



Carbonio, suoi stati allotropici e Grafite

M. Riccò



PERIODIC TABLE

Atomic Properties of the Elements

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
IA	IIA	IIIB	IVB	VB	VIB	VII	VIII	VIII	VIII	IB	IIB	IIIA	IIIA	IVA	VA	VIA	VIIA	VIIIA	
1	H Hydrogen 1.00794 1s																	He Helium 4.002602 1s ²	
2	Li Lithium 6.941 1s ² 2s ¹	Be Beryllium 9.012182 1s ² 2s ²																B Boron 10.811 1s ² 2s ² 2p ¹	Ne Neon 20.1797 1s ² 2s ² 2p ⁶
3	Na Sodium 22.989770 [Ne]3s ¹	Mg Magnesium 24.3050 [Ne]3s ²																Ar Argon 39.948 [Ne]3s ² 3p ⁶	
4	K Potassium 39.0983 [Ar]4s ¹	Ca Calcium 40.078 [Ar]4s ²	Sc Scandium 44.955910 [Ar]3d ¹ 4s ²	Ti Titanium 47.88 [Ar]3d ² 4s ²	V Vanadium 50.9415 [Ar]3d ³ 4s ²	Cr Chromium 51.9961 [Ar]3d ⁵ 4s ¹	Mn Manganese 54.938049 [Ar]3d ⁵ 4s ²	Fe Iron 55.845 [Ar]3d ⁶ 4s ²	Co Cobalt 58.933200 [Ar]3d ⁷ 4s ²	Ni Nickel 58.6934 [Ar]3d ⁸ 4s ²	Cu Copper 63.546 [Ar]3d ¹⁰ 4s ¹							Kr Krypton 83.798 [Ar]3d ¹⁰ 4s ² 4p ⁶	
5	Rb Rubidium 85.4678 [Kr]5s ¹	Sr Strontium 87.62 [Kr]5s ²	Y Yttrium 88.90585 [Kr]4d ¹ 5s ²	Zr Zirconium 91.224 [Kr]4d ² 5s ²	Nb Niobium 92.90638 [Kr]4d ⁴ 5s ¹	Mo Molybdenum 95.94 [Kr]4d ⁵ 5s ¹	Tc Technetium (98) [Kr]4d ⁵ 5s ²	Ru Ruthenium 101.07 [Kr]4d ⁷ 5s ¹	Rh Rhodium 102.90550 [Kr]4d ⁸ 5s ¹	Pd Palladium 106.42 [Kr]4d ¹⁰	Ag Silver 107.8682 [Kr]4d ¹⁰ 5s ¹							Xe Xenon 131.293 [Kr]4d ¹⁰ 5s ² 5p ⁶	
6	Cs Cesium 132.90545 [Xe]6s ¹	Ba Barium 137.327 [Xe]6s ²		Hf Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s ²	Ta Tantalum 180.9479 [Xe]4f ¹⁴ 5d ³ 6s ²	W Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s ²	Re Rhenium 186.207 [Xe]4f ¹⁴ 5d ⁵ 6s ¹	Os Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s ²	Ir Iridium 192.221 [Xe]4f ¹⁴ 5d ⁷ 6s ²	Pt Platinum 195.078 [Xe]4f ¹⁴ 5d ⁹ 6s ¹	Au Gold 196.96655 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹	Hg Mercury 200.59 [Xe]4f ¹⁴ 5d ¹⁰ 6s ²	Tl Thallium 204.3833 [Hg]6p ¹	Pb Lead 207.2 [Hg]6p ²	Bi Bismuth 208.98038 [Hg]6p ³	Po Polonium (209) [Hg]6p ⁴	At Astatine (210) [Hg]6p ⁵	Rn Radon (222) [Hg]6p ⁶	
7	Fr Francium (223) [Rn]7s ¹	Ra Radium (226) [Rn]7s ²		Rf Rutherfordium (261) [Rn]5f ¹⁴ 6d ² 7s ²	Db Dubnium (262) [Rn]5f ¹⁴ 6d ³ 7s ²	Sg Seaborgium (266) [Rn]5f ¹⁴ 6d ⁴ 7s ²	Bh Bohrium (264) [Rn]5f ¹⁴ 6d ⁵ 7s ²	Hs Hassium (277) [Rn]5f ¹⁴ 6d ⁶ 7s ²	Mt Meitnerium (268) [Rn]5f ¹⁴ 6d ⁷ 7s ²	Uun Ununium (281) [Rn]5f ¹⁴ 6d ⁸ 7s ²	Uuu Ununium (272) [Rn]5f ¹⁴ 6d ⁹ 7s ²	Uub Ununium (285) [Rn]5f ¹⁴ 6d ¹⁰ 7s ²		Uuq Ununium (289) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ¹		Uuh Ununium (292) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ²			
			Lanthanides	La Lanthanum 138.9055 [Xe]5d ¹ 6s ²	Ce Cerium 140.116 [Xe]4f ¹ 5d ¹ 6s ²	Pr Praseodymium 140.90785 [Xe]4f ² 6s ²	Nd Neodymium 144.24 [Xe]4f ³ 6s ²	Pm Promethium (145) [Xe]4f ⁴ 6s ²	Sm Samarium 150.36 [Xe]4f ⁶ 6s ²	Eu Europium 151.964 [Xe]4f ⁷ 6s ²	Gd Gadolinium 157.25 [Xe]4f ⁷ 5d ¹ 6s ²	Tb Terbium 158.92534 [Xe]4f ⁹ 6s ²	Dy Dysprosium 162.500 [Xe]4f ¹⁰ 6s ²	Ho Holmium 164.93032 [Xe]4f ¹¹ 6s ²	Er Erbium 167.259 [Xe]4f ¹² 6s ²	Tm Thulium 168.93421 [Xe]4f ¹³ 6s ²	Yb Ytterbium 173.04 [Xe]4f ¹⁴ 6s ²	Lu Lutetium 174.967 [Xe]4f ¹⁴ 5d ¹ 6s ²	
			Actinides	Ac Actinium (227) [Rn]6d ¹ 7s ²	Th Thorium 232.0381 [Rn]6s ² 7s ²	Pa Protactinium 231.03688 [Rn]5f ² 6d ¹ 7s ²	U Uranium 238.02891 [Rn]5f ³ 6d ¹ 7s ²	Np Neptunium (237) [Rn]5f ⁴ 6d ¹ 7s ²	Pu Plutonium (244) [Rn]5f ⁶ 7s ²	Am Americium (243) [Rn]5f ⁷ 7s ²	Cm Curium (247) [Rn]5f ⁸ 6d ¹ 7s ²	Bk Berkelium (247) [Rn]5f ⁹ 7s ²	Cf Californium (251) [Rn]5f ¹⁰ 7s ²	Es Einsteinium (252) [Rn]5f ¹¹ 7s ²	Fm Fermium (257) [Rn]5f ¹² 7s ²	Md Mendelevium (258) [Rn]5f ¹³ 7s ²	No Nobelium (259) [Rn]5f ¹⁴ 7s ²	Lr Lawrencium (262) [Rn]5f ¹⁴ 7s ² 7p ¹	

Frequently used fundamental physical constants
 For the most accurate values of these and other constants, visit physics.nist.gov/constants
 1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs

speed of light in vacuum	<i>c</i>	299 792 458 m s ⁻¹ (exact)
Planck constant	<i>h</i>	6.6261 × 10 ⁻³⁴ J s
elementary charge	<i>e</i>	1.6022 × 10 ⁻¹⁹ C
electron mass	<i>m_e</i>	9.1094 × 10 ⁻³¹ kg
	<i>m_ec²</i>	0.5110 MeV
proton mass	<i>m_p</i>	1.6726 × 10 ⁻²⁷ kg
fine-structure constant	<i>α</i>	1/137.036
Rydberg constant	<i>R_∞</i>	10 973 732 m ⁻¹
	<i>R_{H,C}</i>	3.289 842 × 10 ¹⁵ Hz
	<i>R_∞hc</i>	13.6057 eV
Boltzmann constant	<i>k</i>	1.3807 × 10 ⁻²³ J K ⁻¹

- Solids
- Liquids
- Gases
- Artificially Prepared

Atomic Number: 58
 Ground-state Level: 1G₄
 Symbol: **Ce**
 Name: Cerium
 Atomic Weight: 140.116
 Ground-state Configuration: [Xe]4f¹5d¹6s²
 Ionization Energy (eV): 5.5387

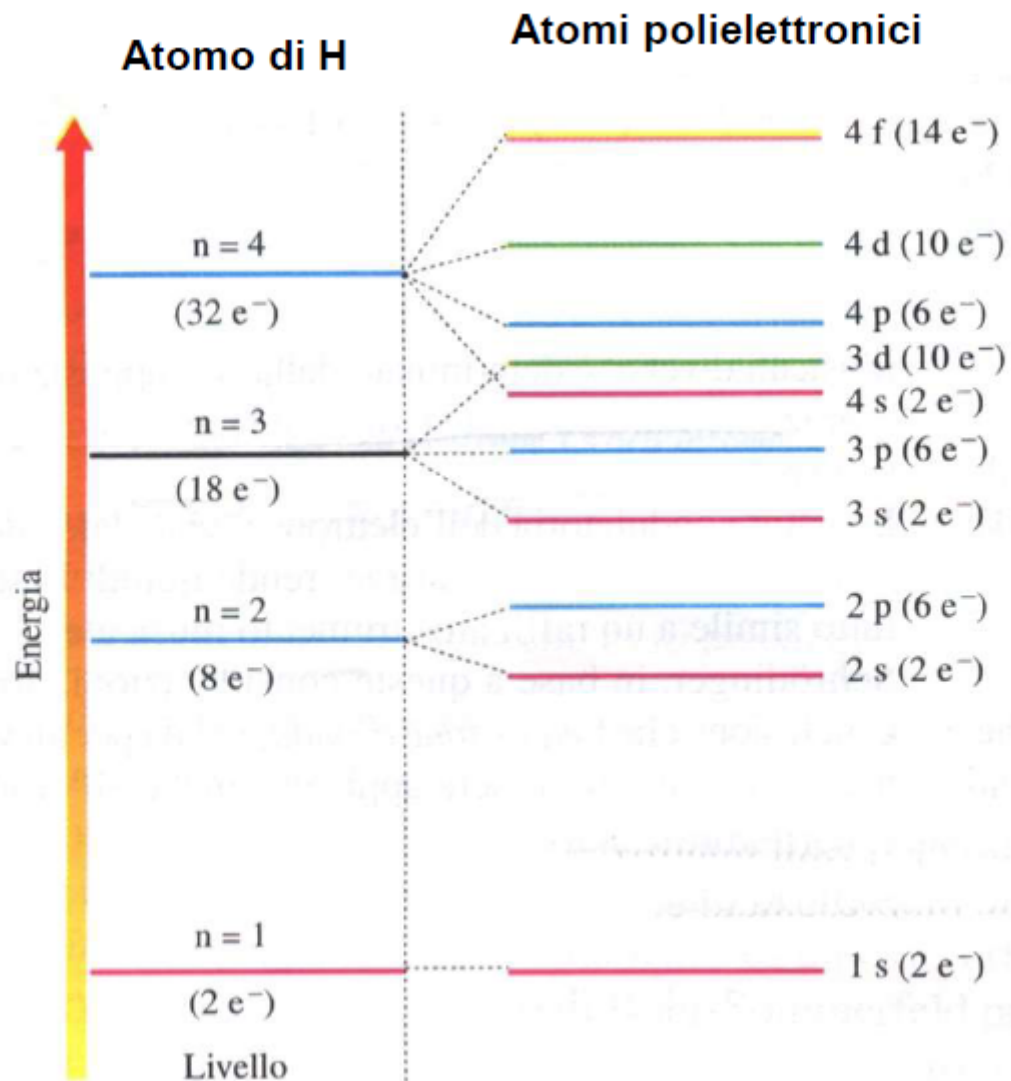
[†]Based upon ¹²C. () indicates the mass number of the most stable isotope.

For a description of the data, visit physics.nist.gov/data

NIST SP 966 (September 2003)



- Isotopo ^{12}C \rightarrow abbondanza naturale (98.93%, $S=0$)
- Isotopo ^{13}C \rightarrow importante per l'NMR (1.07%, $S=1/2$)
- Isotopo ^{14}C \rightarrow importante per la datazione archeologica (vita media 5730 anni)



L'energia di ogni elettrone negli atomi polielettronici dipende non solo da n , ma anche da l ; conseguenza fondamentale delle interazioni interelettroniche

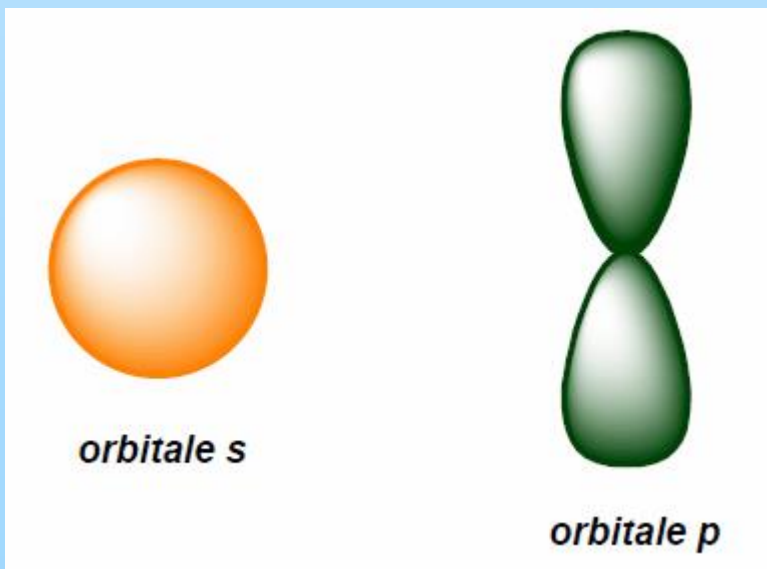
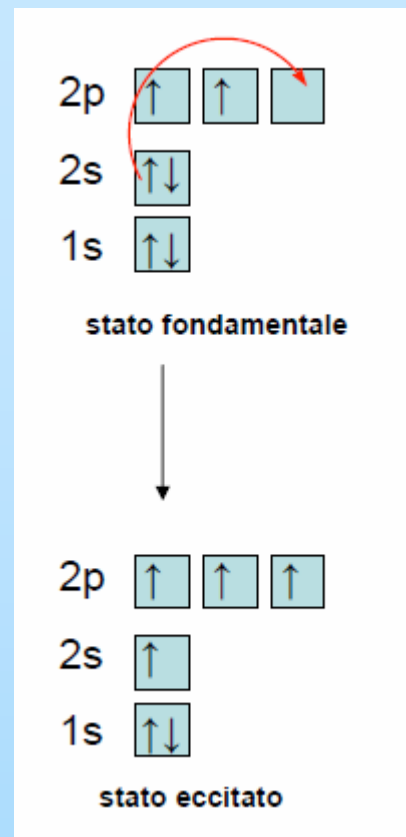
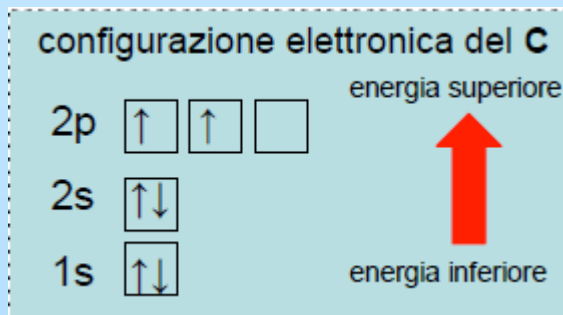
Scissione dei livelli energetici in più sottolivelli distinti di energia crescente, per un dato valore di n , con il crescere di l .

