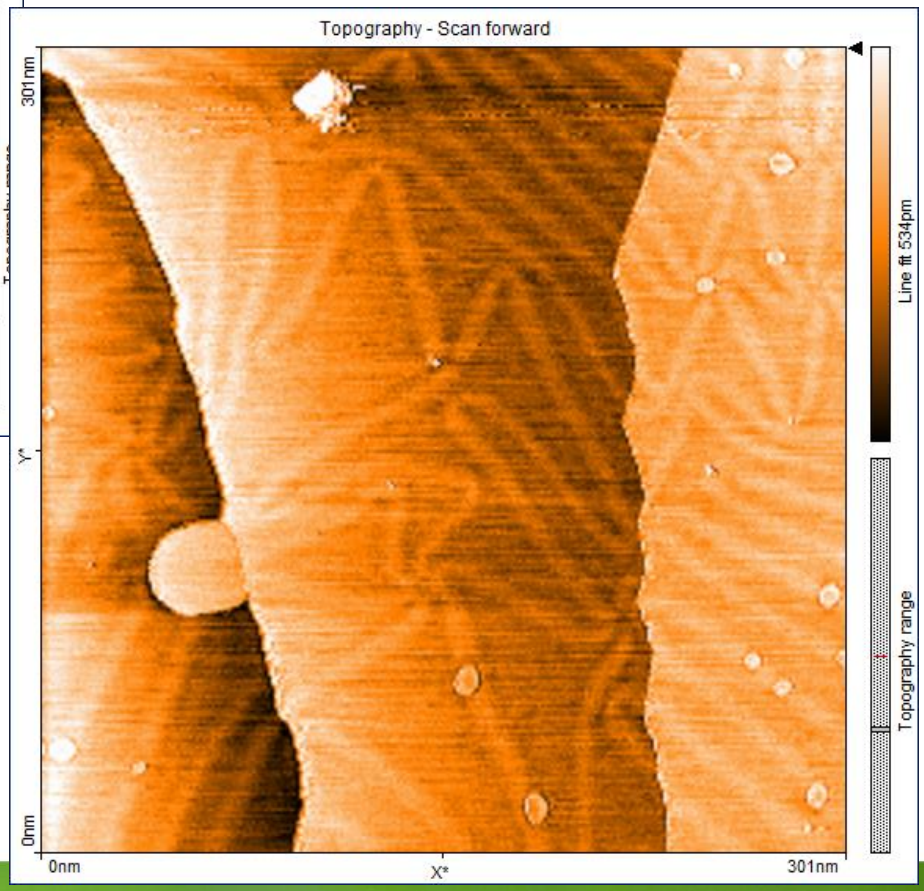
WYDZIAŁ FIZYKI

UNIWERSYTET WARSZAWSKI

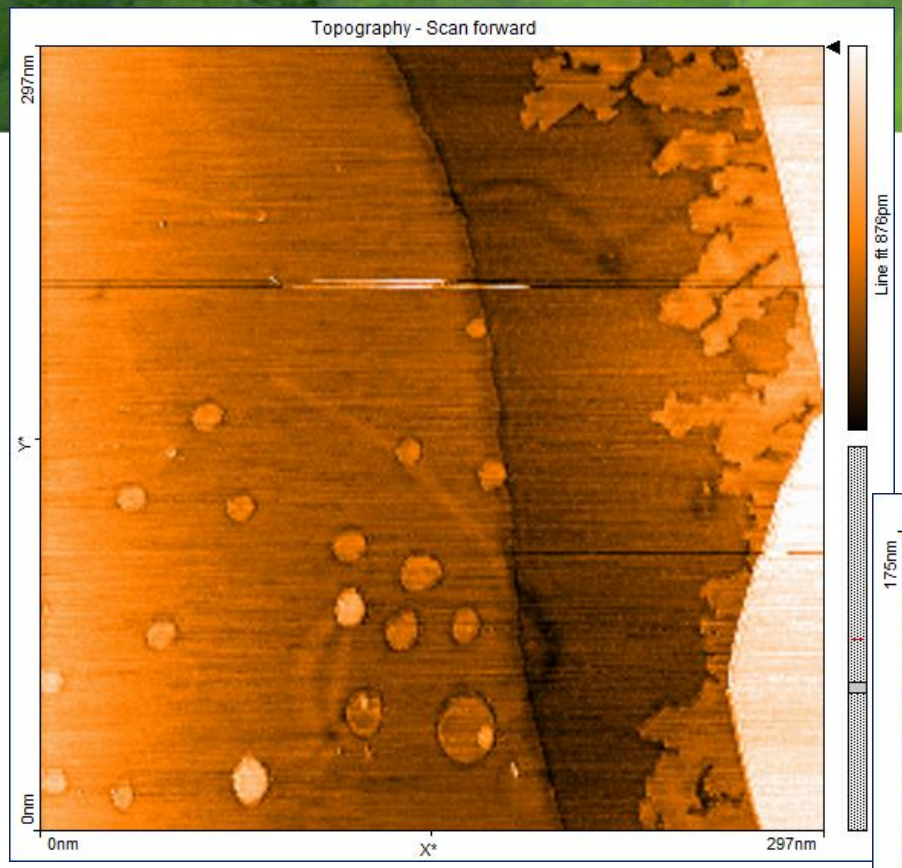
ITME

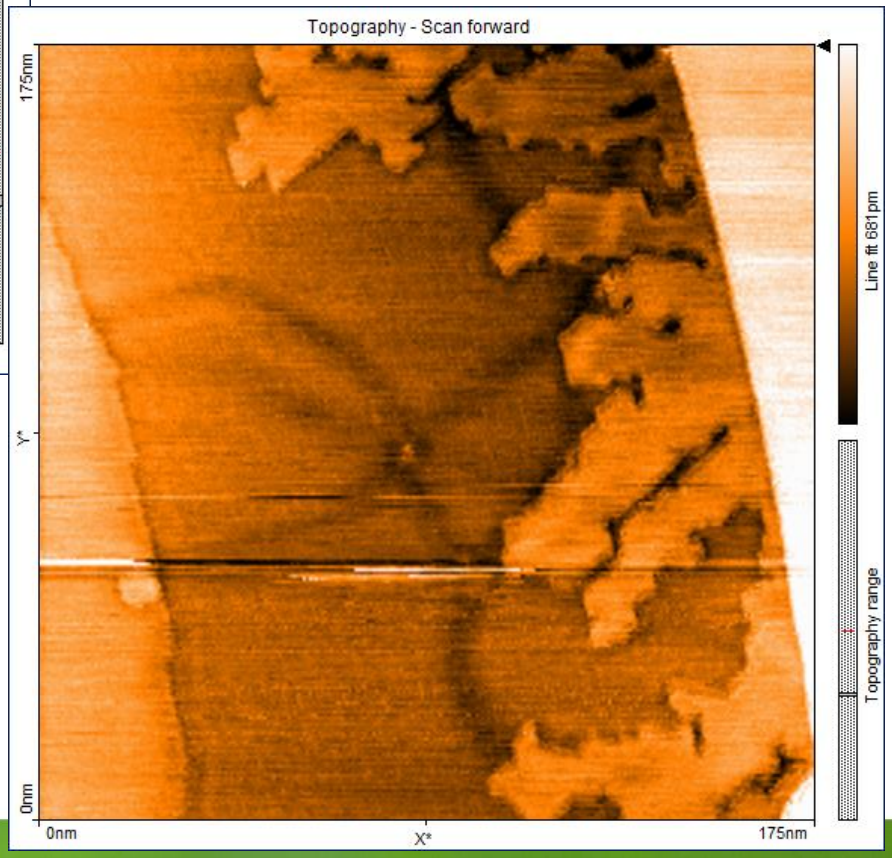




dr Jacek Szczytko
Michał Kluz
Izabela Rytarowska

Inżynieria nanostruktur





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Inżynieria nanostruktur

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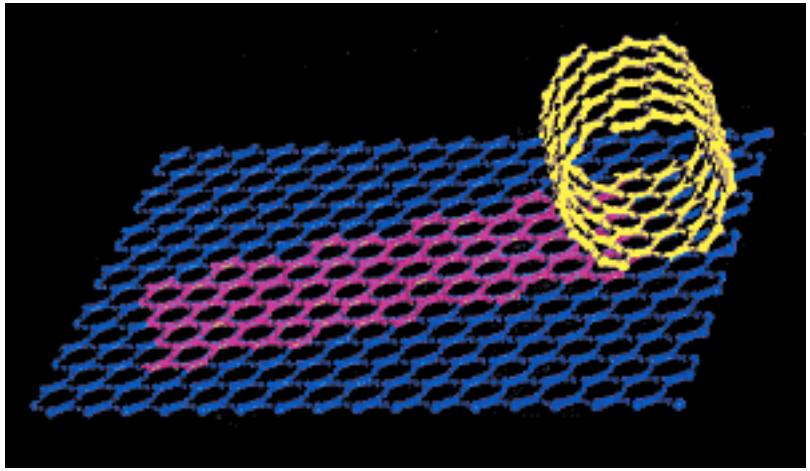
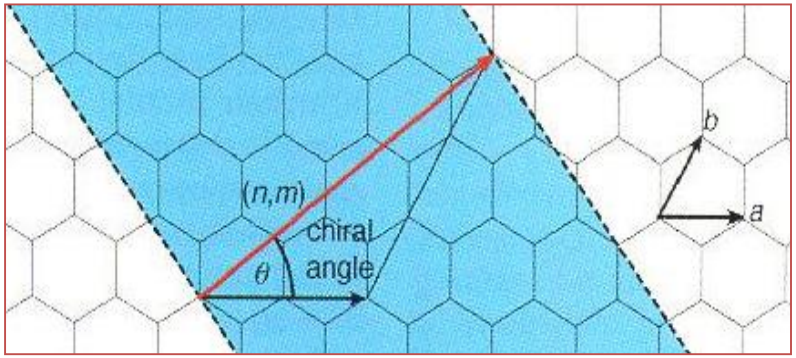
Michał Kluz
Izabela Rytarowsk

Inżynieria nanostruktur

Nanotubes

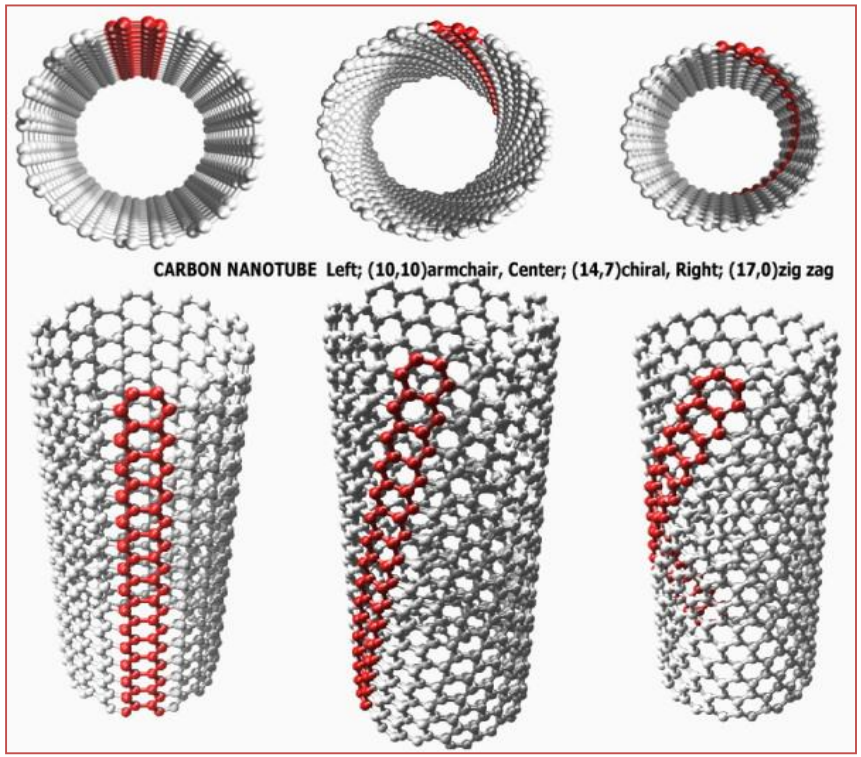




Orientation is defined by the chiral vector (n, m): $c_h = n\,a + m\,b$

Different orientations:

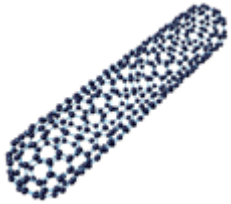
- **Armchair**
- **Zig-zag**
- **Chiral**



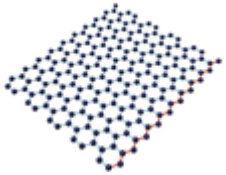
J.Basak, D.Mitra, S.Sinha „*Carbon nanotube: the next generation sensors*" presentation

Paweł Tomasz Pęczkowski

Nanotubes

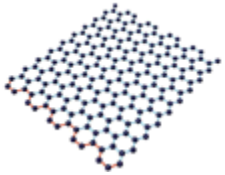


Single Wall Nanotube
(Zig-Zag Type)

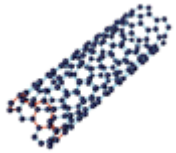


Uprolling a Graphene
(Zig-Zag Type)

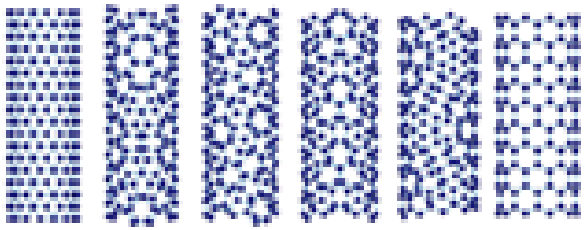
Single Wall Nanotube
(Arm-Chair Type)

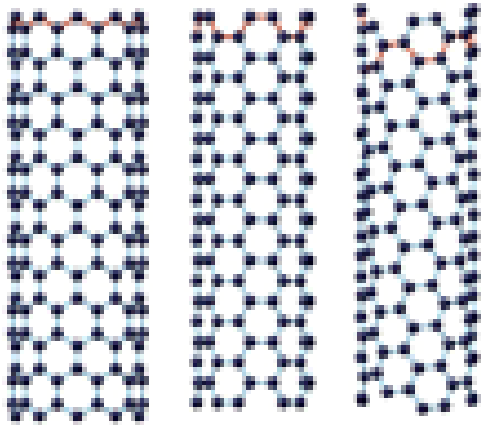


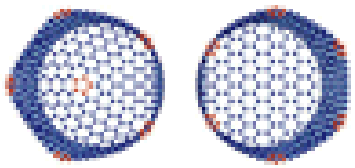
Uprolling a Graphene
(Arm-Chair Type)