Tra il livello 3 ed il livello 4 vi è una sovrapposizione dei livelli energetici



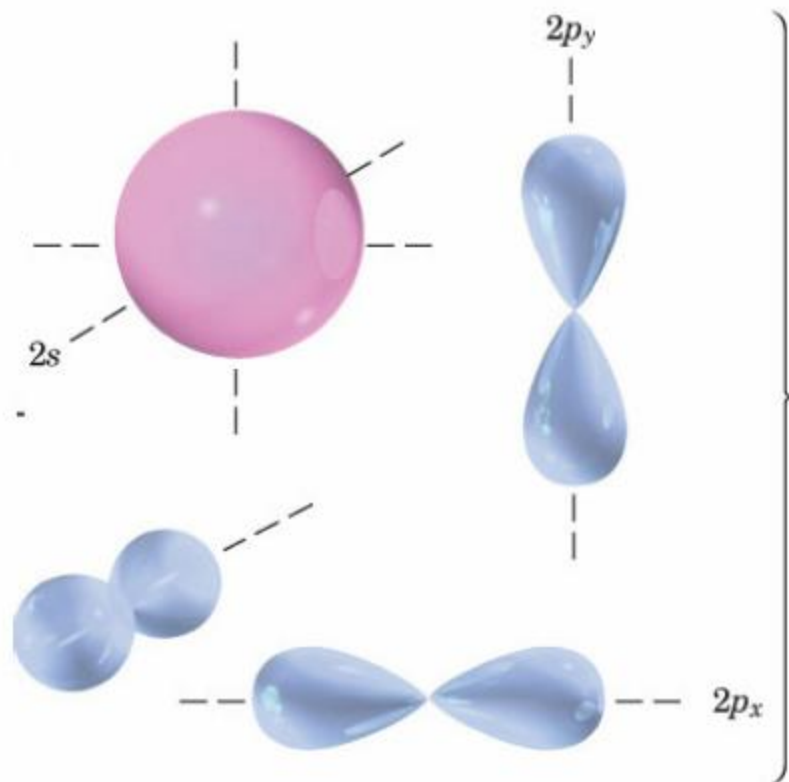
Ibridizzazione sp^3

Configurazione: $[\text{He}] 2s^2 2p^2$





Ibridizzazione sp^3



Ibridizzazione →



Quattro orbitali sp^3 tetraedrici



Orbitale sp^3

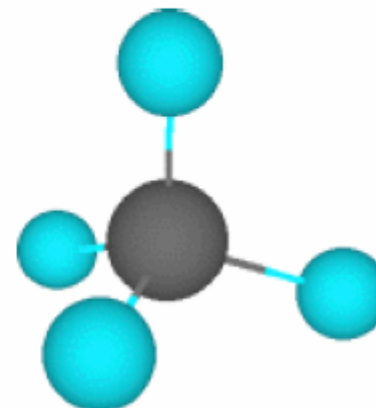


Ibridizzazione sp^3

Metano

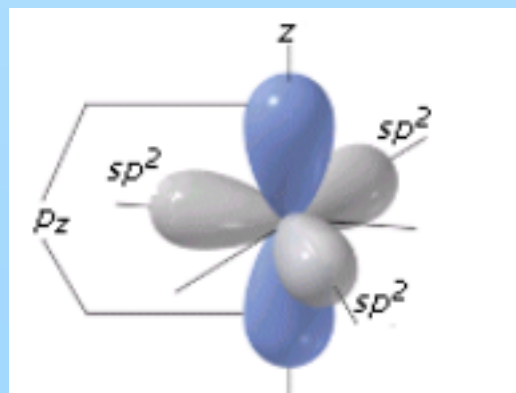
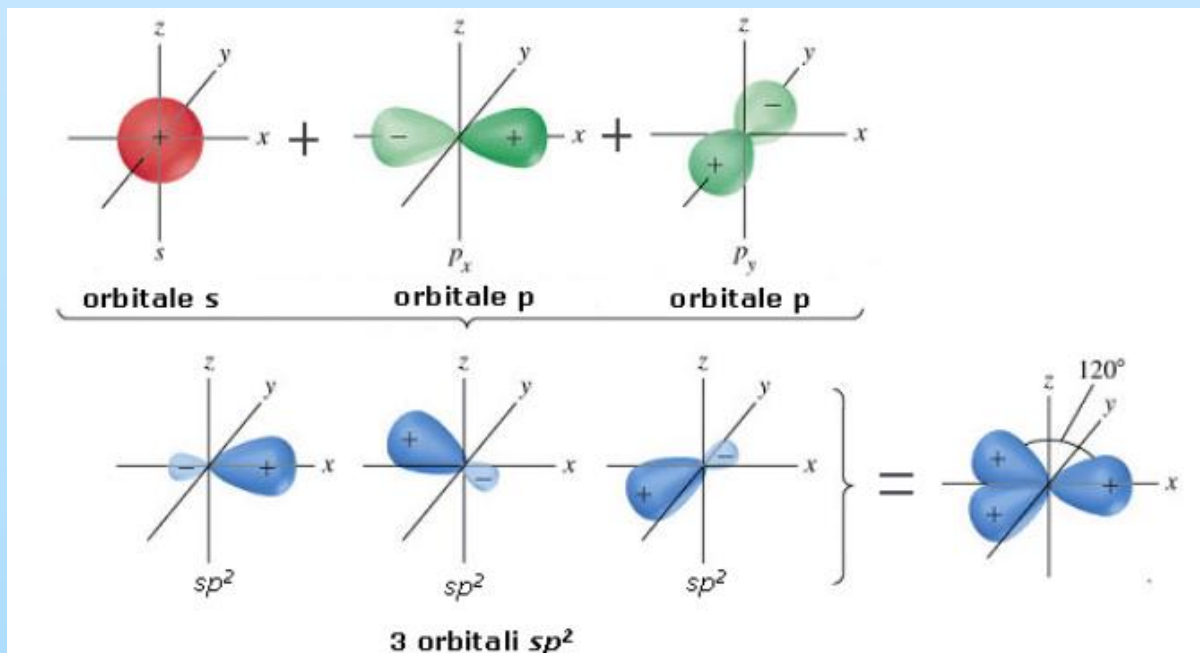


L'angolo di legame formato da ciascun H-C-H vale esattamente $109,5^\circ$ (angolo tetraedrico)



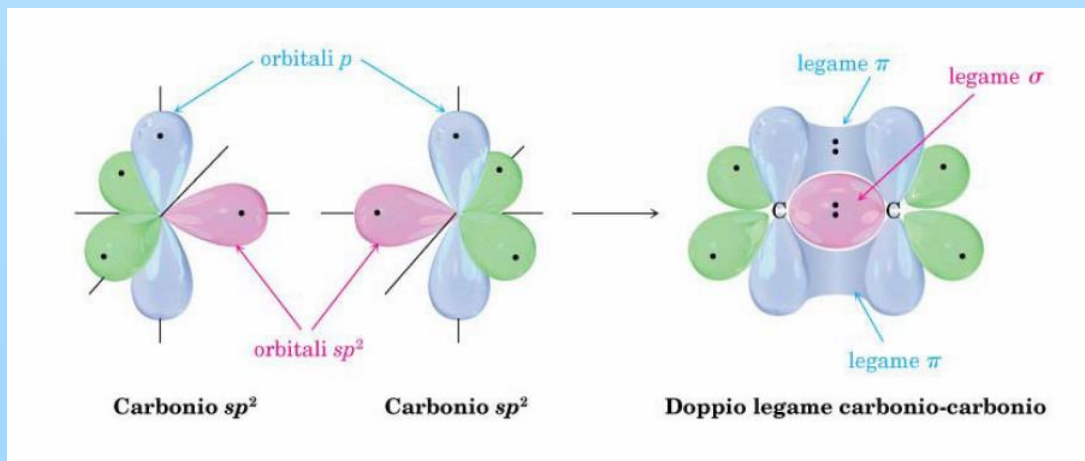
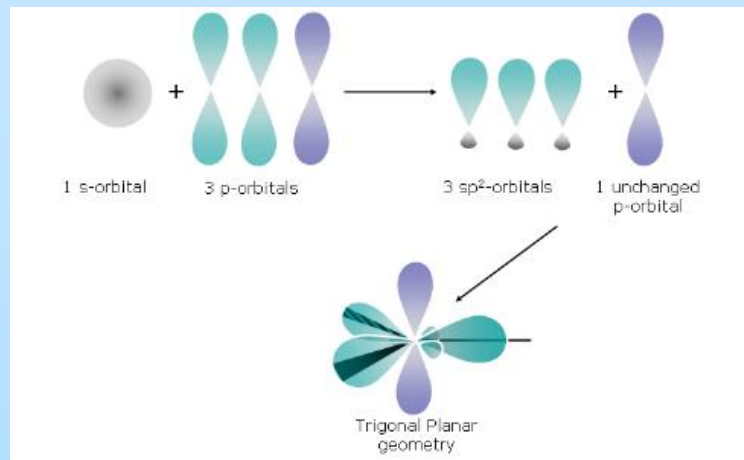
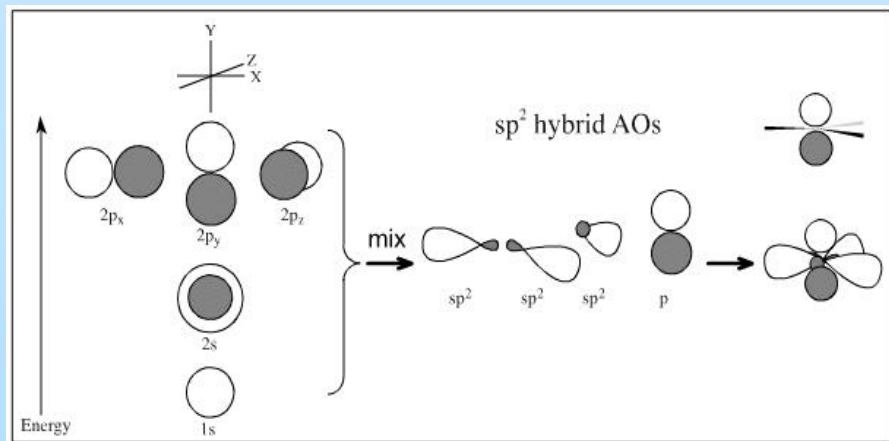


Ibridizzazione sp^2





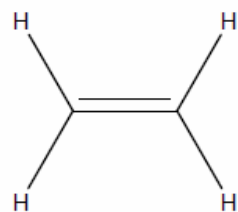
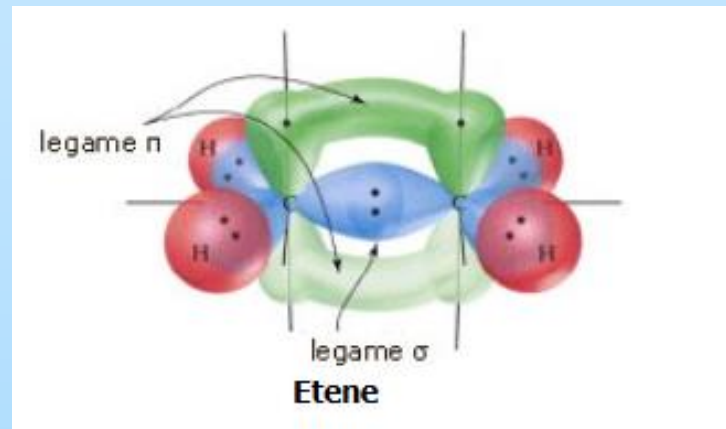
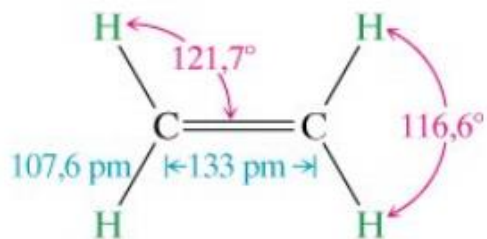
Ibridizzazione sp^2



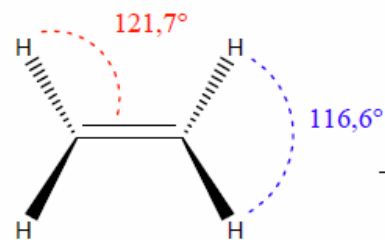


Ibridizzazione sp^2

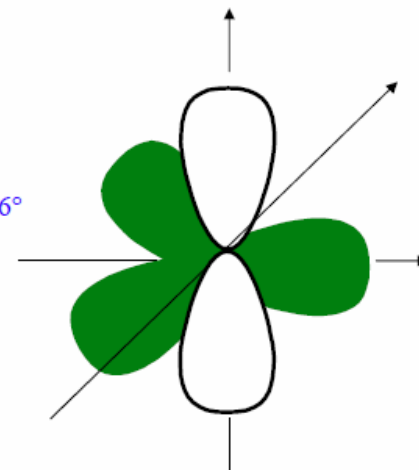
Etilene



vista dall'alto

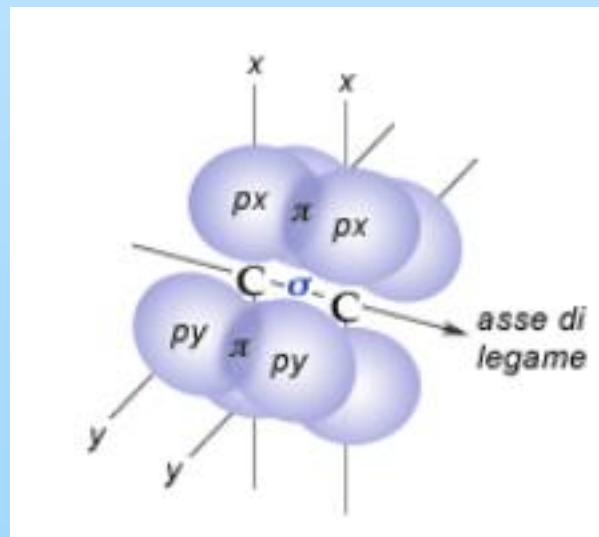
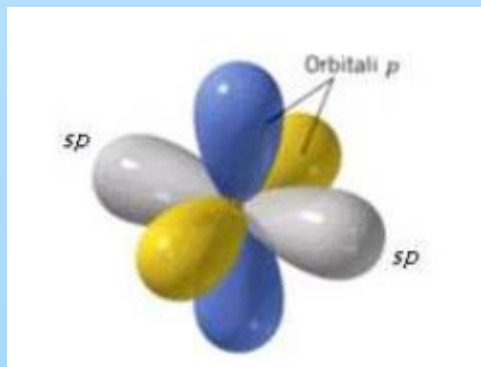
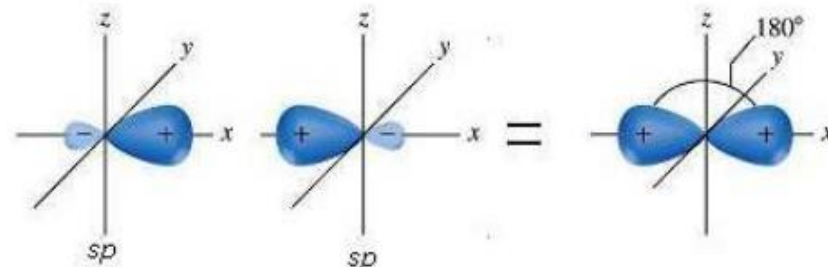
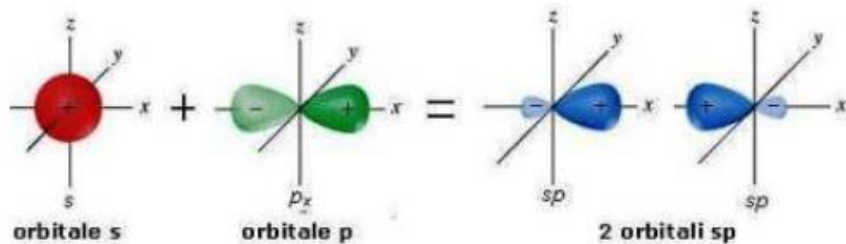


vista laterale



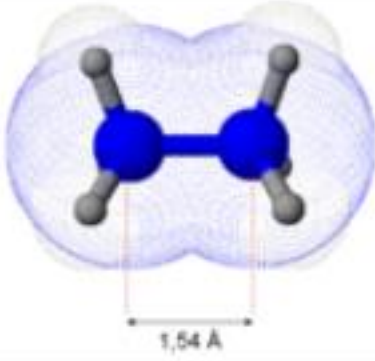
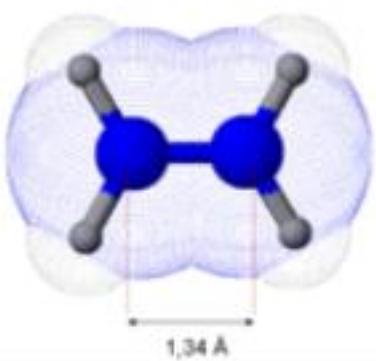
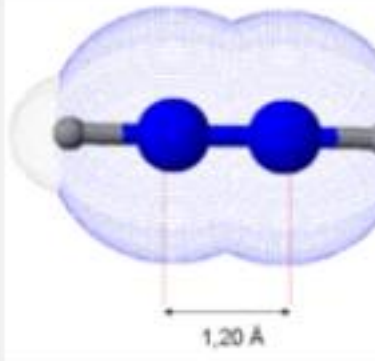


Ibridizzazione sp



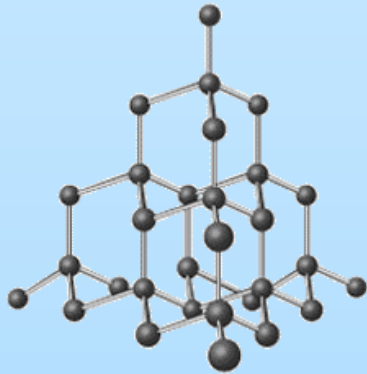


Ibridizzazione sp^n

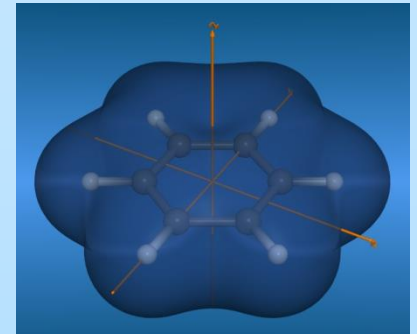
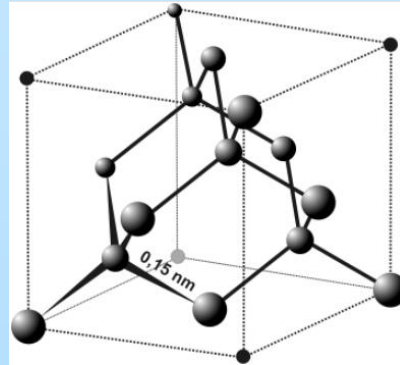
		
1,54 Å	1,34 Å	1,20 Å
Legame singolo Carbonio-Carbonio	Legame doppio Carbonio-Carbonio	Legame triplo Carbonio-Carbonio
Ibridizzazione sp^3	Ibridizzazione sp^2	Ibridizzazione sp



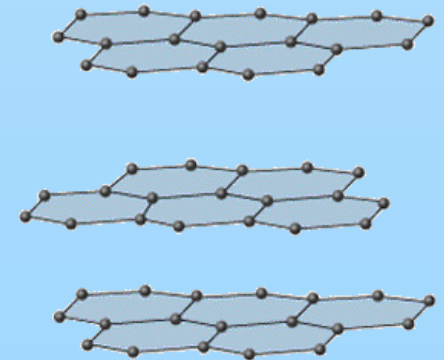
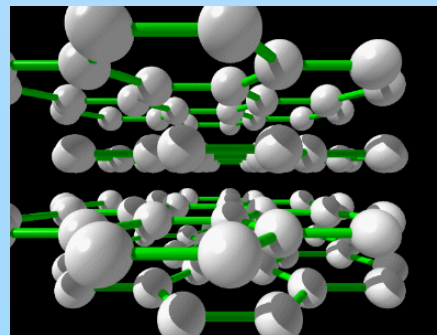
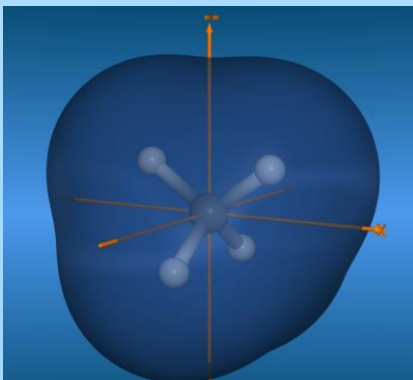
Stati allotropici del carbonio



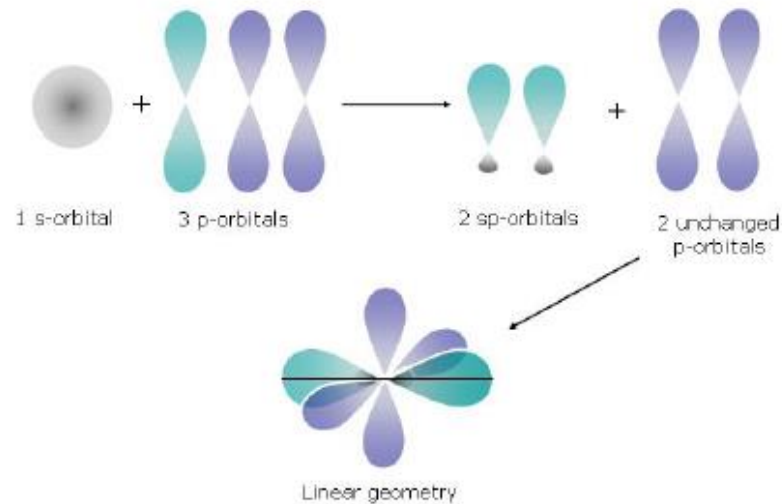
Diamante



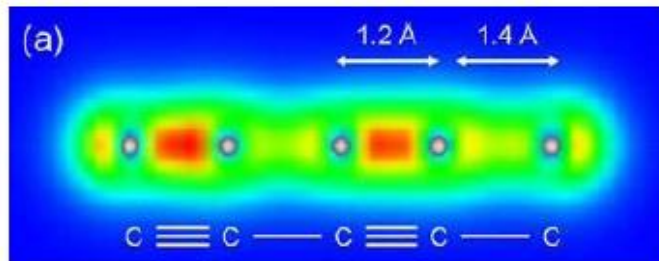
Grafite



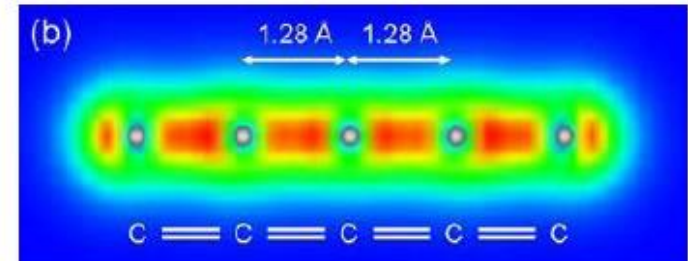
Ibridizzazione sp



Due possibilità: (a) **poliini**, alternanza legami tripli e doppi



(b) **cumuleni**, catena di legami doppi



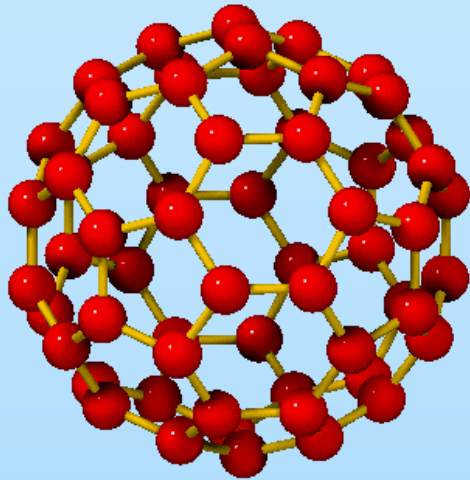
Problema: i sistemi di carbonio sp sono instabili

- reattività delle catene insature (es. O_2);
- tendenza a formare *cross-links* fra le catene, favorendo l'evoluzione verso la più stabile fase sp^2 .

Catene sp isolate sono state osservate solo in fase gassosa o in matrici di gas inerti a basse temperature.

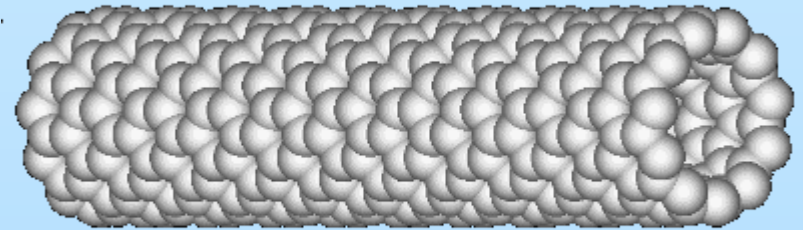


Stati allotropici del carbonio



Fullerene (C₆₀)

Curl, Kroto e Smalley,
premio Nobel per la Chimica 1996



Nanotubi

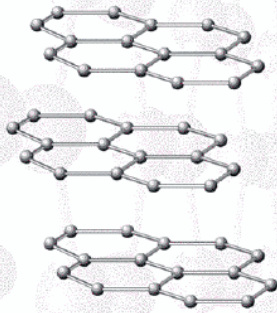
(Iijima 1991)

Nanostrutture.....