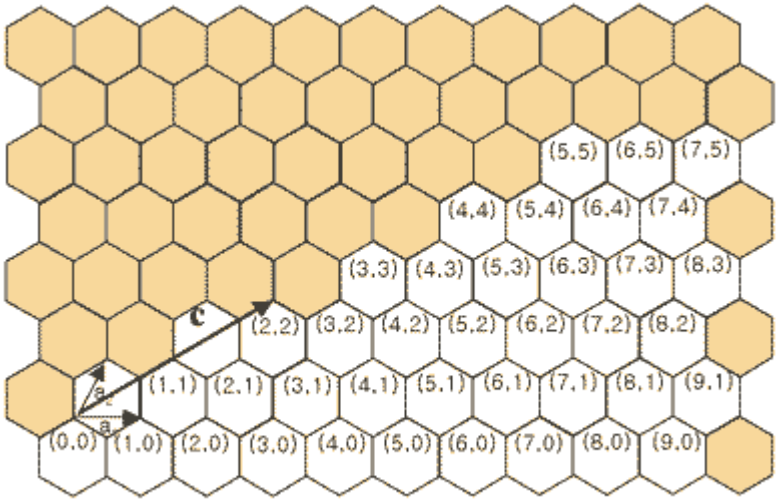


Single Wall Nanotube
(Chiral Type)





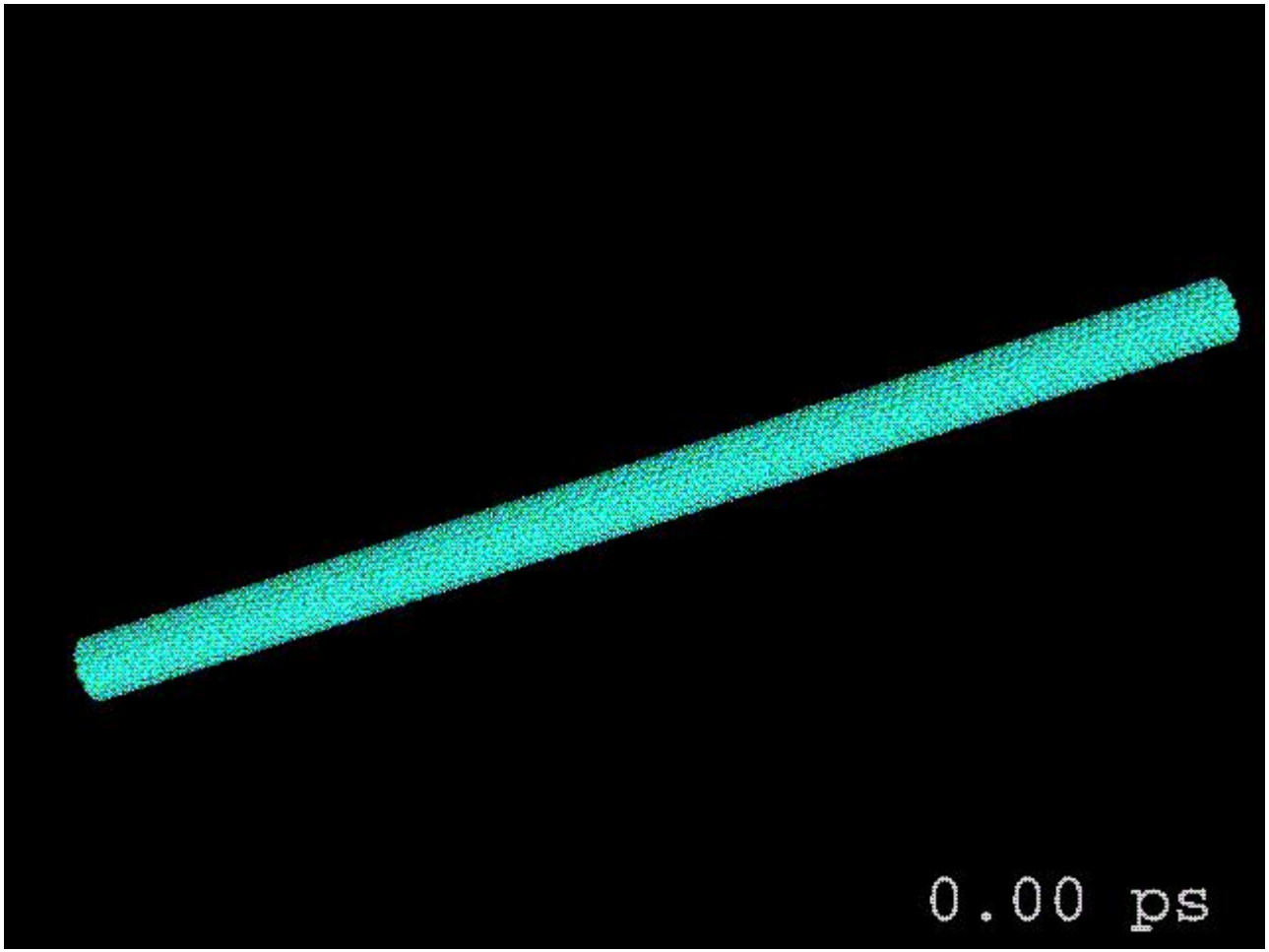




$$\phi = 0.246\ (n^2+nm+m^2)^{1/2} / \pi\ (nm)$$

www.surf.nuqe.nagoya-u.ac.jp/nanotubes/omake/nanotubes/nanotubes.html

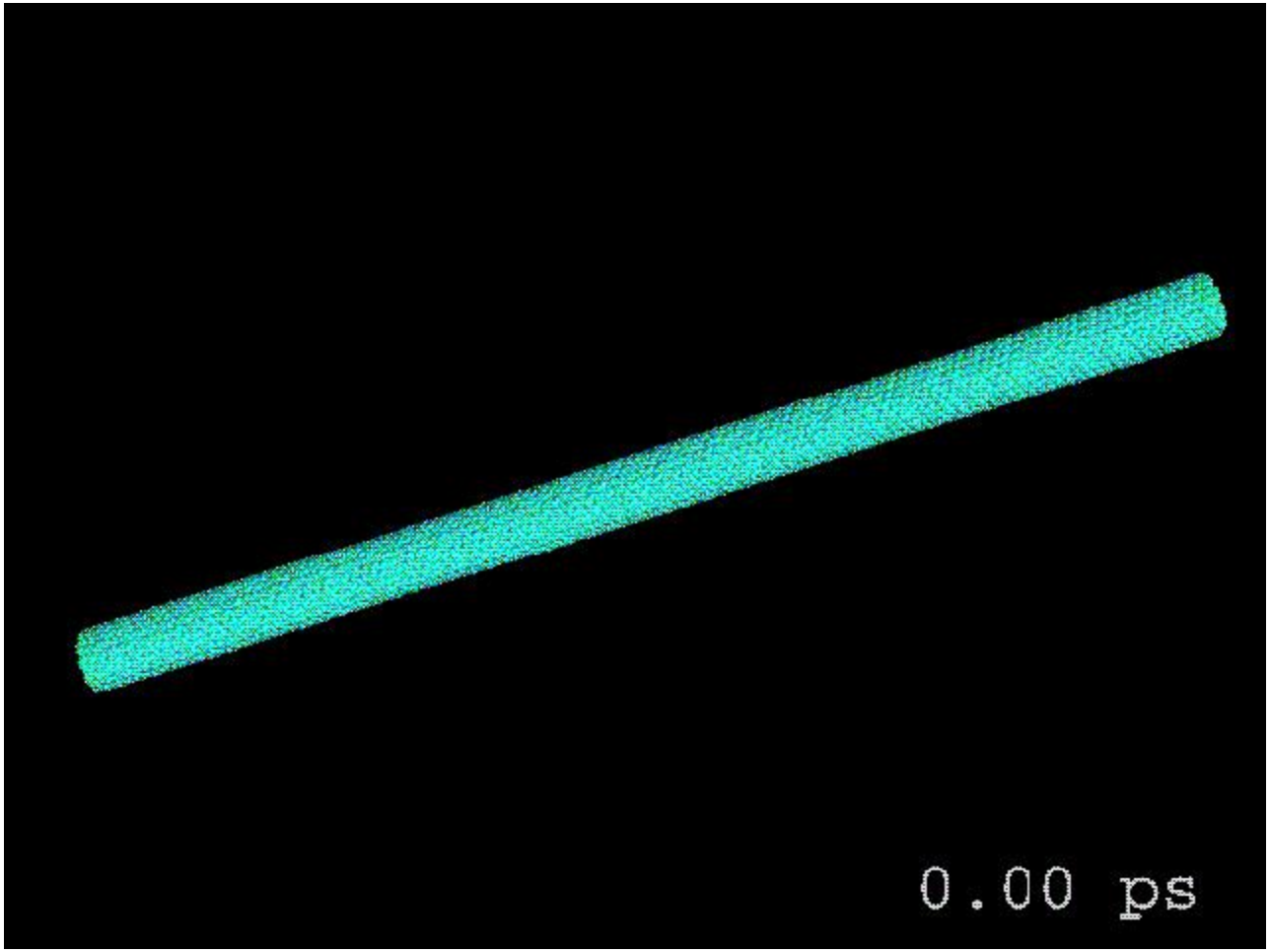
Nanomachines



Single – twist

http://www.ipt.arc.nasa.gov

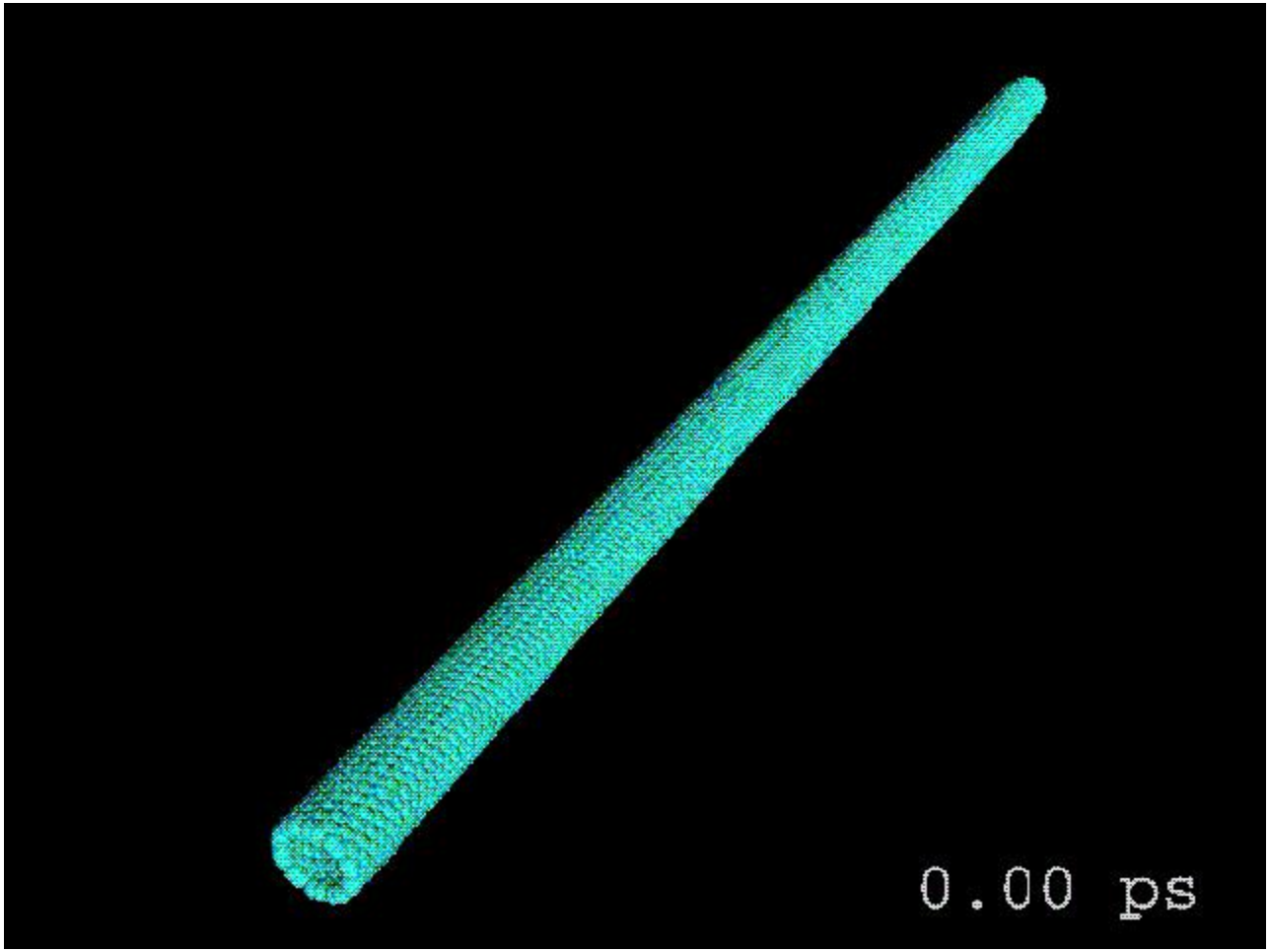
Nanomachines



Single – bend

http://www.ipt.arc.nasa.gov

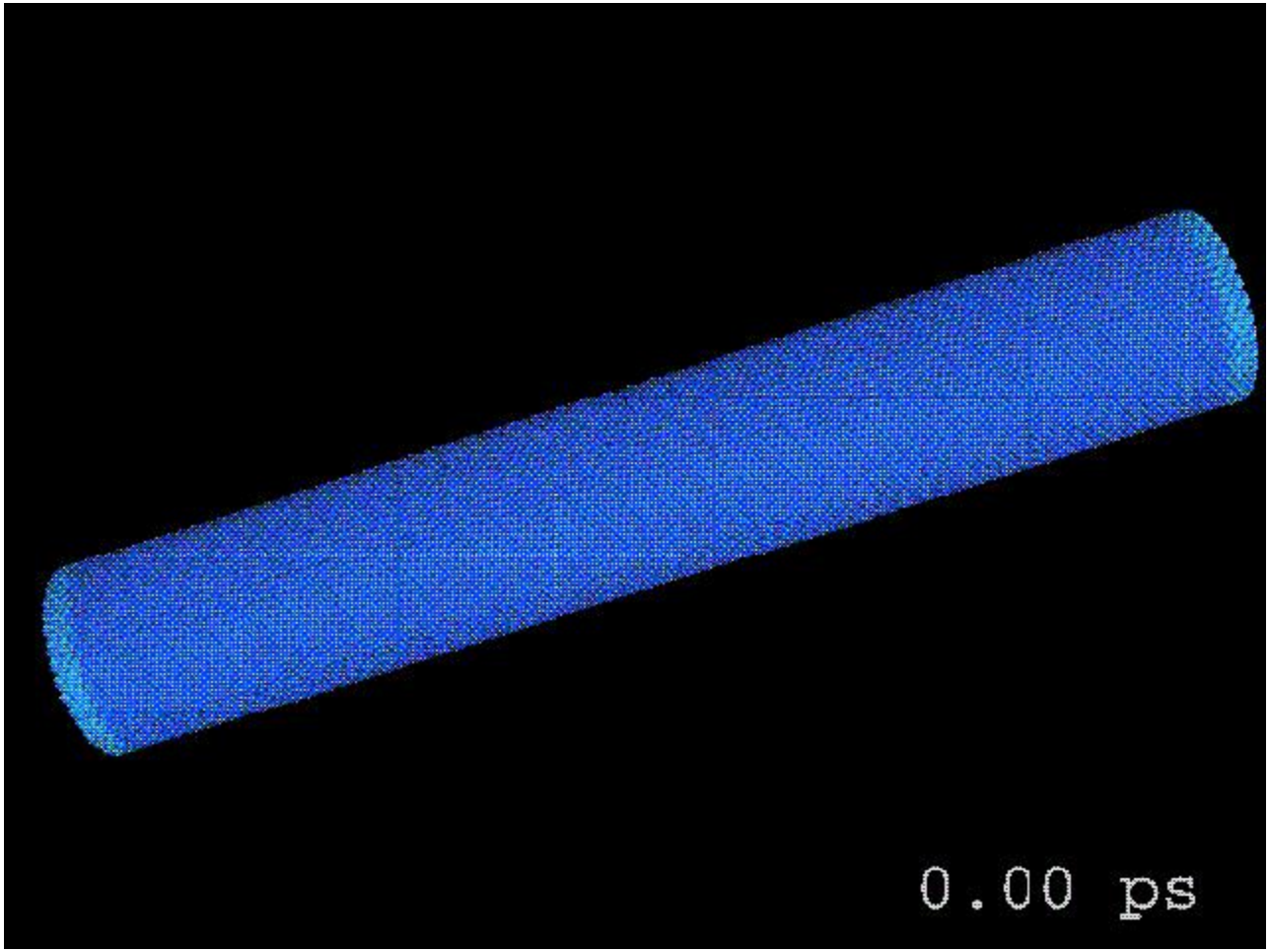
Nanomachines



Single – compress

http://www.ipt.arc.nasa.gov

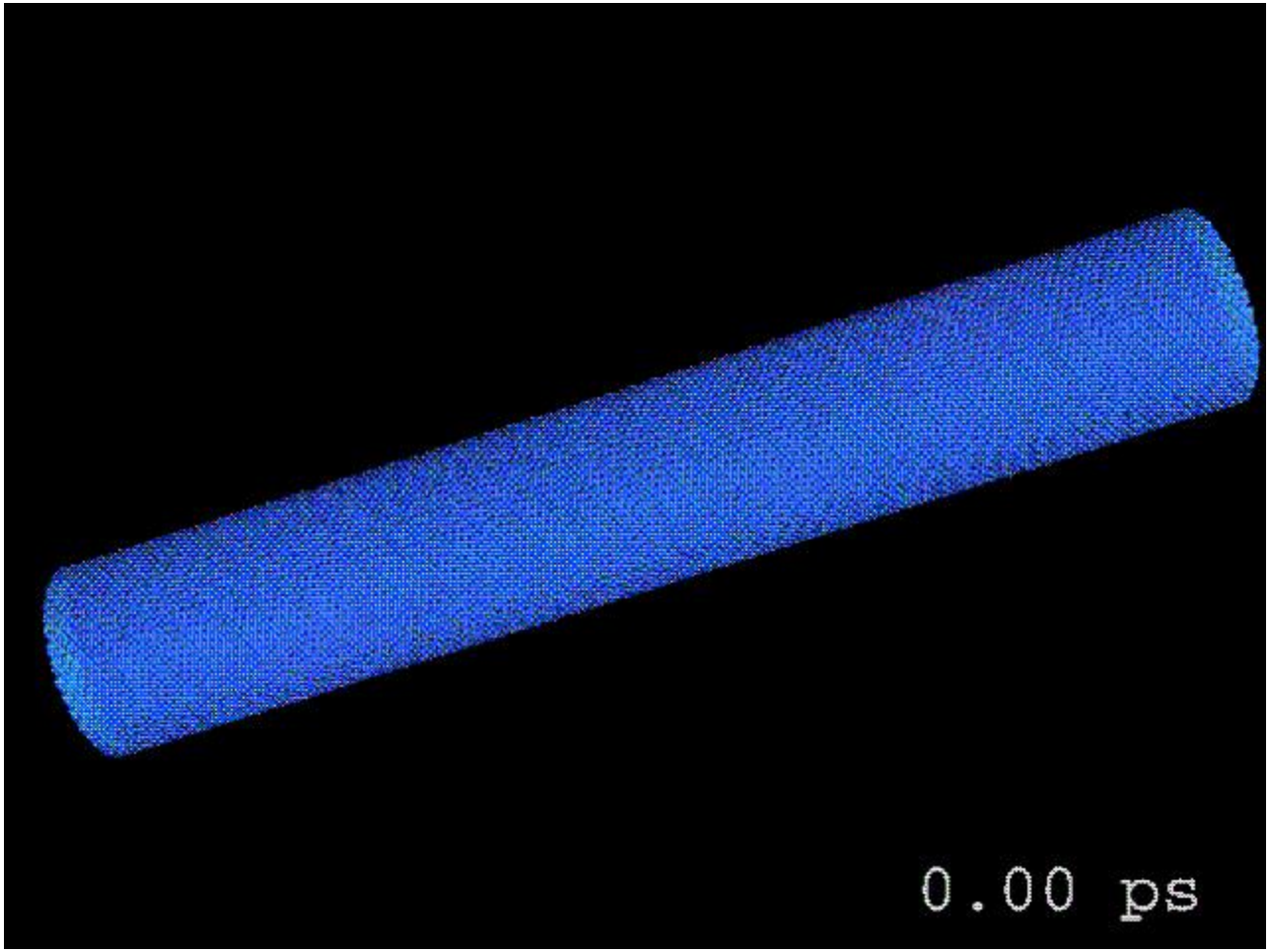
Nanomachines



Multi – twist

http://www.ipt.arc.nasa.gov

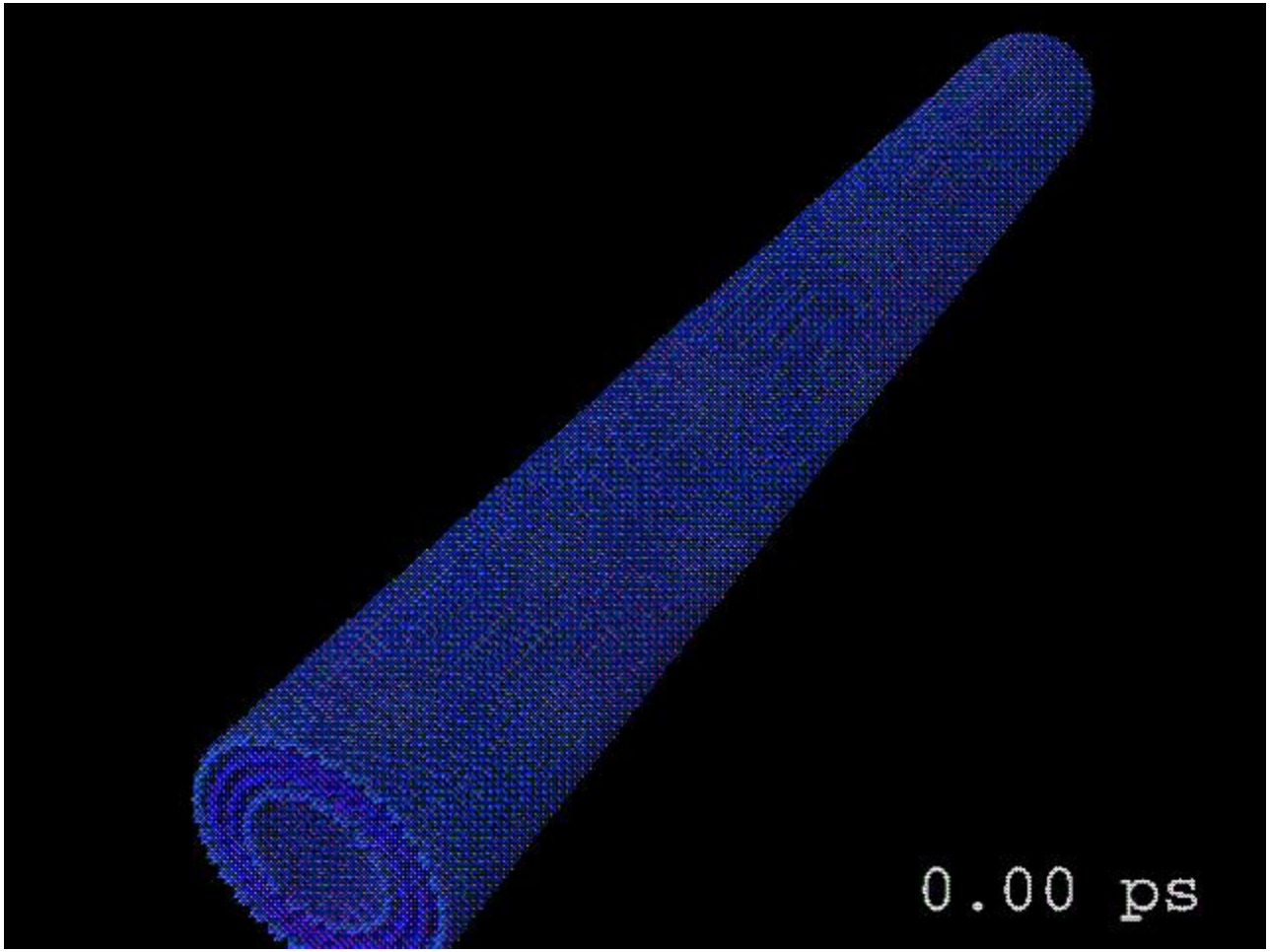
Nanomachines



Multi – bend

http://www.ipt.arc.nasa.gov

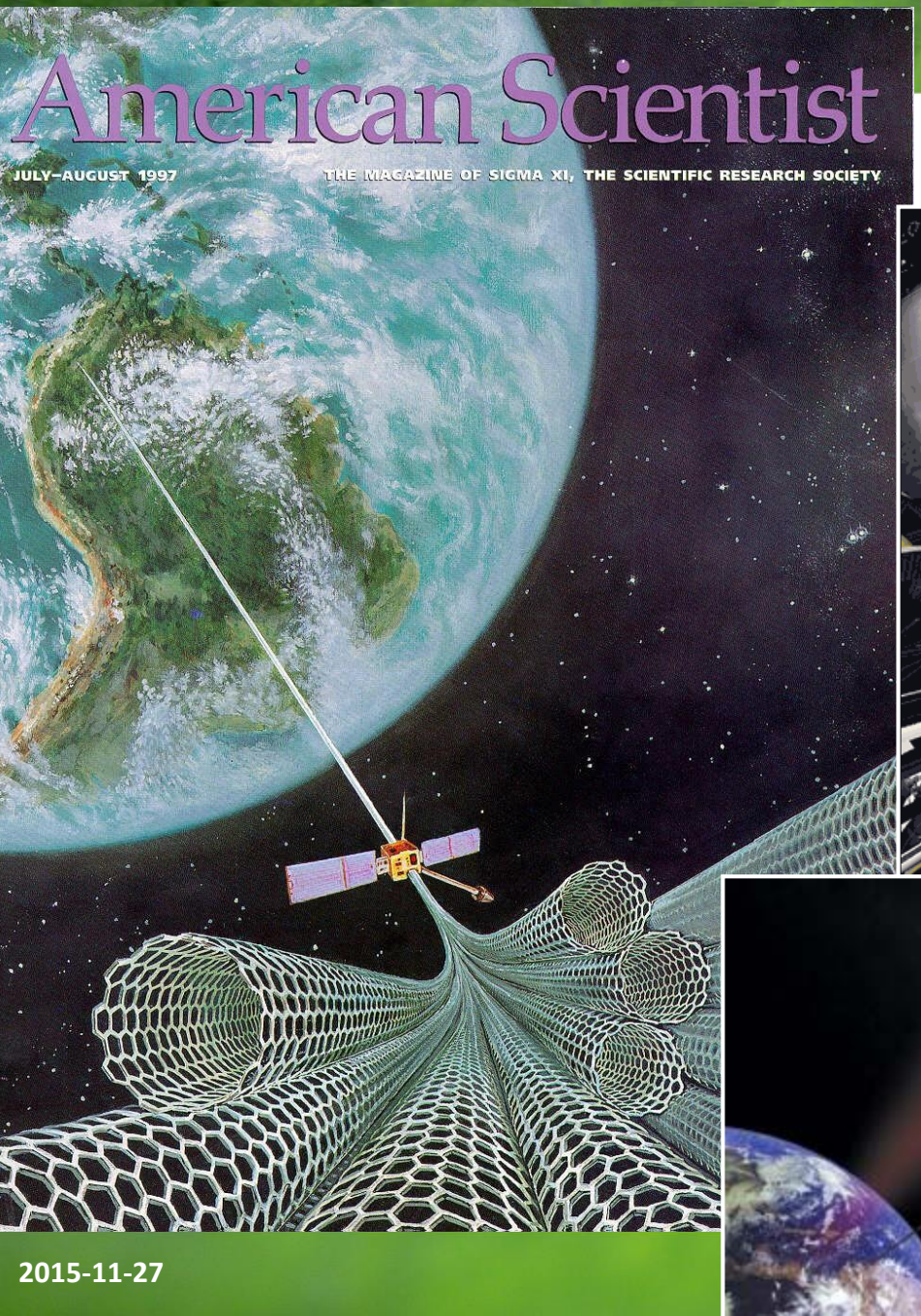
Nanomachines

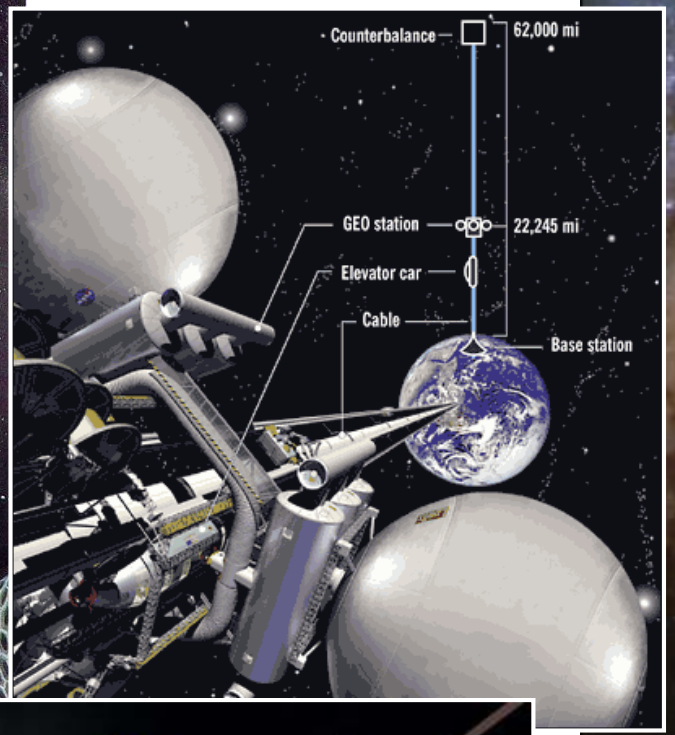