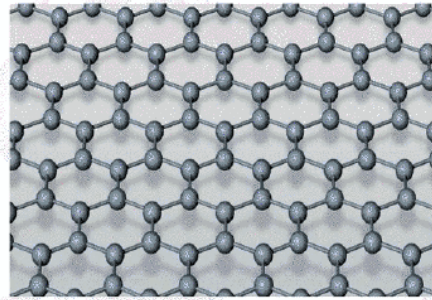
GRAPHENE ALLOTROPES

3D



Graphite

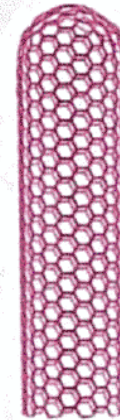
2D



graphene

**PRESUMED
NOT TO EXIST
IN THE FREE STATE**

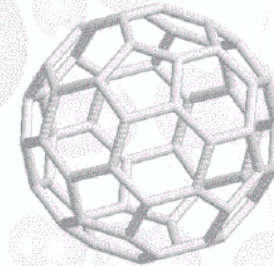
1D



**Carbon
Nanotube**

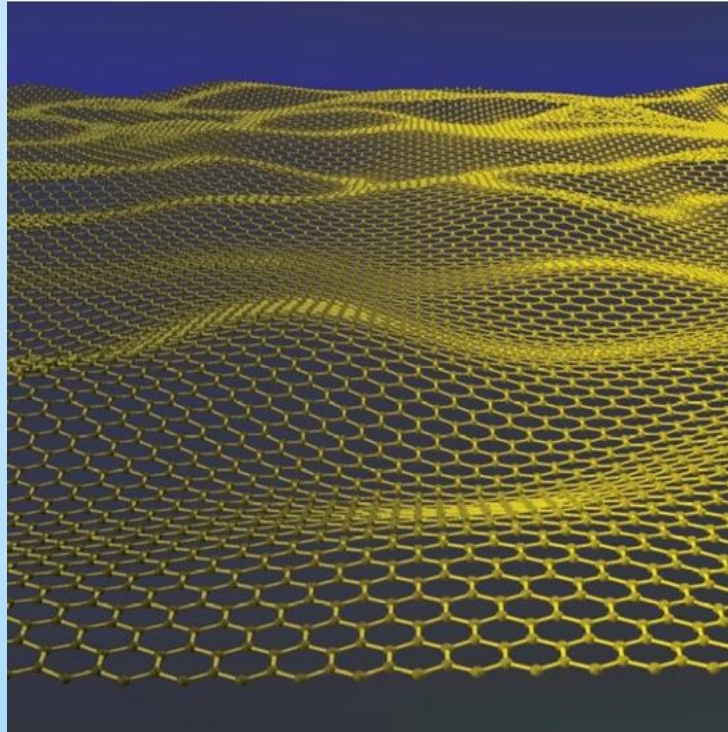
multi-wall:
1952 to *Iijima* 1991
single-wall: 1993

0D



Buckyballs

Kroto et al 1985



Grafene

K. Novoselov, A. Geim

Premio Nobel per la Fisica 2010



Diamante ↔ Grafite

Table 2.1
Properties of graphite and diamond

Property	Graphite ^a		Diamond
Lattice structure	Hexagonal		Cubic
Space group	$P6_3/mmc (D_{6h}^4)$		$Fd\bar{3}m (O_h^7)$
Lattice constant ^b (Å)	2.462	6.708	3.567
Atomic density (C atoms/cm ³)	1.14×10^{23}		1.77×10^{23}
Specific gravity (g/cm ³)	2.26		3.515
Specific heat (cal/g·K)	0.17		0.12
Thermal conductivity ^b (W/cm·K) ^c	30	0.06	~25
Binding energy (eV/C atom)	7.4		7.2
Debye temperature (K)	2500	950	1860
Bulk modulus (GPa)	286		42.2
Elastic moduli (GPa)	1060 ^d	36.5 ^d	107.6 ^e
Compressibility (cm ² /dyn)	2.98×10^{-12}		2.26×10^{-13}
Mohs hardness ^f	9		10
Band gap (eV)	-0.04 ^g		5.47
Carrier density (10 ¹⁸ /cm ³ at 4 K)	5		0
Electron mobility ^b (cm ² /Vsec)	20,000	100	1800
Hole mobility ^b (cm ² /Vsec)	15,000	90	1500
Resistivity (Ωcm)	50×10^{-6}	1	~10 ²⁰
Dielectric constant ^b (low ω)	3.0	5.0	5.58
Breakdown field (V/cm)	0		10 ⁷ (highest)
Magnetic susceptibility (10 ⁻⁶ cm ³ /g)	-0.5	-21	—
Refractive index (visible)	—		2.4
Melting point (K)	4450		4500
Thermal expansion ^b (/K)	-1×10^{-6}	$.29 \times 10^{-6}$	$\sim 1 \times 10^{-6}$
Velocity of sound (cm/sec)	$\sim 2.63 \times 10^5$	$\sim 1 \times 10^5$	$\sim 1.96 \times 10^5$
Highest Raman mode (cm ⁻¹)	1582		1332

^aFor anisotropic properties, the in-plane (*ab* plane or *a*-axis) value is given on the left and the *c*-axis value on the right.

^bMeasurements at room temperature (300 K).

^cHighest reported thermal conductivity values are listed.

^dIn-plane elastic constant is C_{11} and *c*-axis value is C_{33} . Other elastic constants for graphite are $C_{12} = 180$, $C_{13} = 15$, $C_{44} = 4.5$ GPa.

^eFor diamond, there are three elastic constants, $C_{11} = 1040$, $C_{12} = 170$, $C_{44} = 550$ GPa.

^fA scale based on values from 0 to 10, where 10 is the hardest material (diamond) and 1 is talc [2.8].

^gA negative band gap implies a band overlap, i.e., semimetallic behavior.



Diagramma di Fase

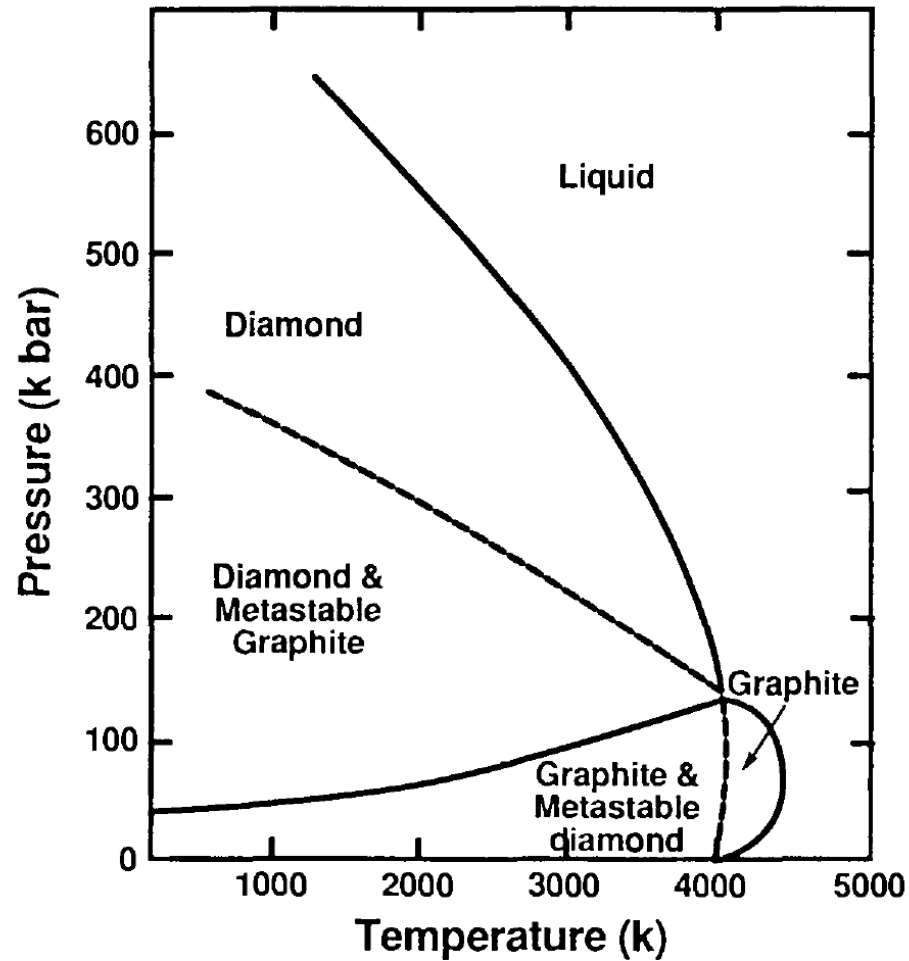
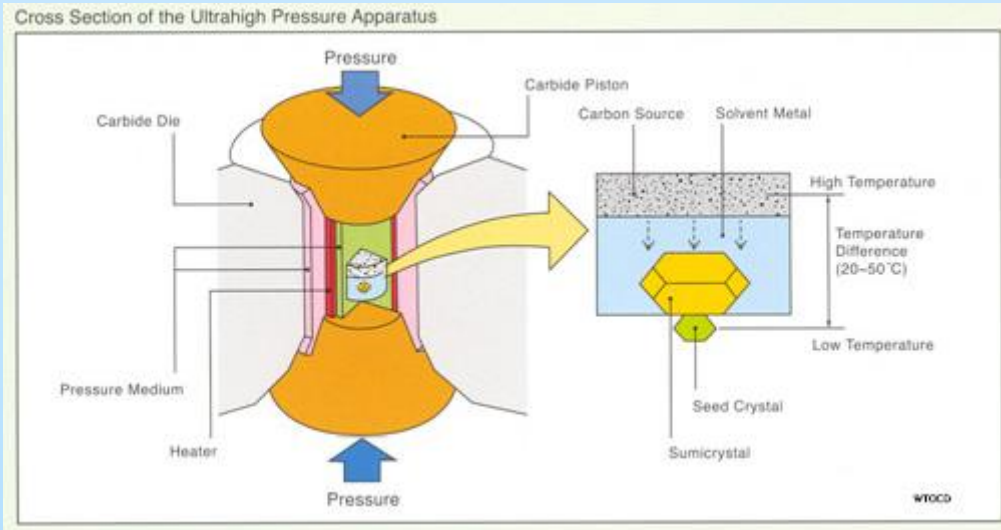


Figure 2.20. Carbon phase diagram.

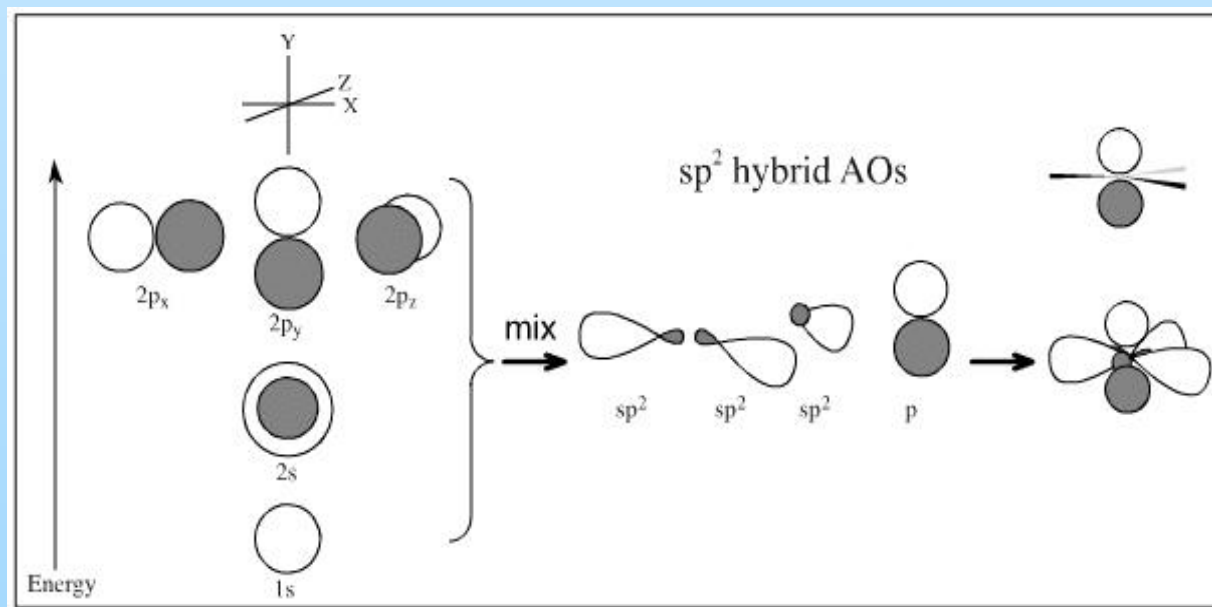
Sintesi dei diamanti





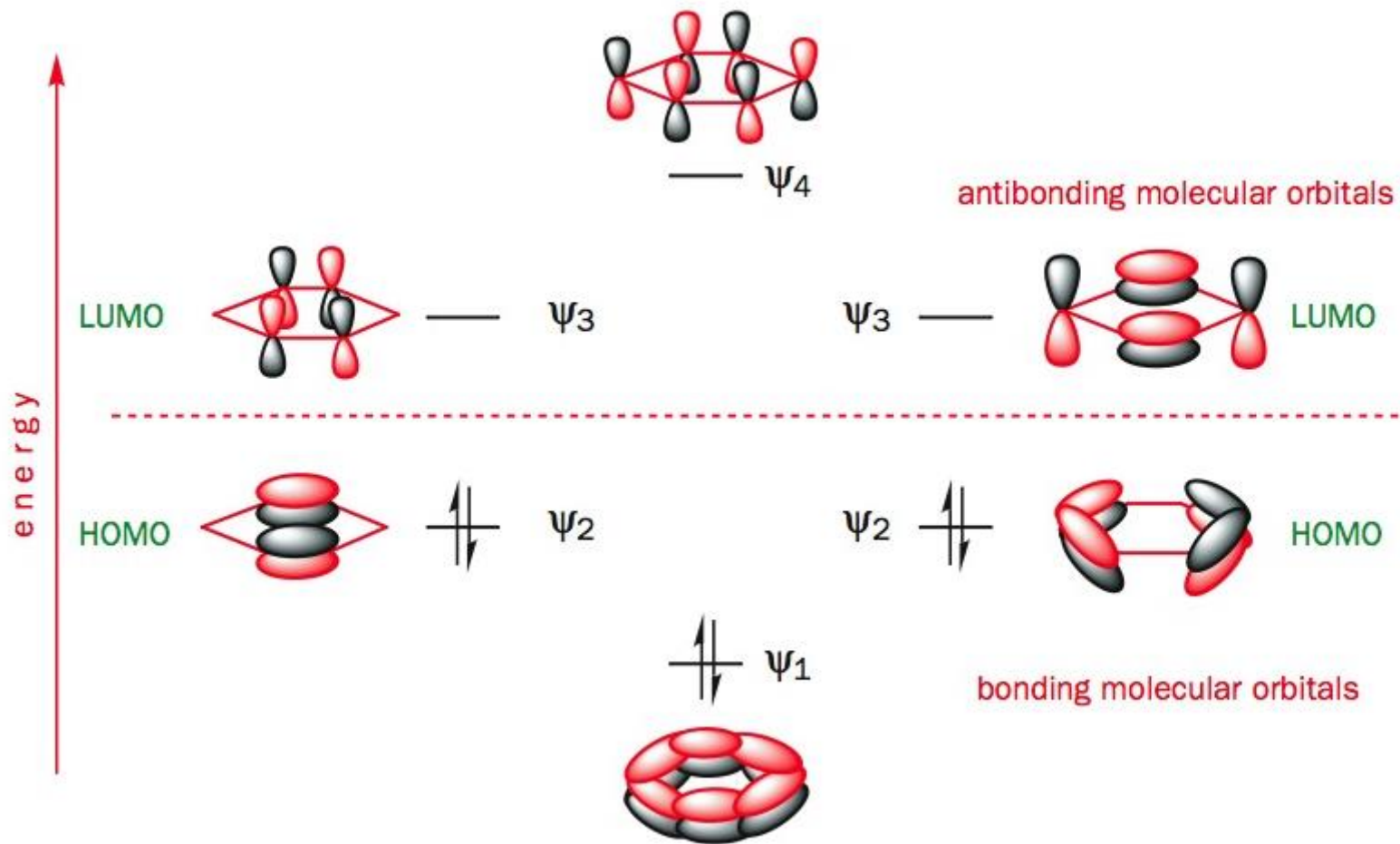
Ibridizzazione sp^2

Configurazione: $[\text{He}] 2s^2 2p^2$



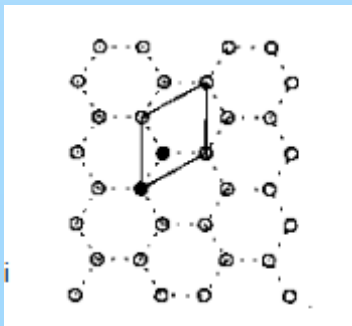
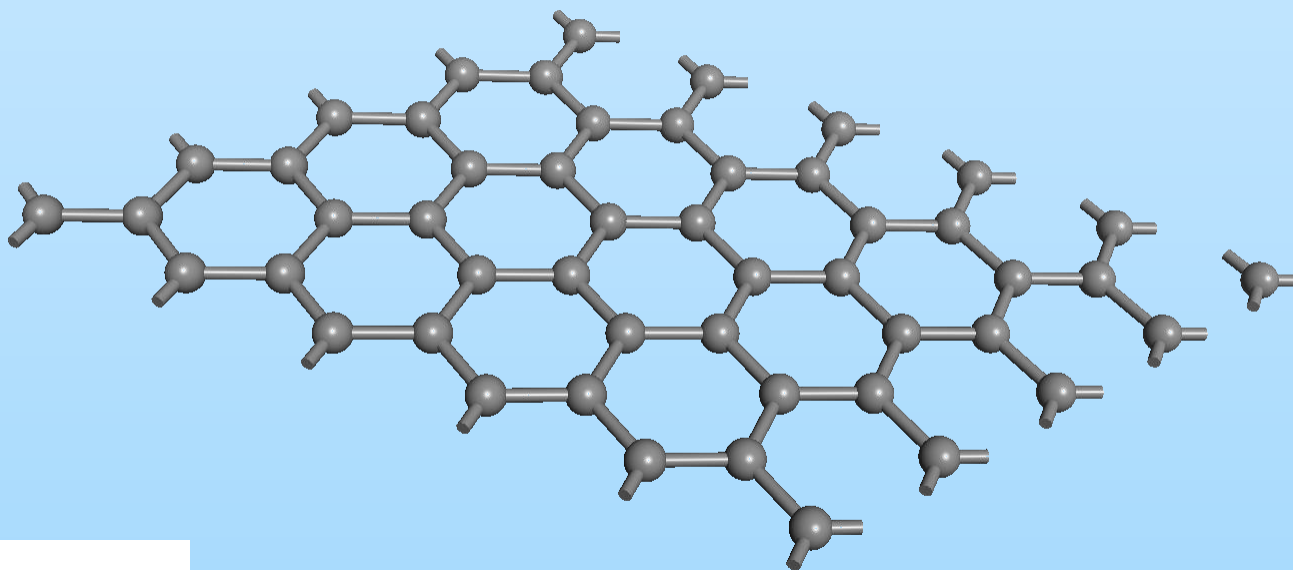