Multi – compress

http://www.ipt.arc.nasa.gov

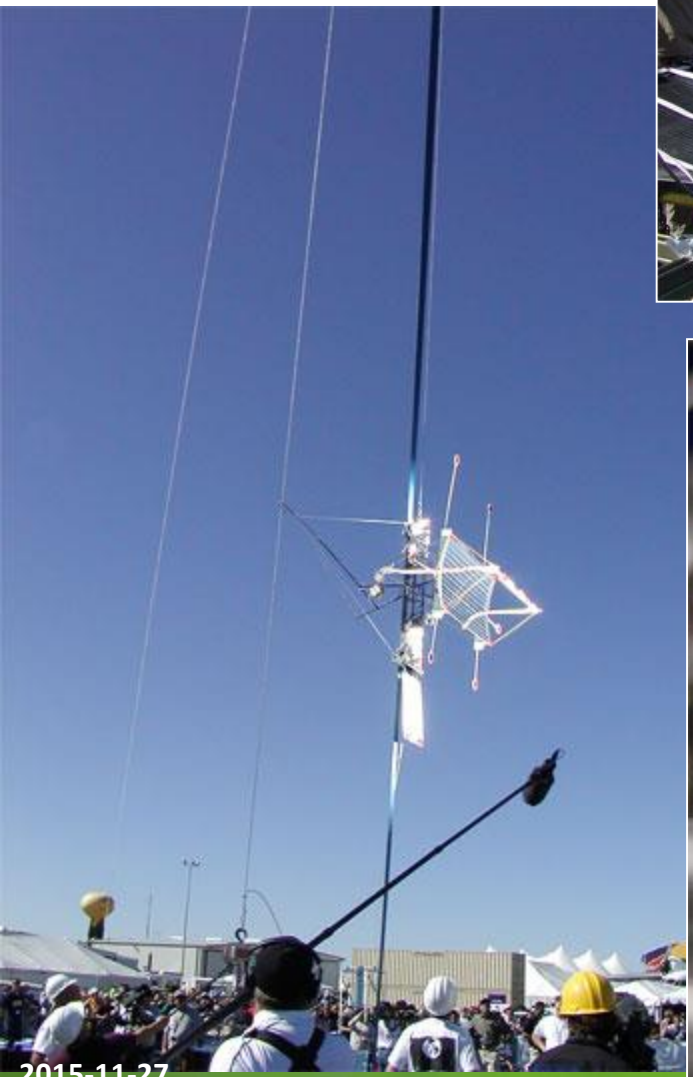
Space elevator

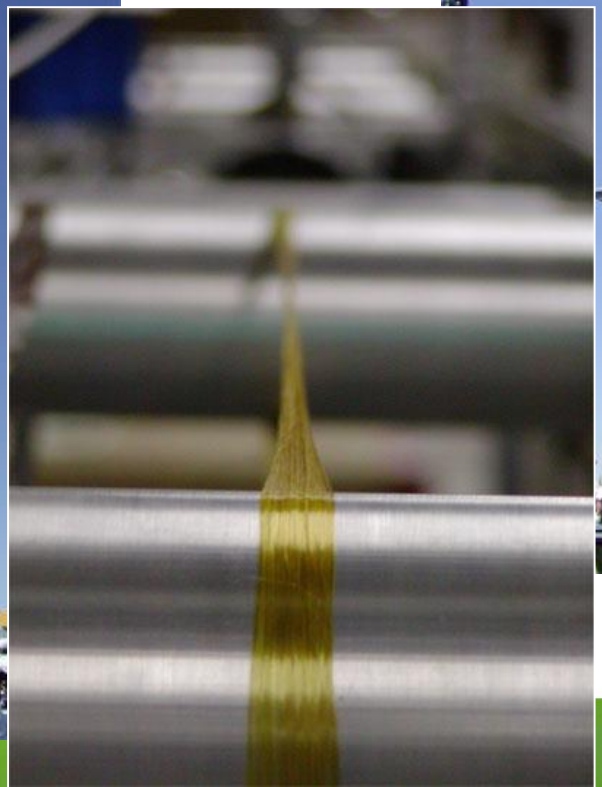




Space elevator

http://www.spaceelevator.com/





Space elevator

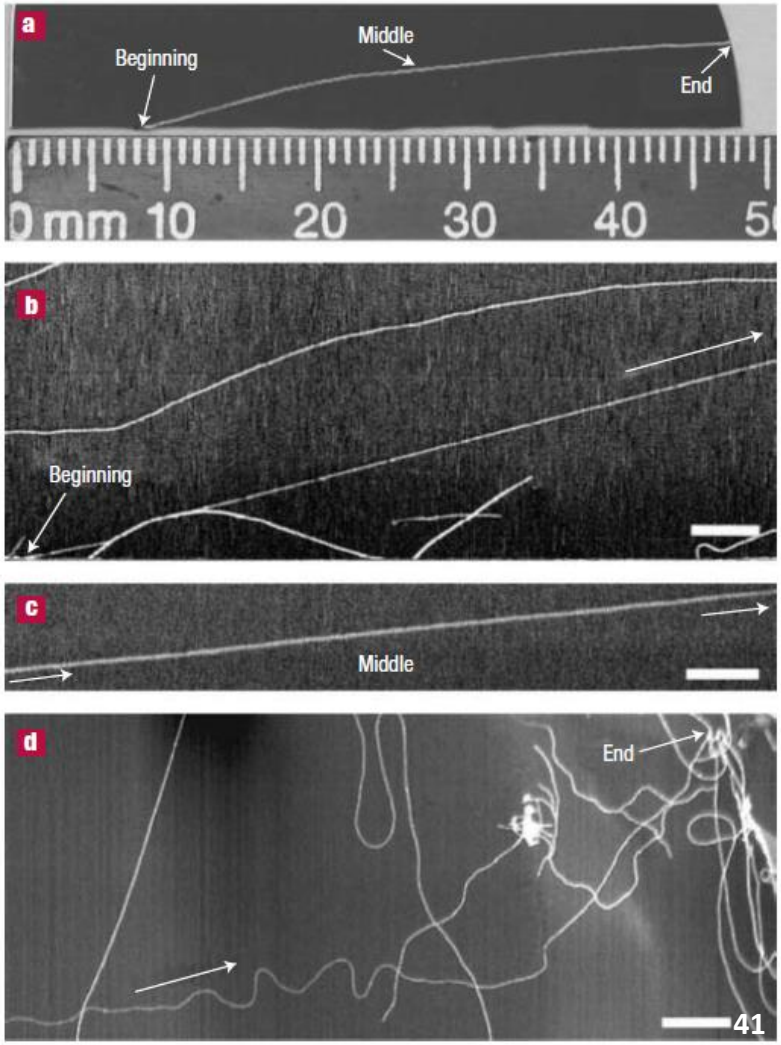
LETTERS

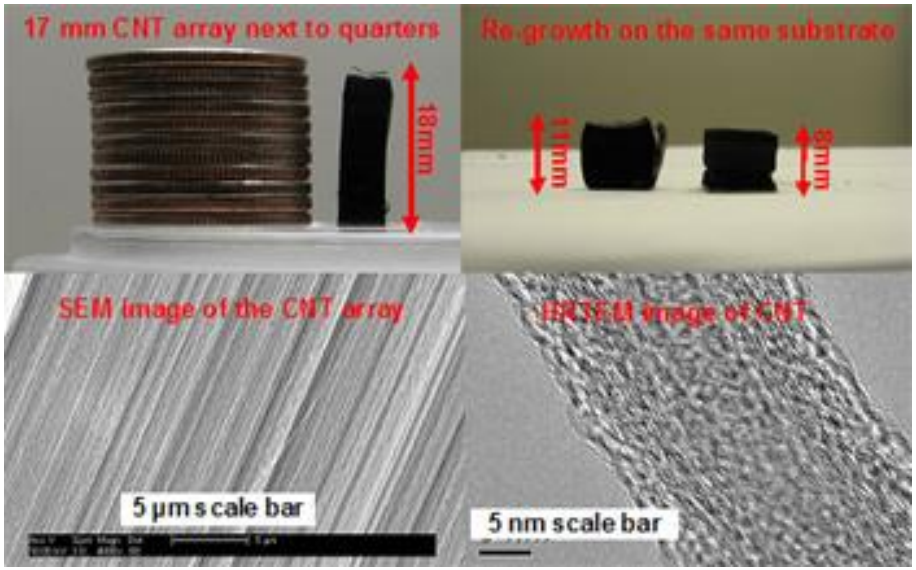
Ultralong single-wall carbon nanotubes

L. X. ZHENG[1], M. J. O'CONNELL[1], S. K. DOORN[1], X. Z. LIAO[1], Y. H. ZHAO[1], E. A. AKHADOV[1], M. A. HOFFBAUER[1], B. J. ROOP[1], Q. X. JIA[1], R. C. DYE[1], D. E. PETERSON[1], S. M. HUANG[2], J. LI[1,2] AND Y. T. ZHU[1]*

[1]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
[2]Chemistry Department, Duke University, Durham, North Carolina 27708, USA
*e-mail: yzhu@lanl.gov