Ibridizzazione sp^2 : benzene





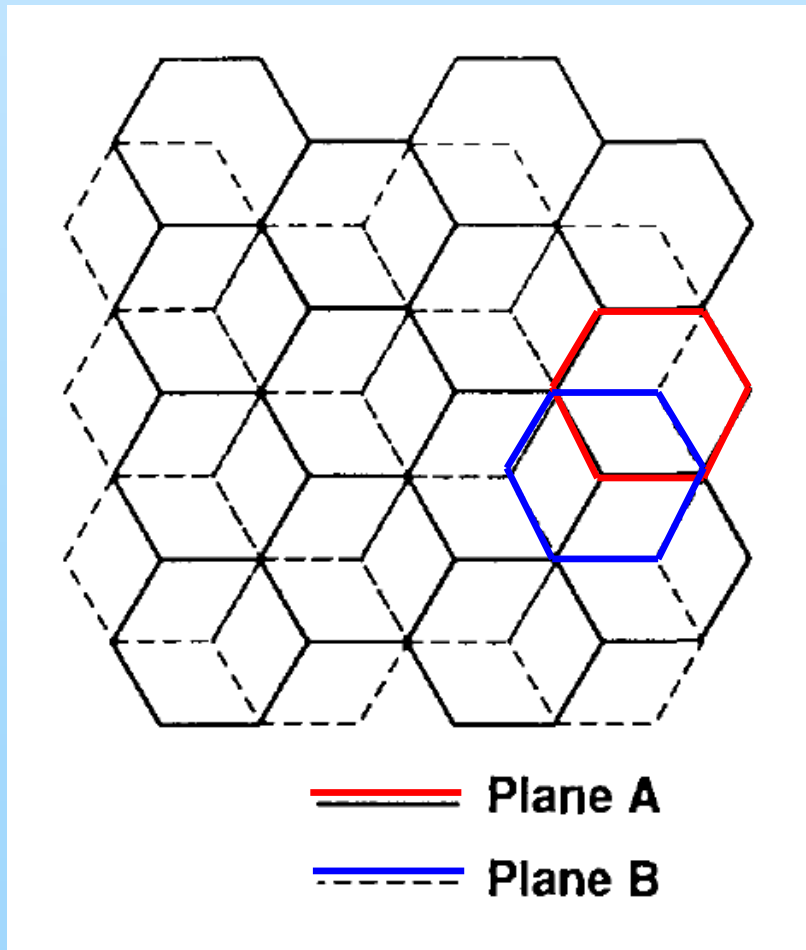
Ibridizzazione sp^2 : grafene



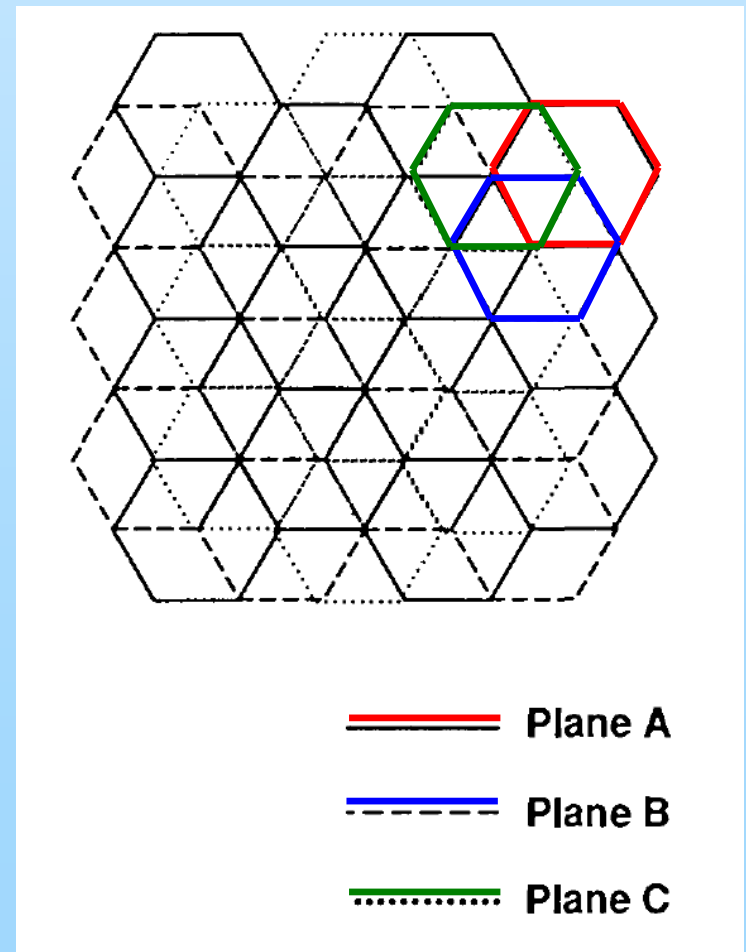


Grafite Struttura

grafite esagonale

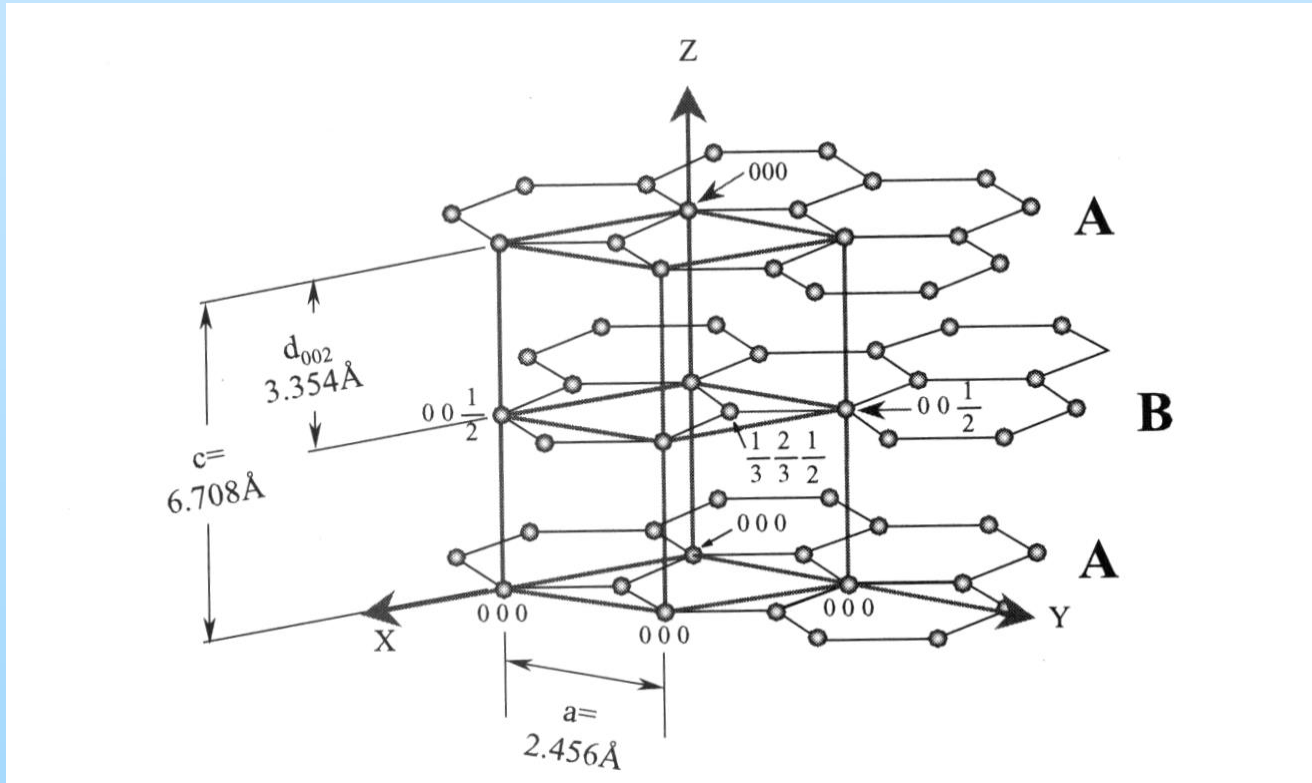


grafite romboedrica





Grafite esagonale: cella unitaria

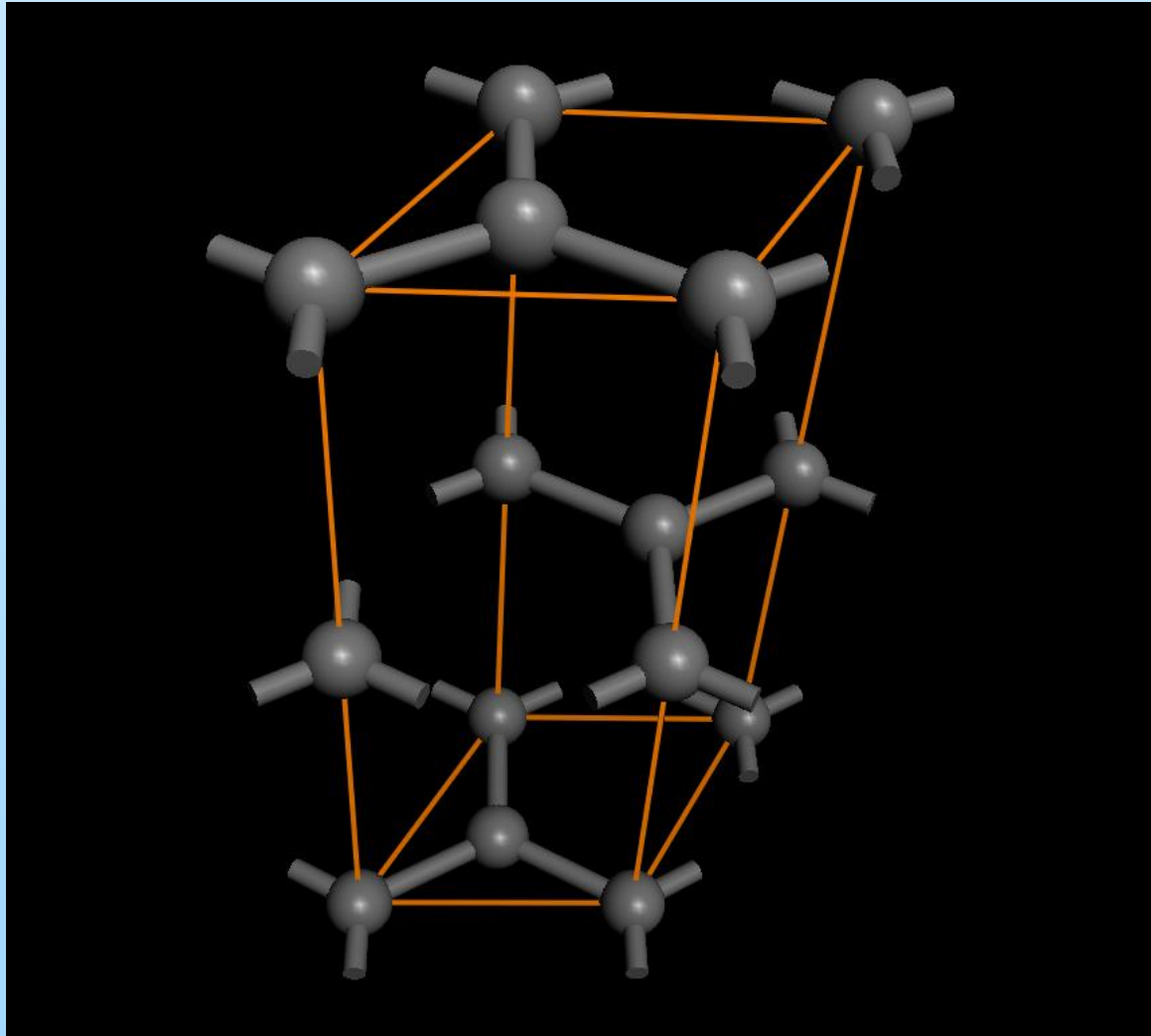


$$d(\text{C}=\text{C}) = 1.42 \text{ \AA}$$



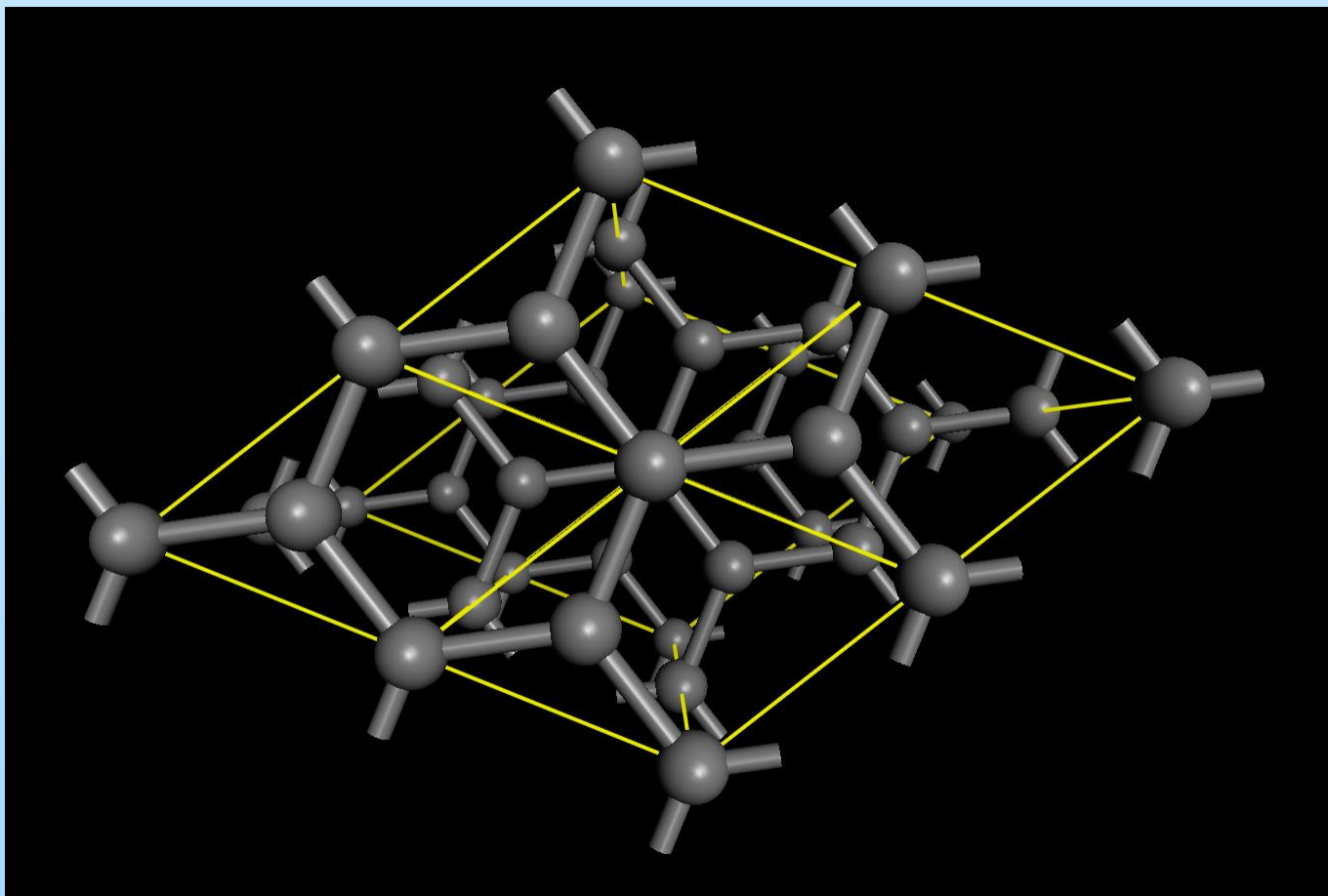
Grafite cella unitaria

Gruppo esagonale P 63 MMC #194





Grafite cella unitaria





Reticolo reciproco 2D

$$\mathbf{A} = 2\pi \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}; \quad \mathbf{B} = 2\pi \frac{\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}; \quad \mathbf{C} = 2\pi \frac{\mathbf{a} \times \mathbf{b}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}.$$

ESEMPIO

Reticolo reciproco in due dimensioni. Un reticolo a due dimensioni (fig. 21) ha i vettori base $\mathbf{a} = 2\hat{x}$; $\mathbf{b} = \hat{x} + 2\hat{y}$. Trovare i vettori base del reticolo reciproco.

Possiamo usare le nostre definizioni per il caso tridimensionale in questo problema in due dimensioni se supponiamo che \mathbf{c} sia parallelo all'asse z , per cui il piano dei vettori \mathbf{A} e \mathbf{B} del reticolo reciproco sarà nel piano di \mathbf{a} e \mathbf{b} . Prendiamo $\mathbf{c} = \hat{z}$. Ora

$$\mathbf{c} \times \mathbf{a} = \hat{z} \times (2\hat{x}) = 2\hat{y};$$

$$\mathbf{b} \times \mathbf{c} = \hat{x} \times \hat{z} + 2\hat{y} \times \hat{z} = -\hat{y} + 2\hat{x}; \quad \mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = 4.$$

Questi risultati sostituiti nelle (33) danno

$$\mathbf{A} = \pi\hat{x} - \frac{1}{2}\pi\hat{y}; \quad \mathbf{B} = \pi\hat{y},$$

come indicato in figura 21.

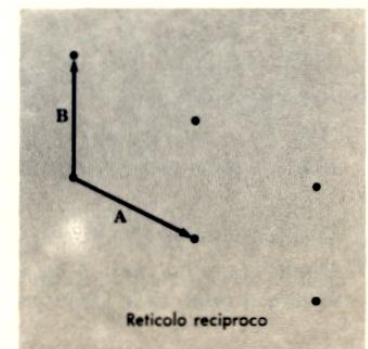
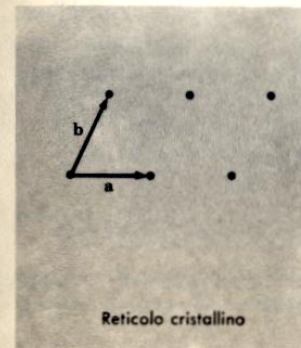
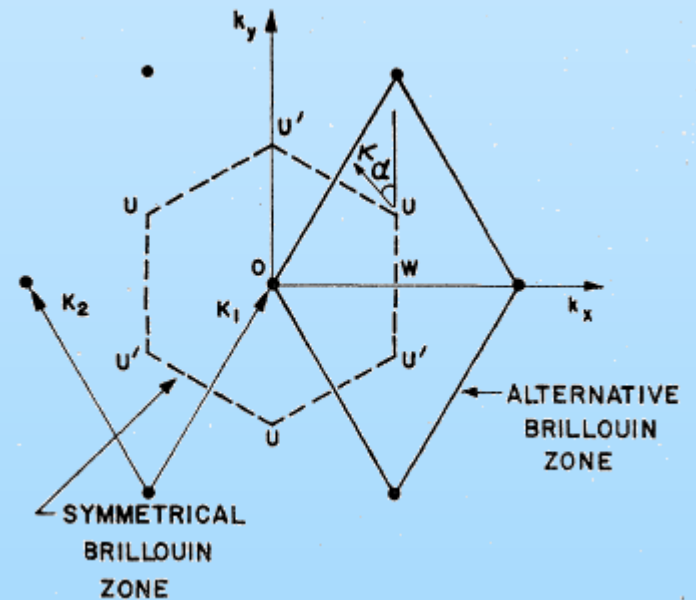
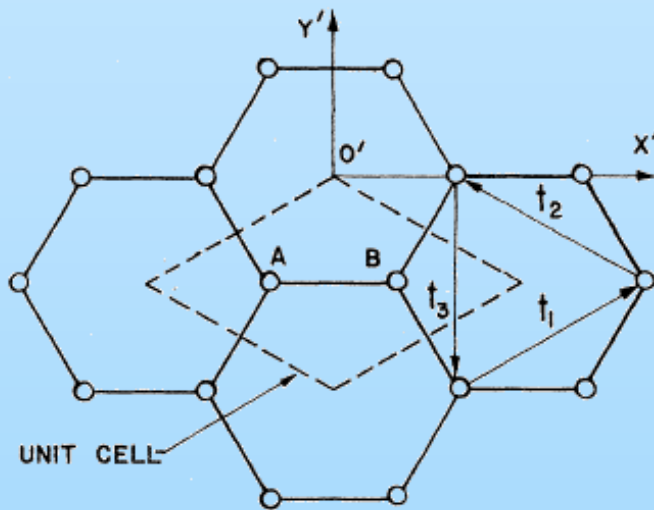


Figura 21 Reticolo reciproco in due dimensioni: \mathbf{A} e \mathbf{B} sono perpendicolari a gruppi di piani (linee) nel reticolo cristallino, cioè alle linee parallele rispettivamente a \mathbf{b} e \mathbf{a} . Qualsiasi vettore fra punti del reticolo reciproco è perpendicolare a qualche piano nel reticolo cristallino.



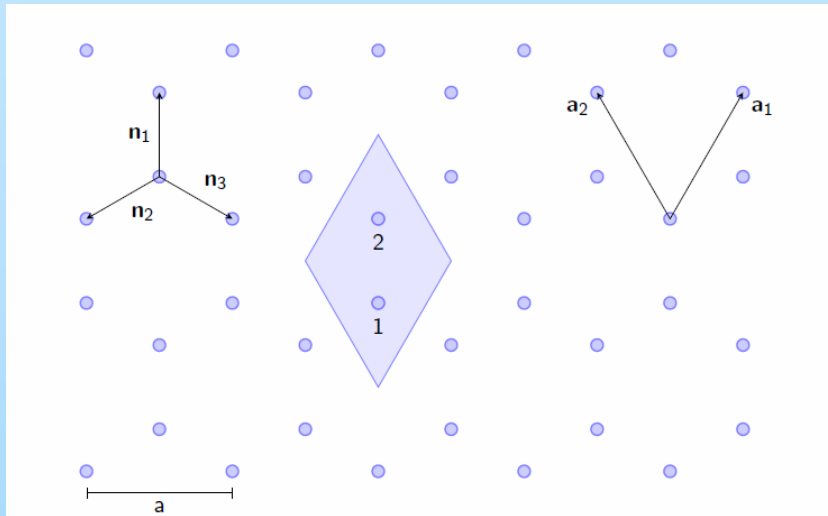
Grafene: cella elementare e I zona di Brillouin



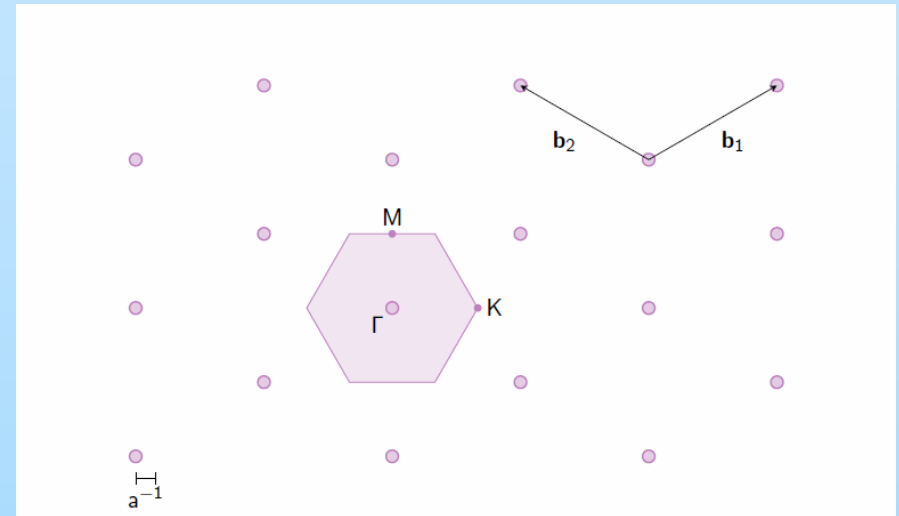
Reticolo reciproco (I zona di B.)



Grafene: cella elementare e I zona di Brillouin



Reticolo diretto: a_1 e a_2 vettori primitivi, n_1 , n_2 e n_3 vettori primi vicini



Reticolo reciproco: b_1 e b_2 vettori primitivi, in rosa I zona di B.



Tight Binding (LCAO)

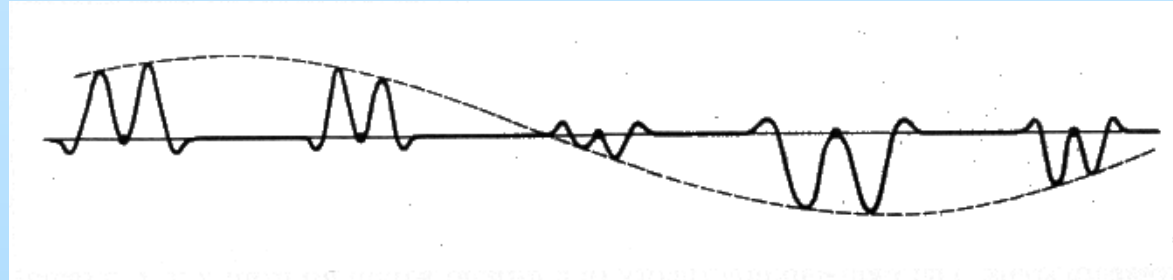
$$\psi(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \phi(\mathbf{r} - \mathbf{R}),$$

ϕ funzioni di Wannier

$$\phi(\mathbf{r}) = \sum_n b_n \psi_n(\mathbf{r}).$$

ψ_n orbitali atomici (indicati con $X(\mathbf{r})$ di seguito)

$$\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi(\mathbf{r}).$$



Condizione di Bloch

Se c 'è una base nella cella.....

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{j\alpha} c_{j\alpha} e^{i\mathbf{k} \cdot \mathbf{d}_j} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \phi_{j\alpha}(\mathbf{r} - \mathbf{R} - \mathbf{d}_j),$$

dove i $\phi_{j\alpha}(\mathbf{r})$ sono gli orbitali di un singolo atomo isolato di numero atomico Z_j centrato nell'origine, individuati dall'indice $\alpha \in \{1s, 2s, 2p_x \dots\}$. \mathbf{R} indica un generico vettore del reticolo di Bravais, j è un indice che individua i siti della base del cristallo, \mathbf{d}_j è la posizione del sito j all'interno della cella unitaria ed infine i $c_{j\alpha}$ sono i coefficienti incogniti della combinazione lineare.



Grafene: Proprietà elettroniche

$$\psi_{2\pi} = \frac{1}{\sqrt{3}} [\psi(2S) + \sqrt{2}\psi(2P_x)]$$

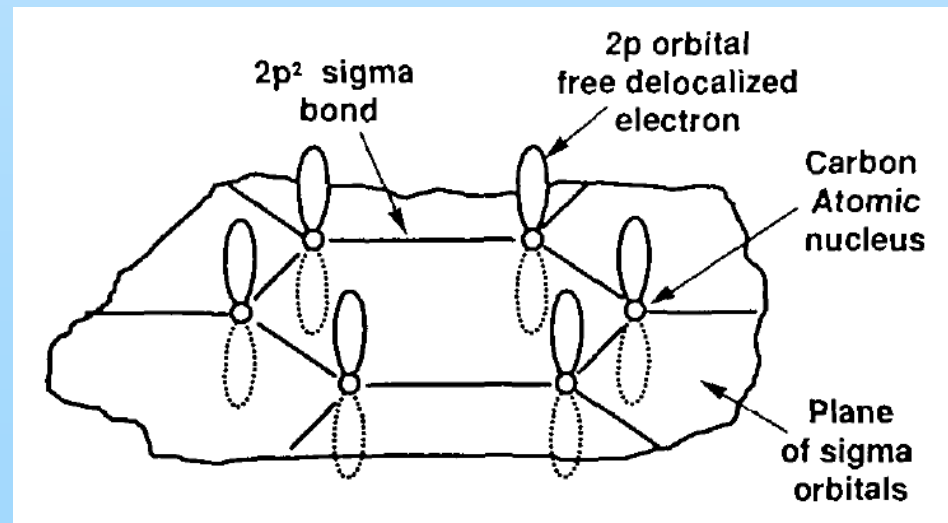
$$\psi_{2\pi/3} = \frac{1}{\sqrt{3}} \left[\psi(2S) - \frac{1}{\sqrt{2}}\psi(2P_x) + \sqrt{\frac{3}{2}}\psi(2P_y) \right]$$

Nel piano

$$\psi_{4\pi/3} = \frac{1}{\sqrt{3}} \left[\psi(2S) - \frac{1}{\sqrt{2}}\psi(2P_x) - \sqrt{\frac{3}{2}}\psi(2P_y) \right]$$

P_z fuori dal piano

$$P_z = \frac{1}{2\sqrt{6}a^5} r e^{-\frac{r}{2a}} \sqrt{\frac{3}{8\pi}} \cos\theta$$





Tight Binding nel grafene

(Wallace 1946)

Phys. Rev. 71 (1947) 622

$$\psi = \varphi_1 + \lambda \varphi_2$$

$$\left. \begin{aligned} \varphi_1 &= \sum_A \exp[2\pi i \mathbf{k} \cdot \mathbf{r}_A] X(\mathbf{r} - \mathbf{r}_A) \\ \varphi_2 &= \sum_B \exp[2\pi i \mathbf{k} \cdot \mathbf{r}_B] X(\mathbf{r} - \mathbf{r}_B) \end{aligned} \right\}$$

$$\int X(\mathbf{r} - \mathbf{r}_A) X(\mathbf{r} - \mathbf{r}_B) d\tau = 0.$$

Nessuna sovrapposizione
tra gli orbitali p^z

$$H\psi = E\psi$$

$$\begin{vmatrix} H_{11} - ES & H_{12} \\ H_{21} & H_{22} - ES \end{vmatrix} = 0$$

$$H_{11} + \lambda H_{12} = ES,$$

$$H_{21} + \lambda H_{22} = \lambda ES,$$

$$H_{11} = \int \phi_1^* H \phi_1 d\tau, \quad H_{12} = H_{21}^* = \int \phi_1^* H \phi_2 d\tau,$$

$$H_{22} = \int \phi_2^* H \phi_2 d\tau$$

$$E = \frac{1}{2S} \{ H_{11} + H_{22} \pm ((H_{11} - H_{22})^2 + 4|H_{12}|^2)^{\frac{1}{2}} \}$$

$$S = \int \phi_1^* \phi_1 d\tau = \int \phi_2^* \phi_2 d\tau = N \text{ (celle nel cr.)}$$




Grafene: Proprietà elettroniche

$H_{11} = H_{22}$ per simmetria

$$H_{11}' = H_{22}' = \frac{1}{N} H_{11} = \frac{1}{N} H_{22},$$

$$H_{12}' = \frac{1}{N} H_{12}$$

$$E = H_{11}' \pm |H_{12}'|.$$


+ fuori, - dentro la zona
di B. esagonale

$$\Delta E = 2 |H_{12}'|$$

$$H_{11}' = \frac{1}{N} \sum_{A, A'} \exp[-2\pi i \mathbf{k} \cdot (\mathbf{r}_A - \mathbf{r}_{A'})] \\ \times \int X^*(\mathbf{r} - \mathbf{r}_A) H X(\mathbf{r} - \mathbf{r}_{A'}) d\tau.$$

ponendo

$$E_0 = \int X^*(\mathbf{r}) H X(\mathbf{r}) d\tau,$$

$$\gamma_0' = - \int X^*(\mathbf{r} - \mathbf{e}') H X(\mathbf{r}) d\tau,$$

$\mathbf{e}' = \mathbf{a}_1$ Vettore che congiunge primi vicini A

$$H_{11}' = E_0 - 2\gamma_0' (\cos 2\pi k_y a + 2 \cos \pi k_x a \sqrt{3} \cos \pi k_y a)$$



Grafene: Proprietà elettroniche

$$H = H_0 + (H - H_0)$$

H_0 Hamiltoniana di un atomo di C isolato

$$H - H_0 = V - U < 0$$

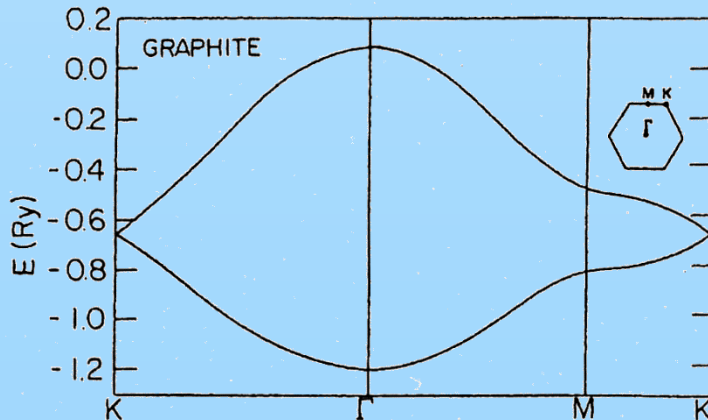
V Potenziale periodico del reticolo

U Potenziale di un atomo di C

$$H_0 X = E_0 X$$

$$E_0 = \bar{E} - \int X^*(\mathbf{r})(U - V)X(\mathbf{r})d\tau$$

$$\gamma_0' = \int X^*(\mathbf{r} - \boldsymbol{\rho}') (U - V)X(\mathbf{r})d\tau > 0$$

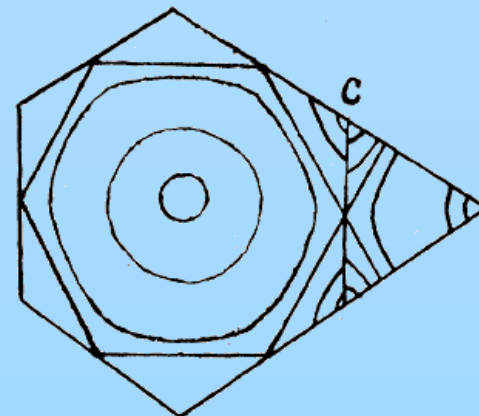


$$\gamma_0 = \int X^*(\mathbf{r} - \boldsymbol{\rho})(U - V)X(\mathbf{r})d\tau > 0$$

$\boldsymbol{\rho} = \mathbf{AB}$ Reticoli contigui

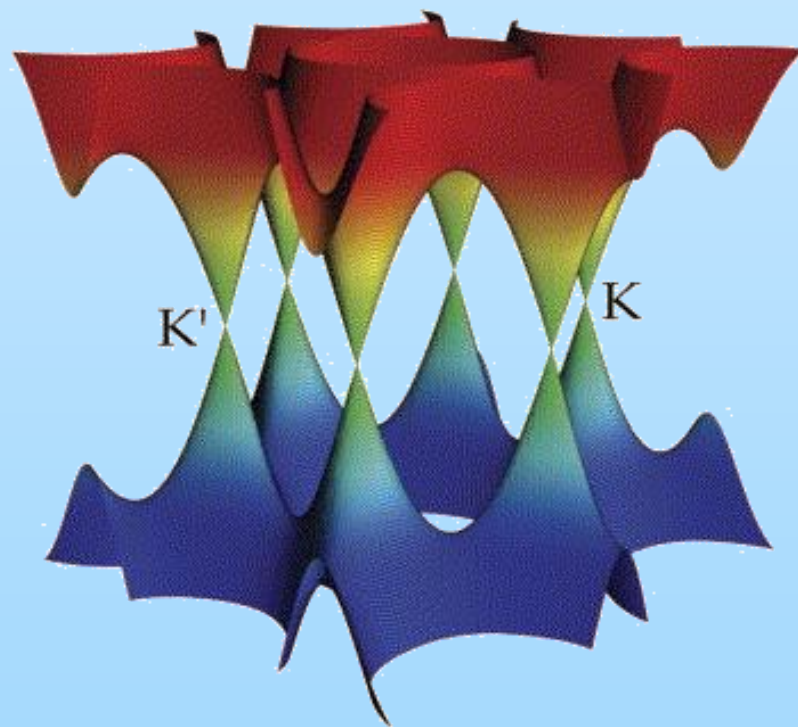
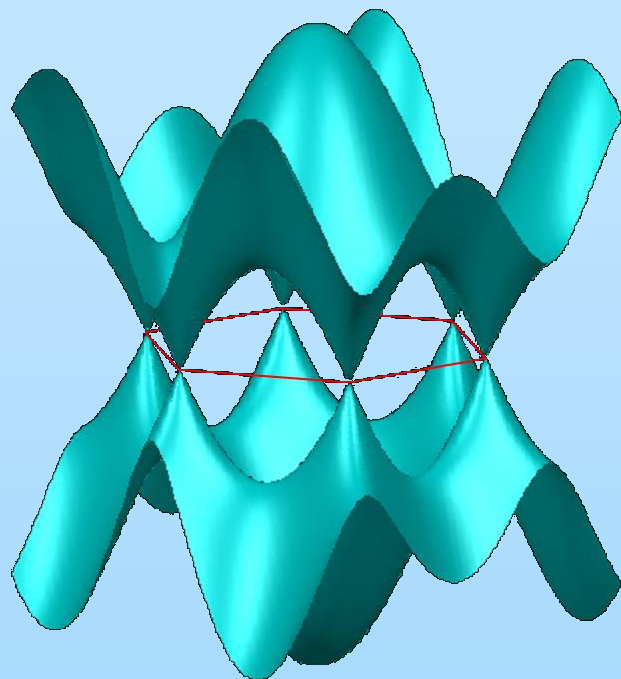
$$H_{12}' = -\gamma_0(\exp[-2\pi i k_x(a/\sqrt{3})] + 2 \cos \pi k_y a \cdot \exp[2\pi i k_x(a/2\sqrt{3})]),$$

$$|H_{12}'|^2 = \gamma_0^2(1 + 4 \cos^2 \pi k_y a + 4 \cos \pi k_y a \cos \pi k_x \sqrt{3} a)$$