nature materials | VOL 3 | OCTOBER 2004 | www.nature.com/naturematerials

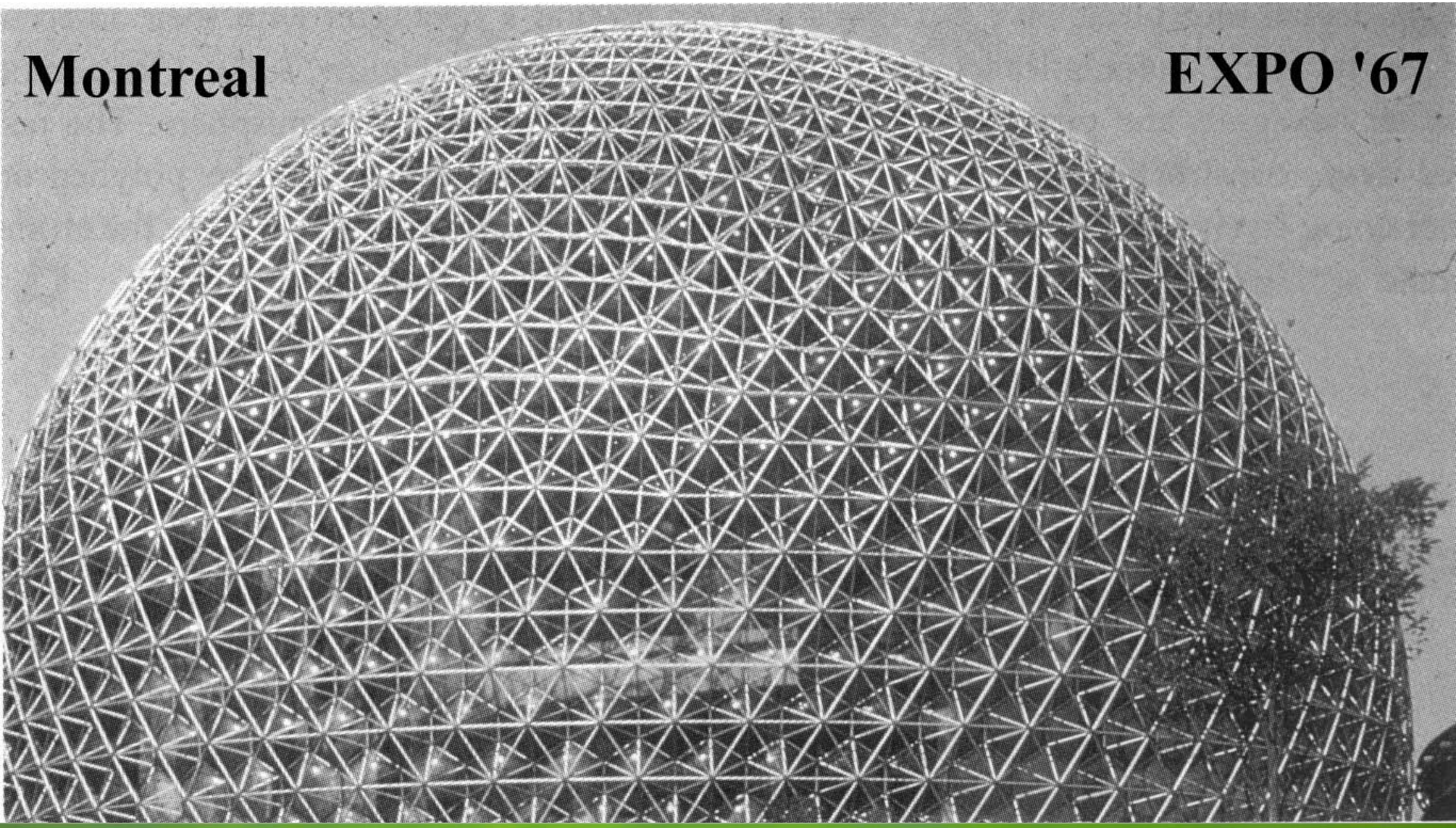




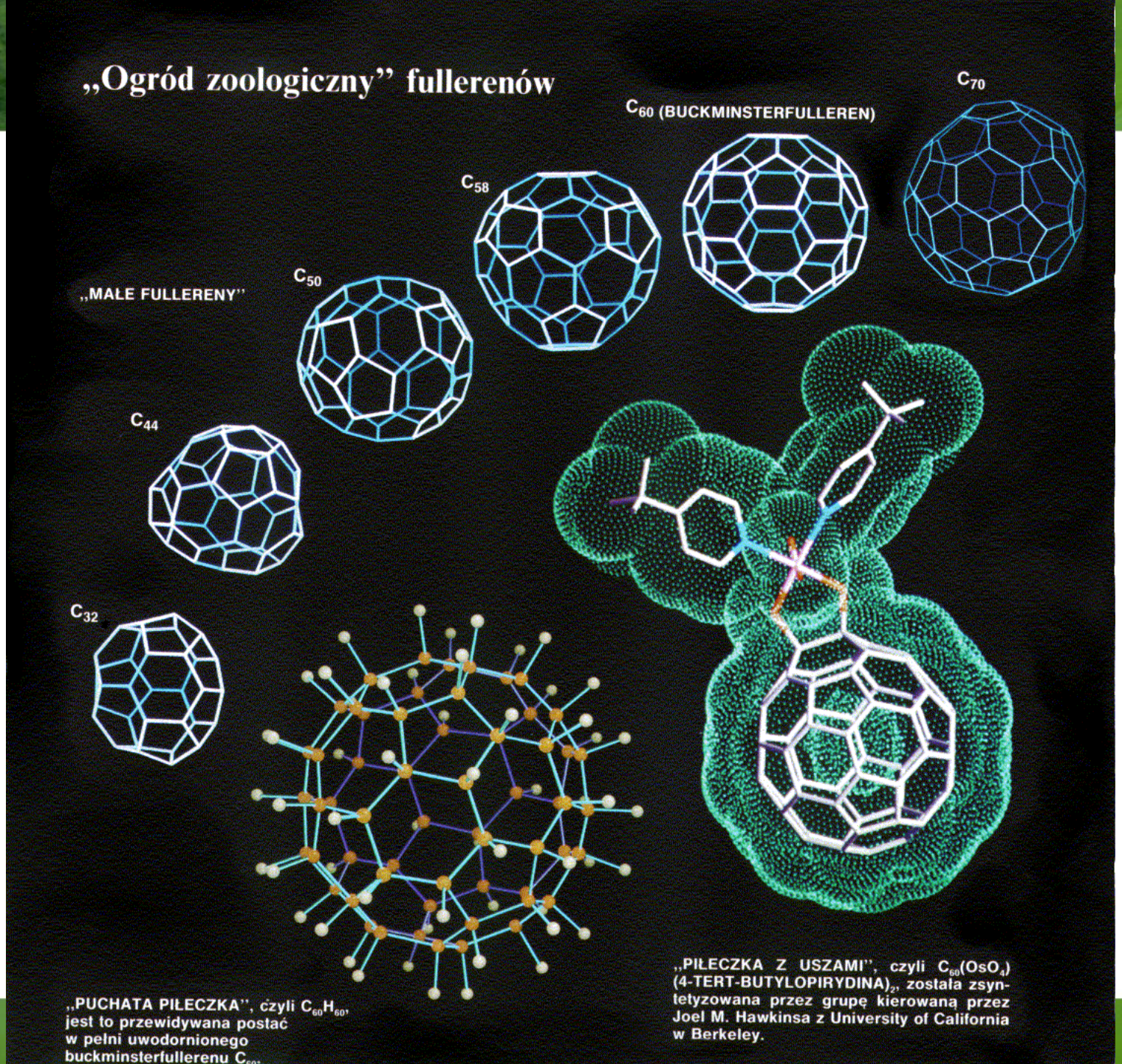
http://www.uc.edu/news/NR.asp?id=5700

Fullerenes

Buckminster Fuller pour un exposition en 1967 à Montréal



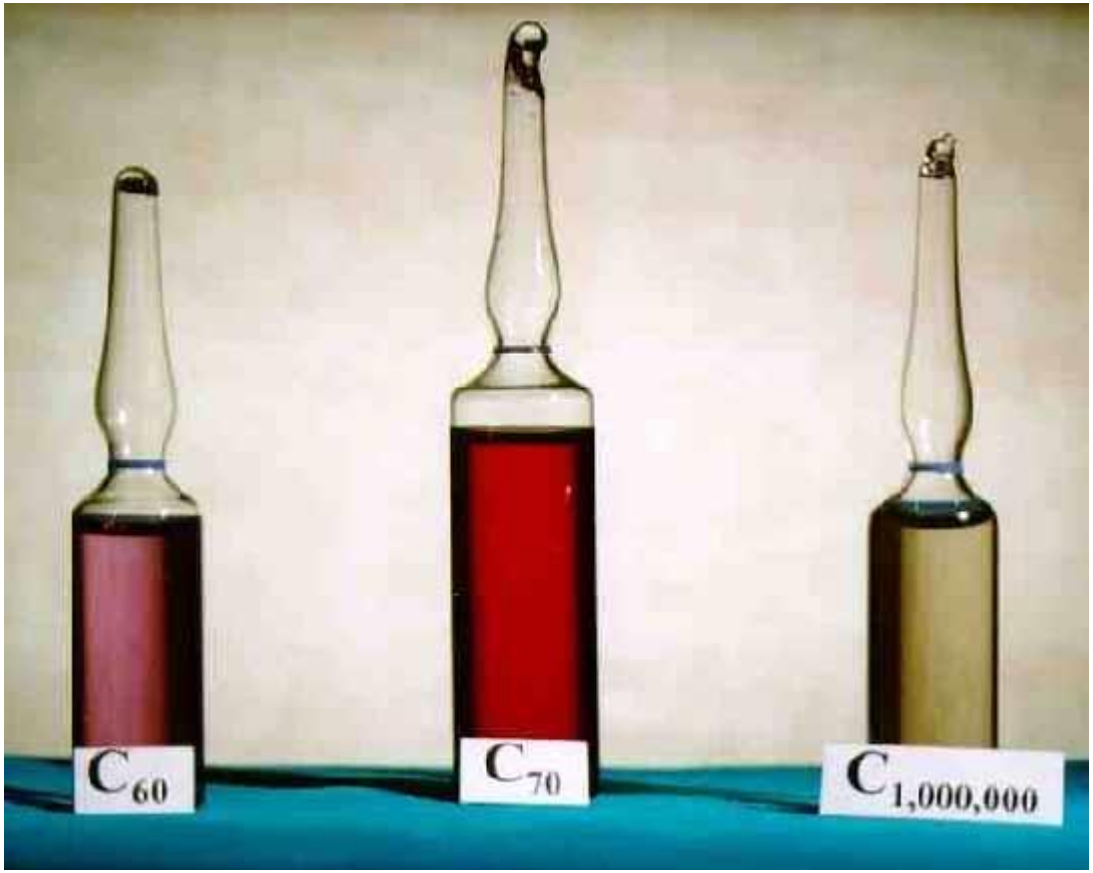
„Ogród zoologiczny" fullerenów



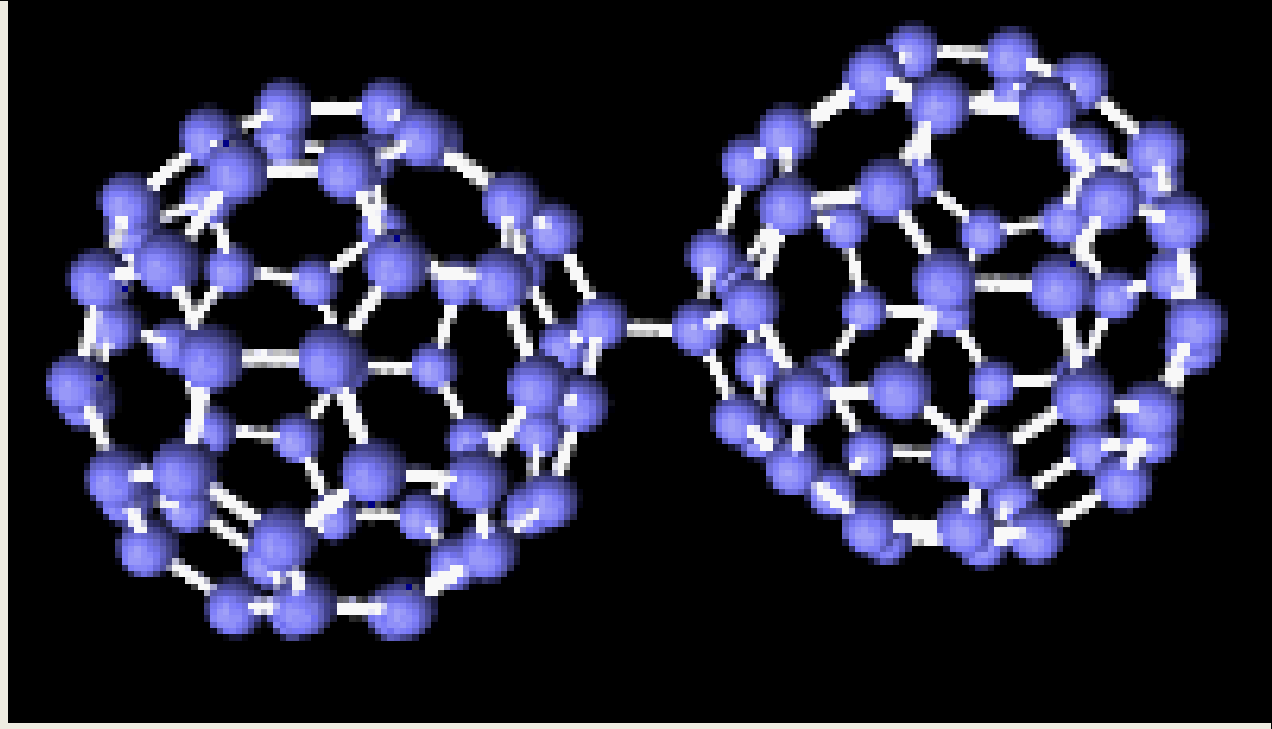
„PUCHATA PIŁECZKA", czyli $C_{60}H_{60}$, jest to przewidywana postać w pełni uwodornionego buckminsterfullerenu C_{60}.

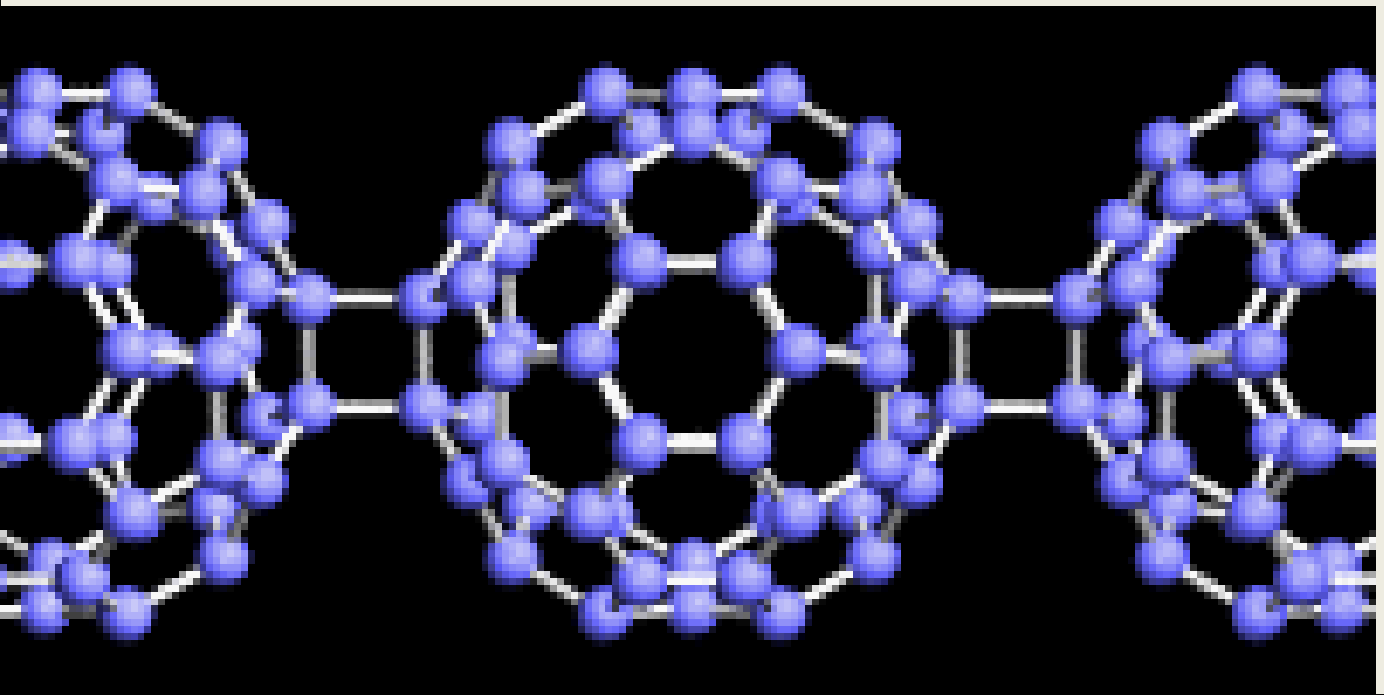
„PIŁECZKA Z USZAMI", czyli $C_{60}(OsO_4)(4\text{-TERT-BUTYLOPIRYDINA})_2$, została zsyntetyzowana przez grupę kierowaną przez Joel M. Hawkinsa z University of California w Berkeley.

Fullerenes

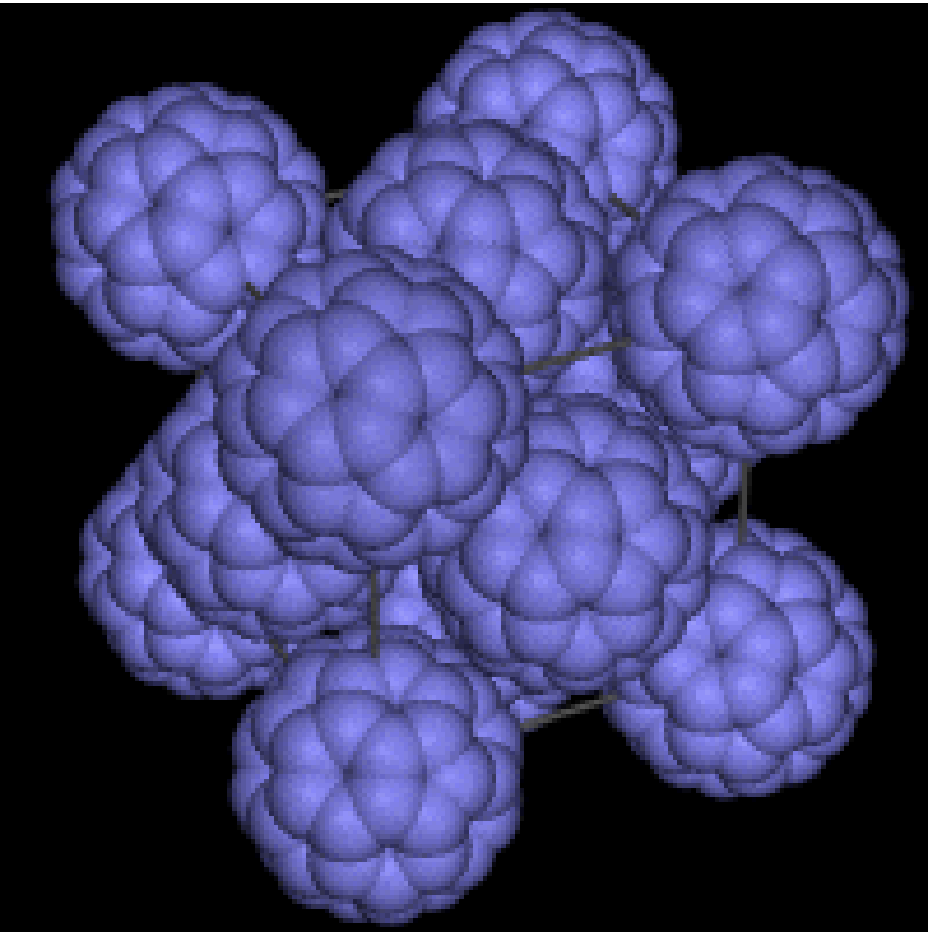


Solutions in toluene

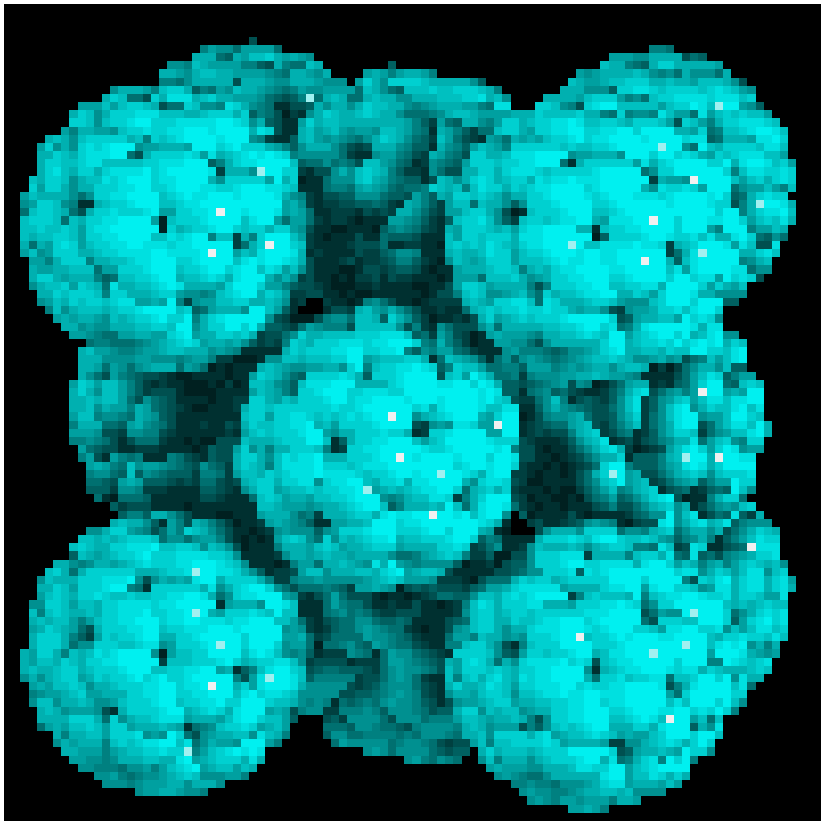




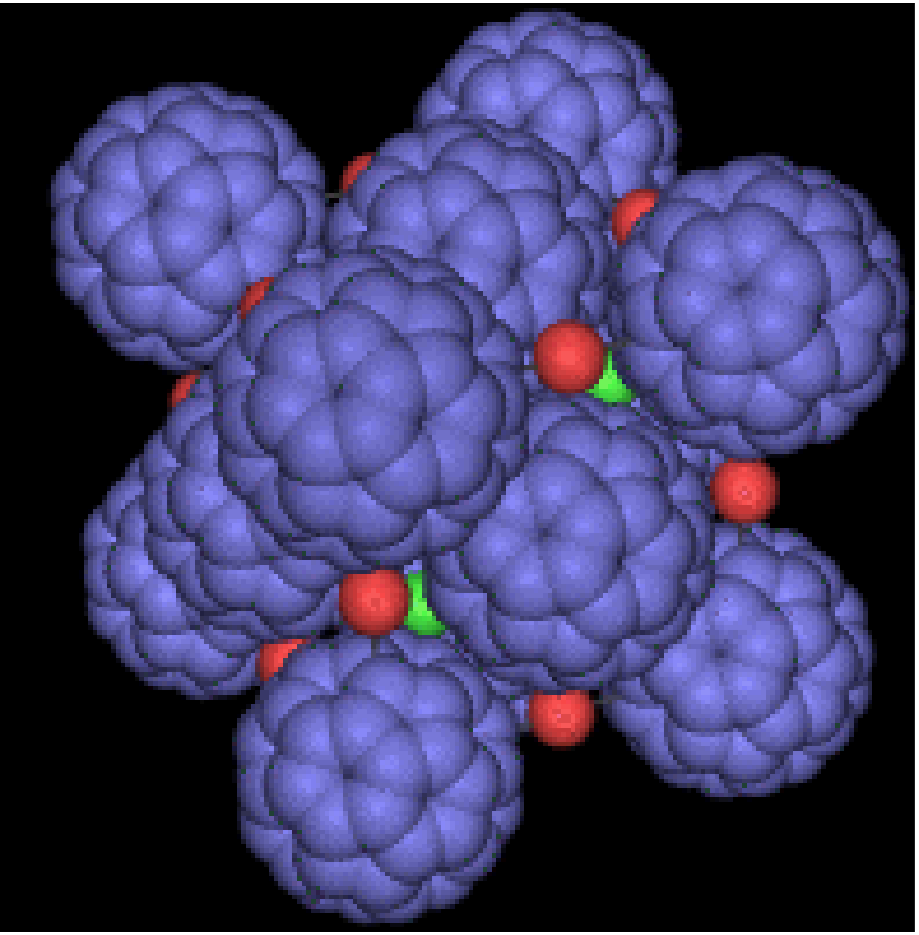
Fullerenes

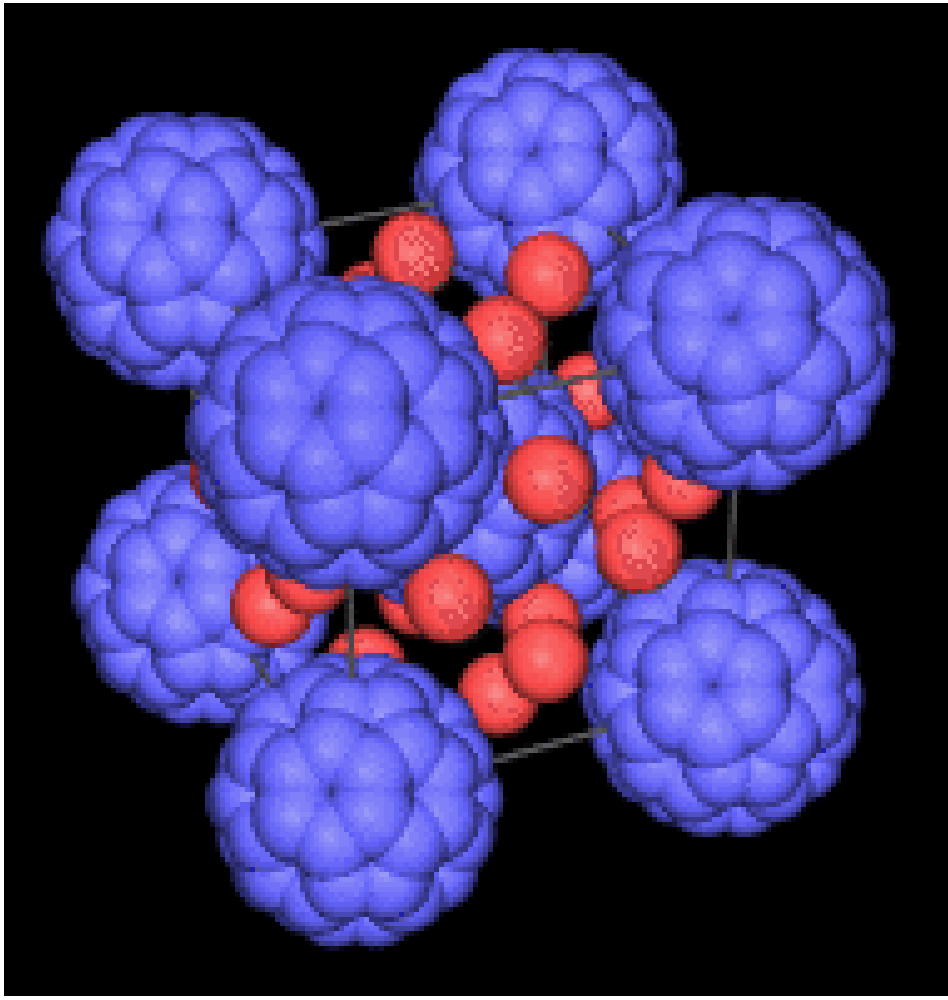


fcc C_{60} crystals



Fullerenes



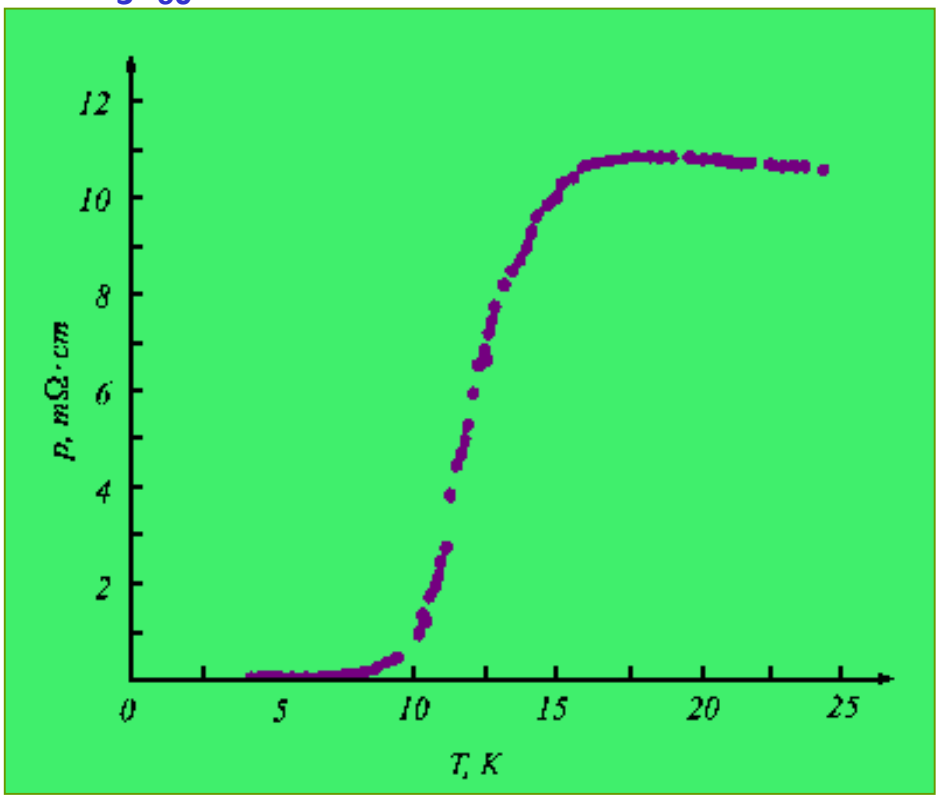


Fullerenes

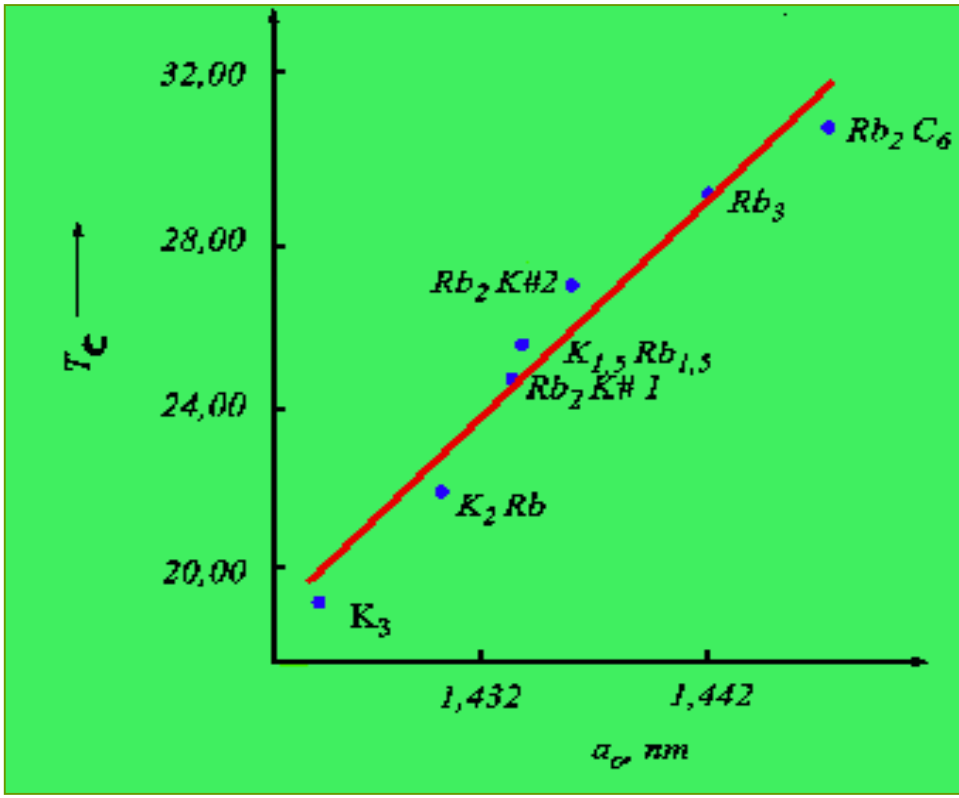
Superconductivity K_3C_{60}

X.D. Xiang, J.G. Hou, et al. Nature 361, 54, 1993

Zależność oporu właściwego K_3C_{60} od temperatury

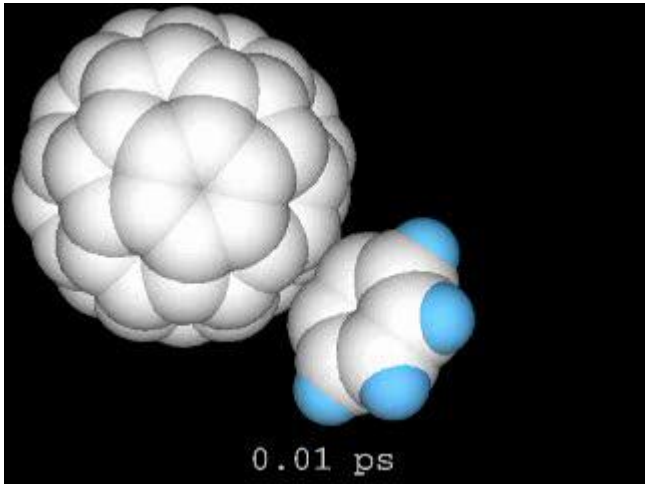


Zależność Tc od stałej sieci

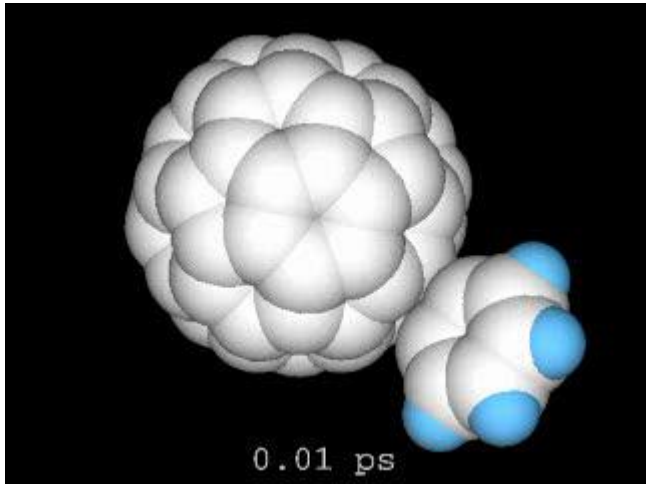


Nanomachines

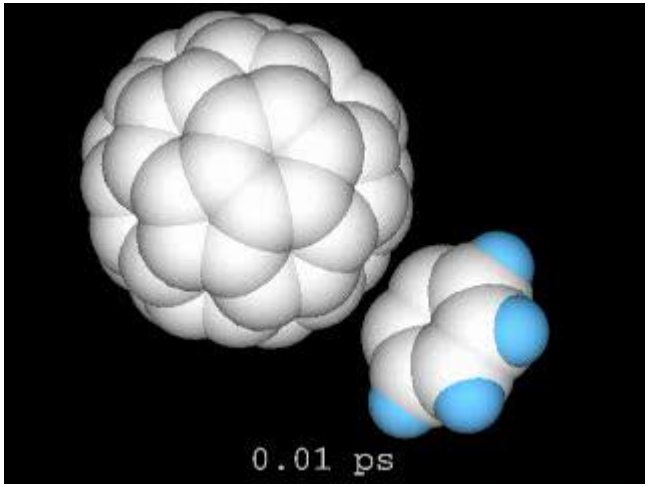
Benzene + C_{60}



Too slow



Too fast

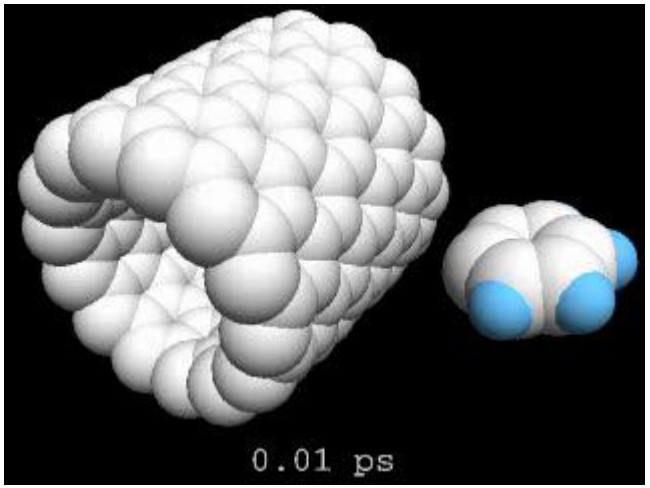


Accurately

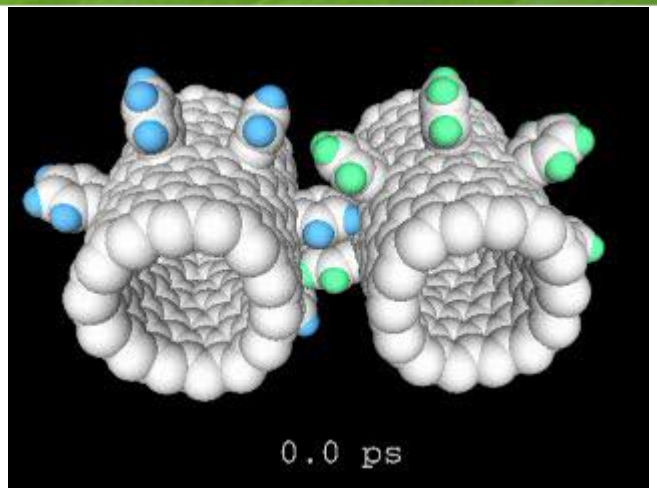
http://www.ipt.arc.nasa.gov

Nanomachines

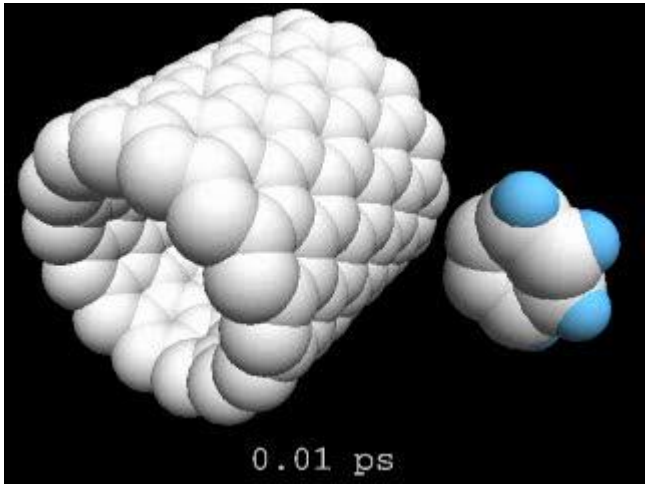
Benzen + CN



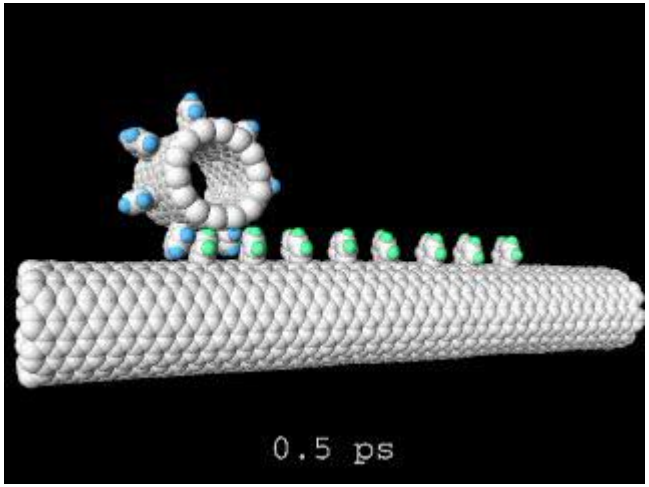
Too slow



Gear Rotation in a Vacuum 200 rot/ns



Accurately



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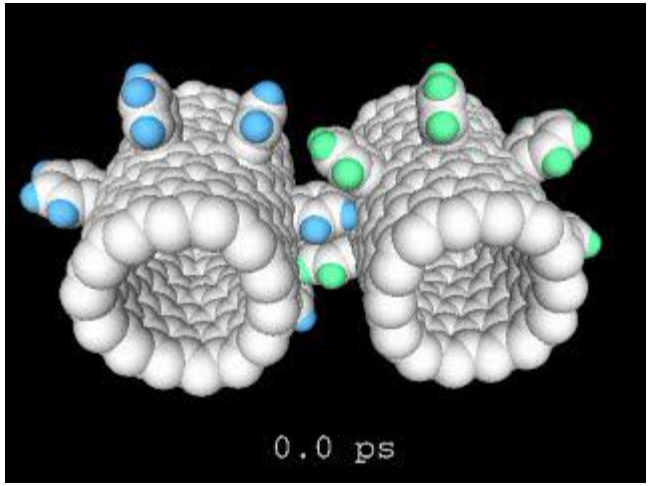
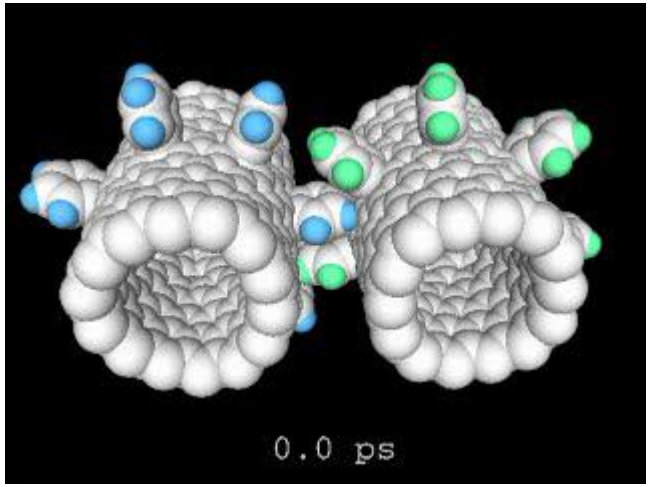
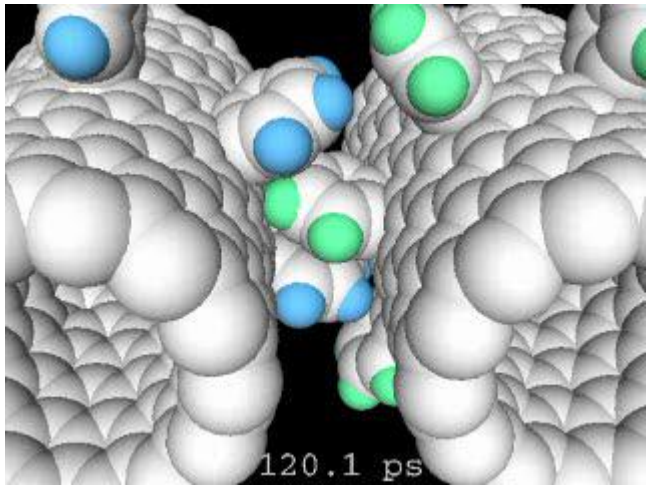


Gear Rotation at RT 50/70/100 rot/ns



Gear Rotation at RT 50 rot/ns



Too fast > 100 rot/ns

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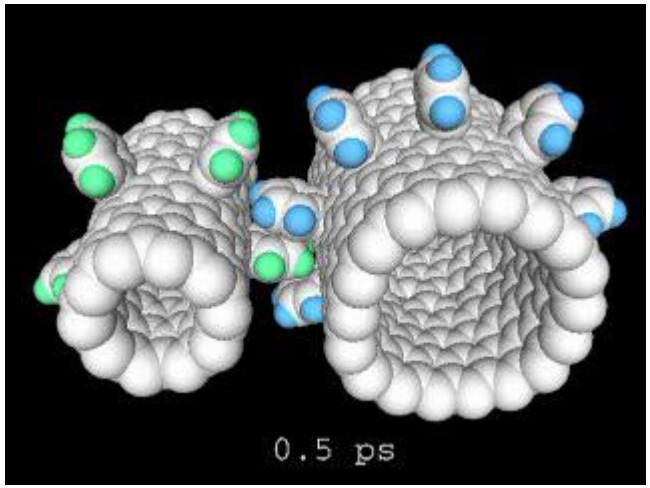
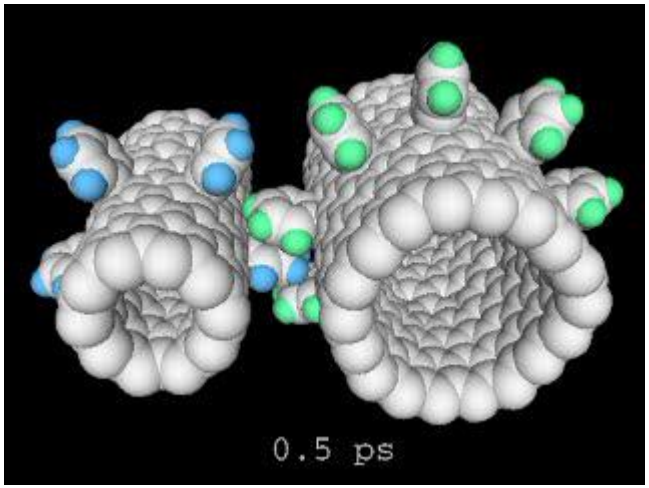
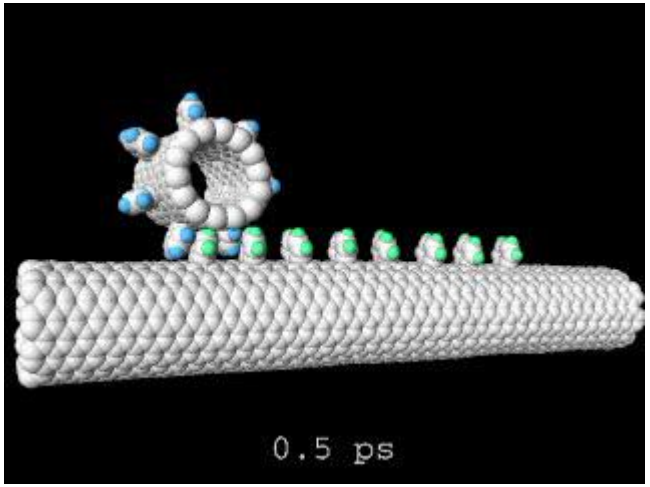
Large Gear Drives Small Gear





Gear and Shaft Operation



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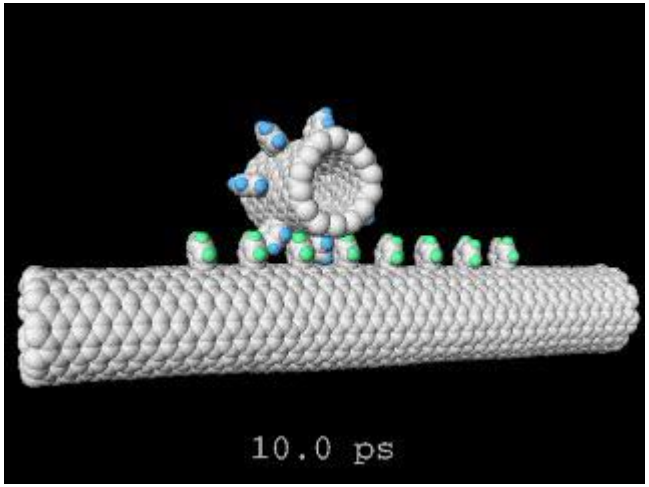

Powered Gear

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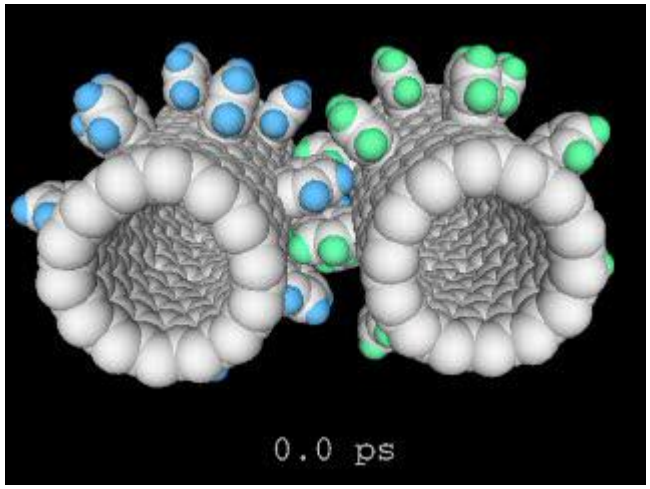
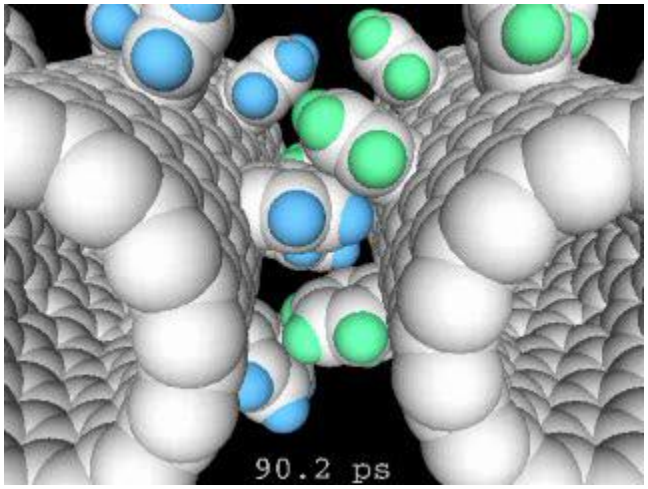
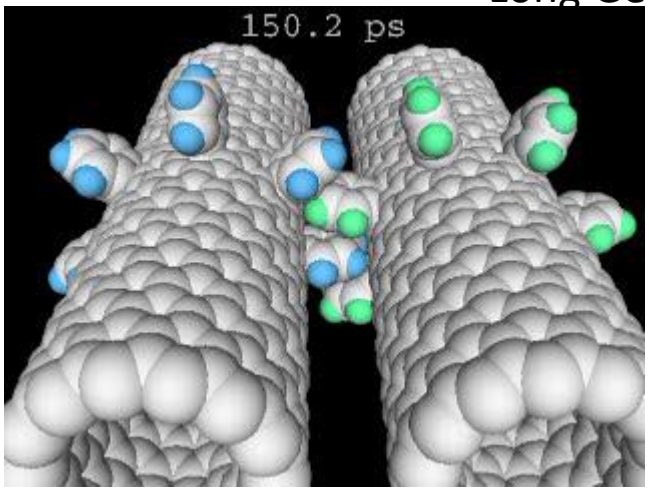
Rotation of Gears with Two Off-line Rows of Teeth

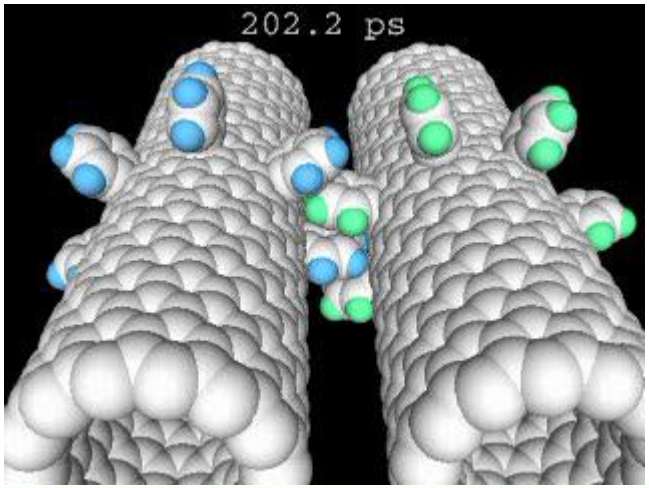




Zbyt szybko

Long Gear Rotation at Room Temperature





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Negatively Curved Graphitic Sheet Model of Amorphous Carbon

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(Received 9 April 1992)

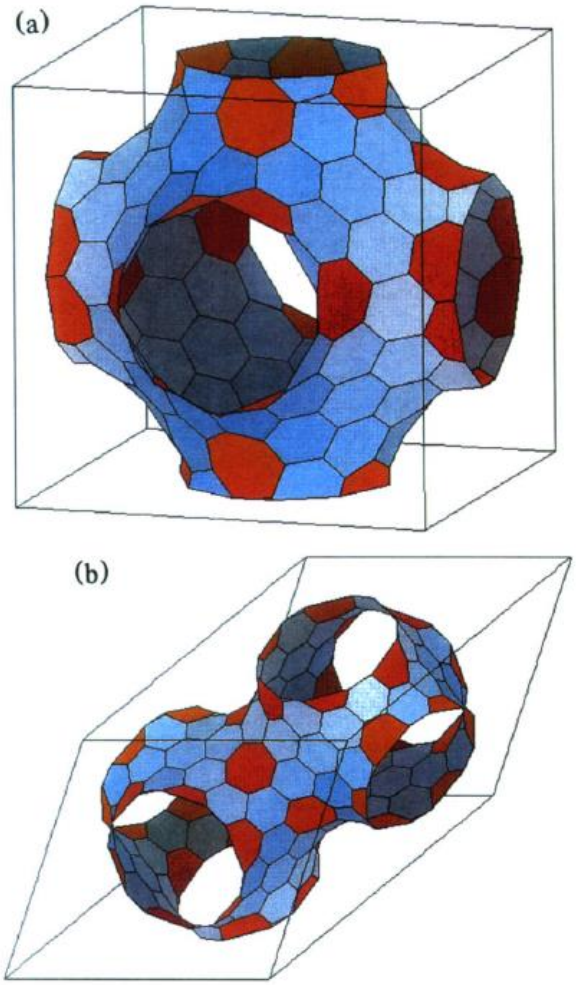

FIG. 1. Views of two new crystalline schwarzites. Each has 216 carbon atoms per primitive unit cell with 80 six-membered rings (blue) and 24 seven-membered rings (orange). The structure in (a) lies on a *P* minimal surface in a cubic cell 15.7 Å on a side. The structure in (b) lies on a *D* minimal surface in an fcc cell whose cubic lattice constant is 24.6 Å.

„plumber's nightmare"

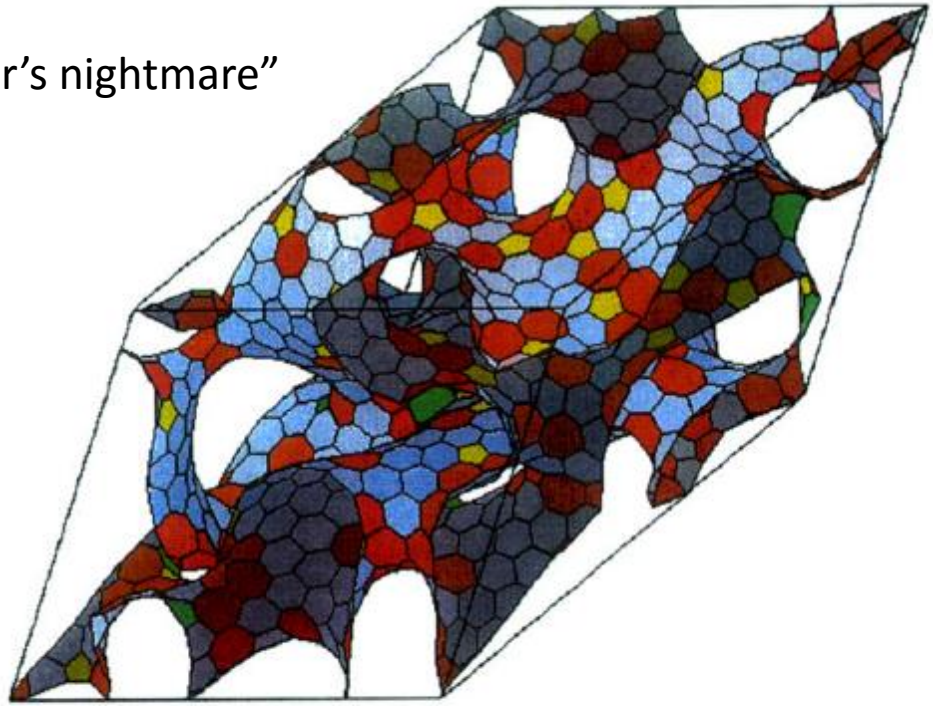

FIG. 2. View of a random schwarzite model on a surface of genus 12 per fcc supercell. The structure has 1248 carbons arranged into 38 five-membered rings (yellow), 394 six-membered rings (blue), 155 seven-membered rings (orange), 12 eight-membered rings (green), and 1 nine-sided ring (pink). Slower annealing produces a structure with many fewer five-membered rings. The cubic unit cell (4 times the volume of the fcc cell shown) is 42.9 Å on a side.

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Schwartzite

IMAGE ANALYSIS OF A NEGATIVELY CURVED GRAPHITIC SHEET MODEL FOR AMORPHOUS CARBON

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Received 4 September 1995

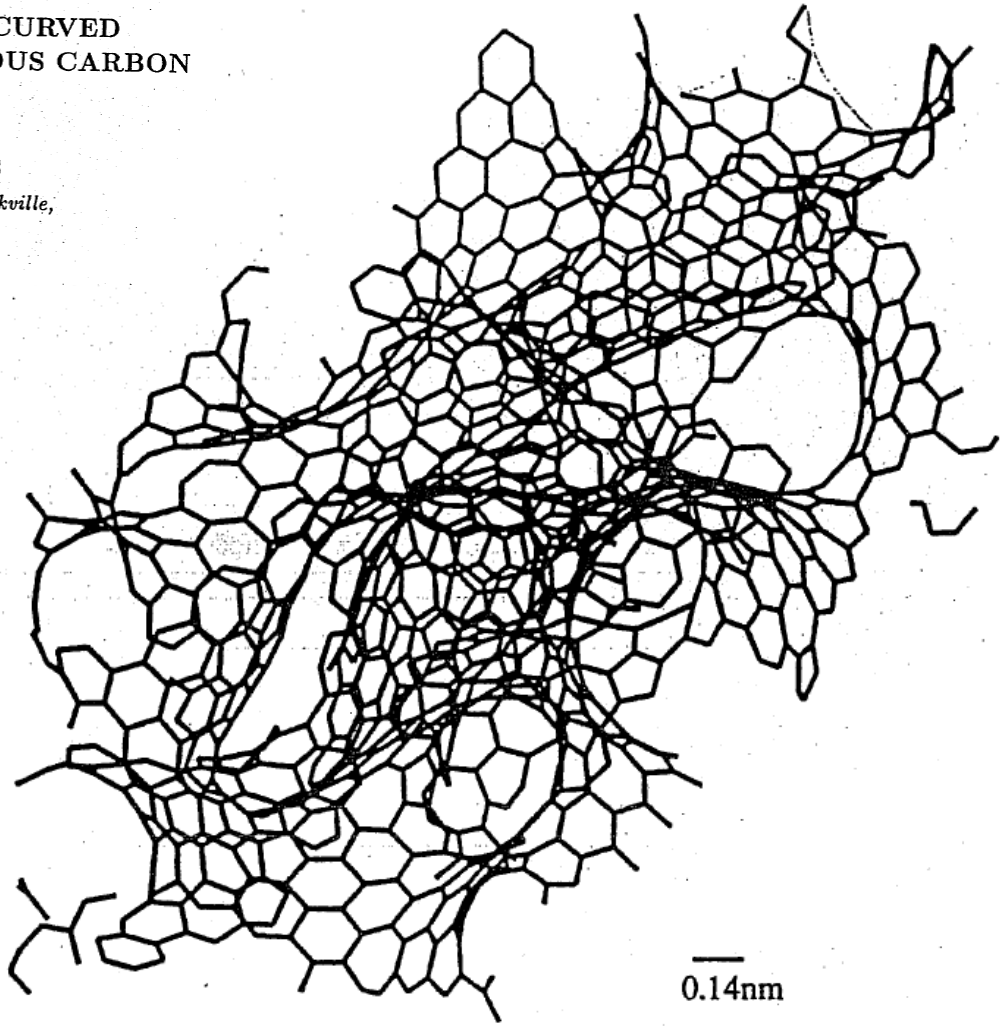

Fig. 2. Random schwartzite model of a surface of genus 12; the volume shown has the shape of a primitive f.c.c cell.

Magnetism in All-Carbon Nanostructures with Negative Gaussian Curvature

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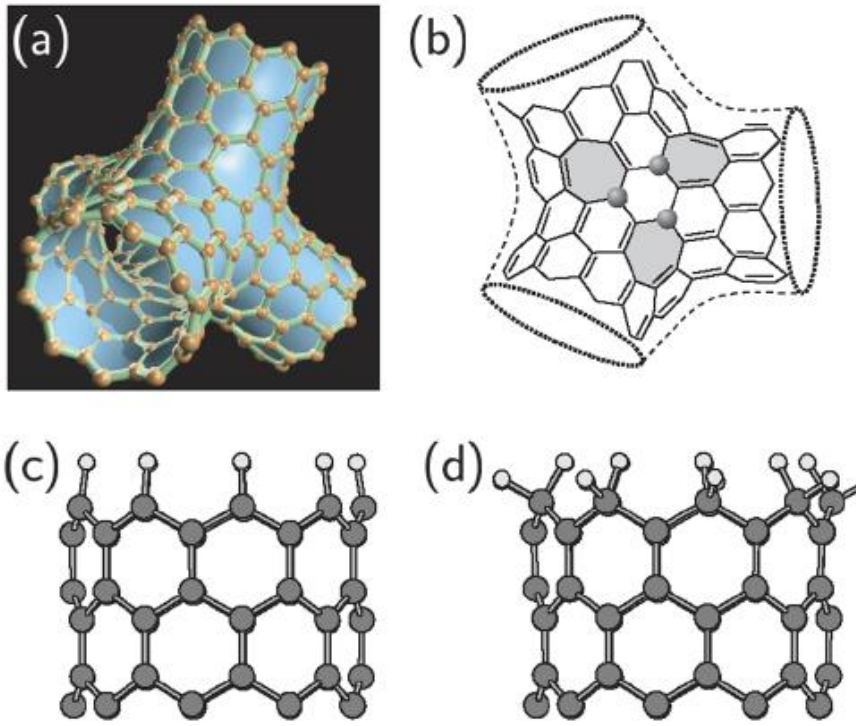

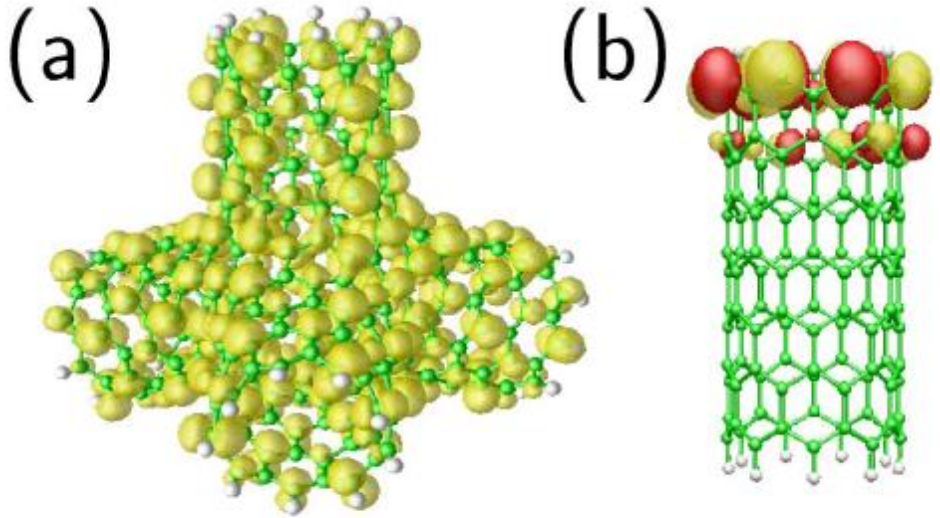

FIG. 3 (color online). (a) Charge density associated with the four unpaired spins, which are unrelated to the edge states in an sp^2 terminated tetrapod. (b) The wave function of a spin-polarized edge state in an sp^2 terminated (9, 0) nanotube. We use color shading to represent the phase of the wave function.