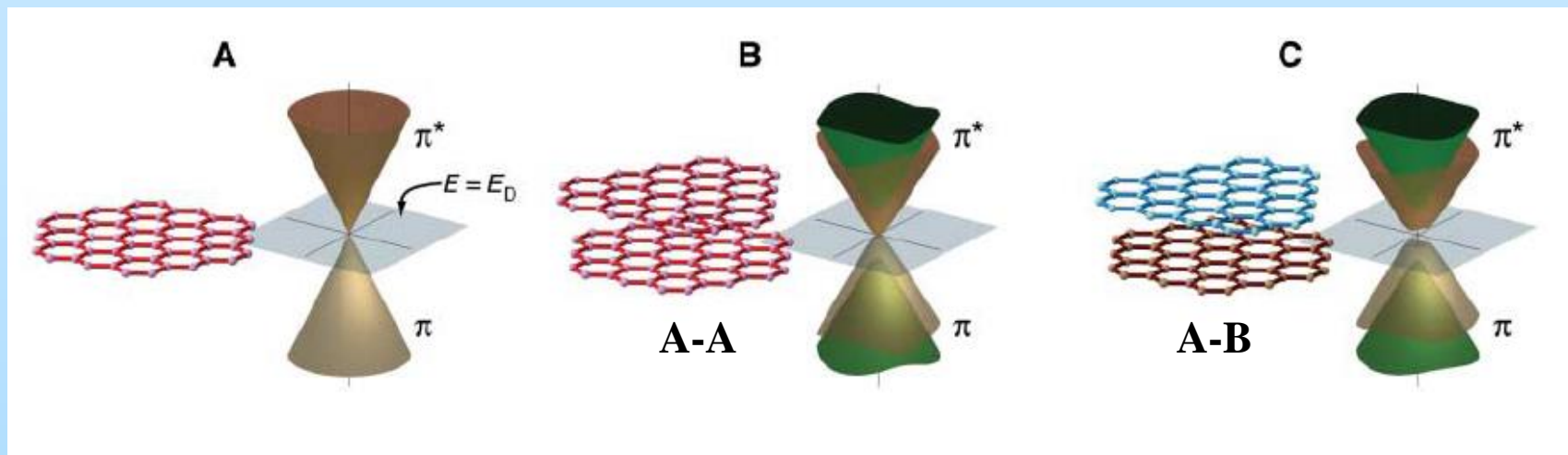


Grafene: Proprietà elettroniche



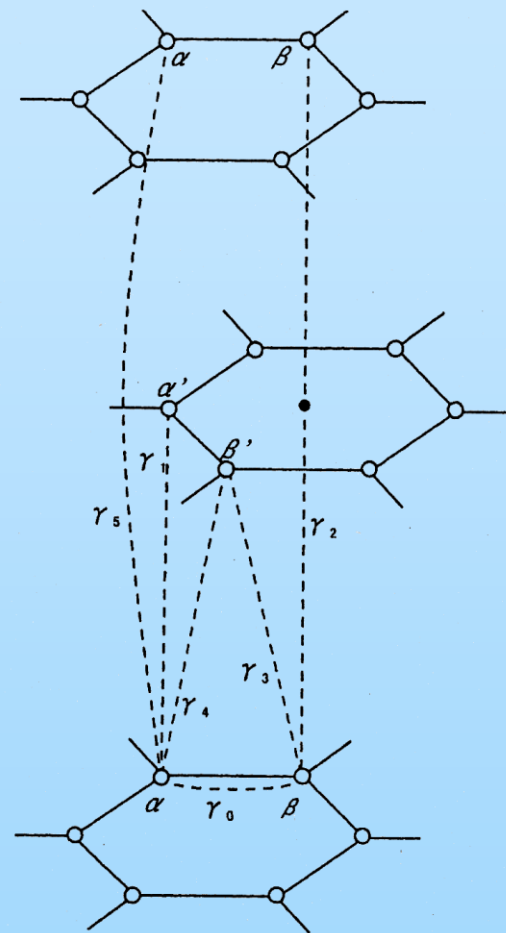
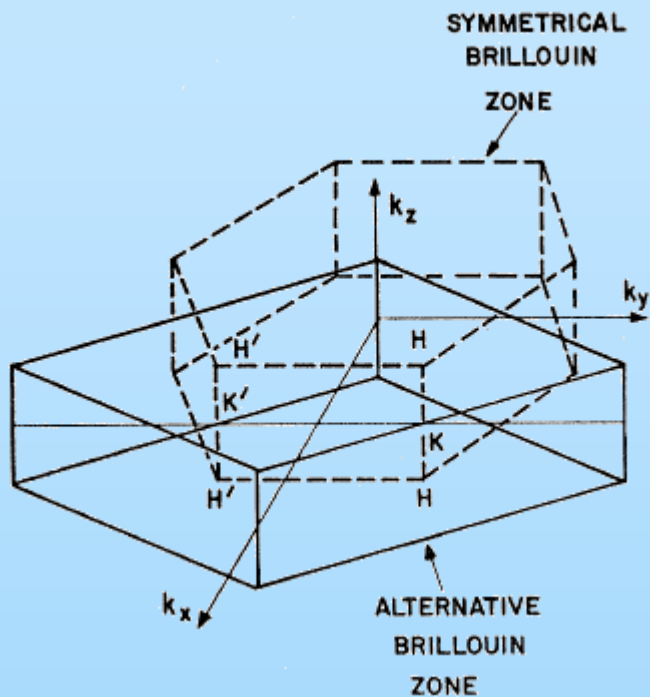


Multigrafene (2 strati)





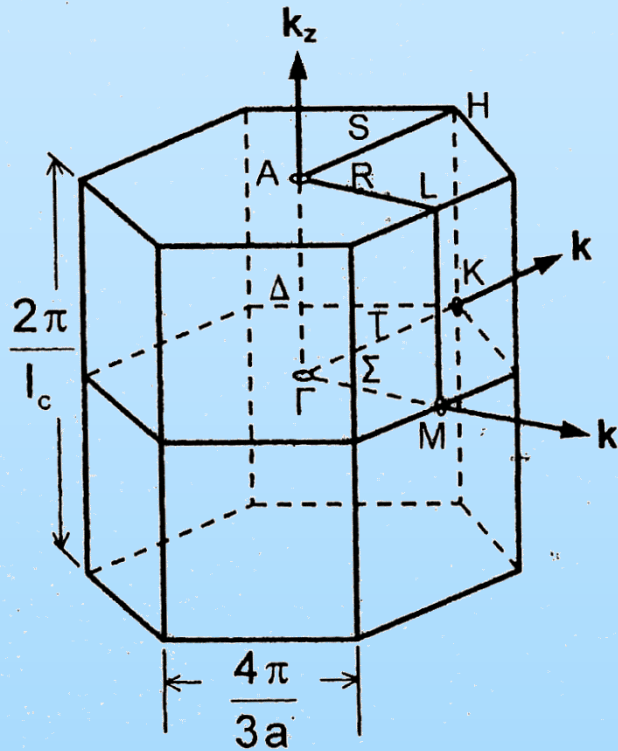
Grafite: Proprietà elettroniche



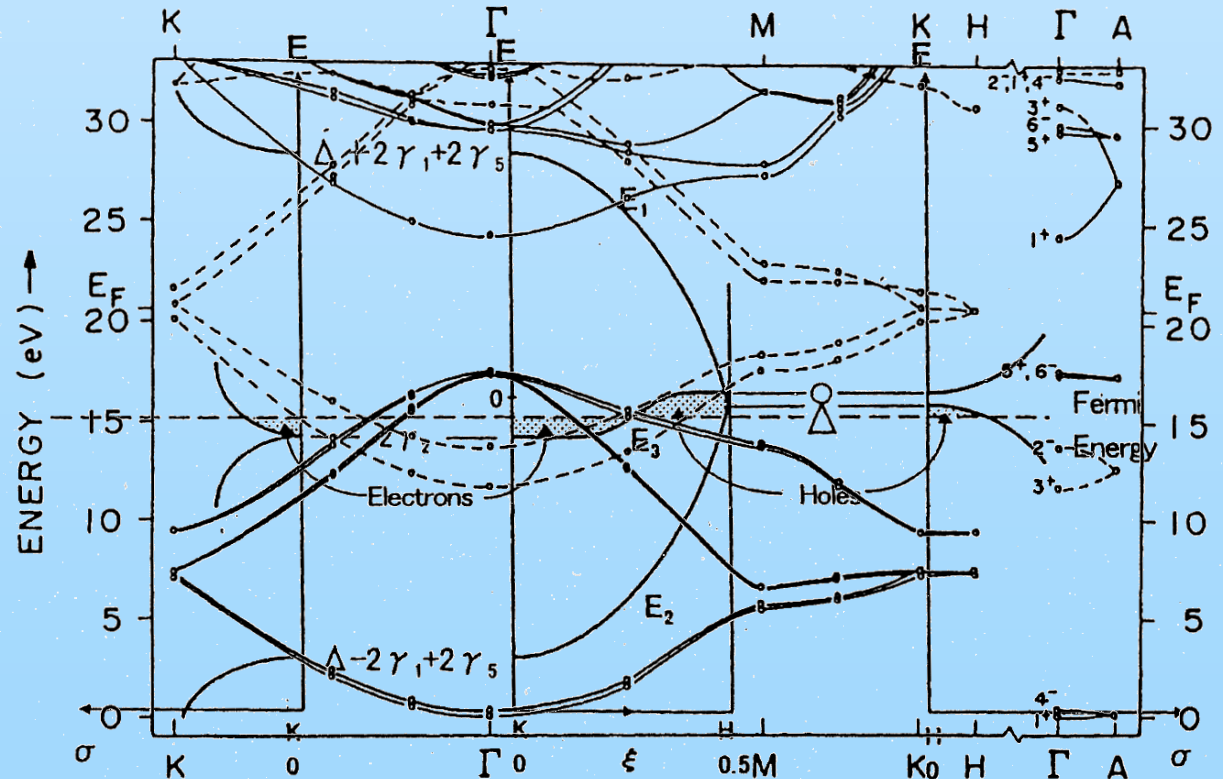
$$\gamma_0 \gg \gamma_n$$

$$\begin{aligned} \gamma_0 &= 3.16, \gamma_1 = 0.39, \\ \gamma_2 &= -0.020, \gamma_3 = 0.315, \gamma_4 \simeq 0.044, \\ \gamma_5 &= 0.038; \Delta = -0.008 \text{ eV} \end{aligned}$$

Grafite: Proprietà elettroniche



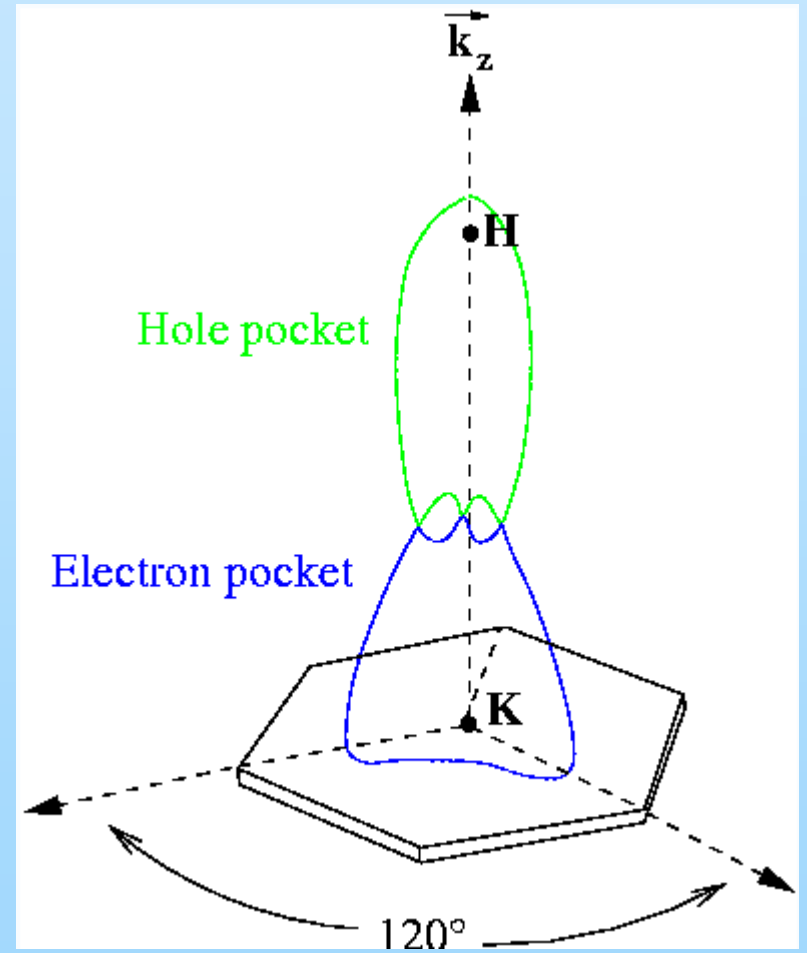
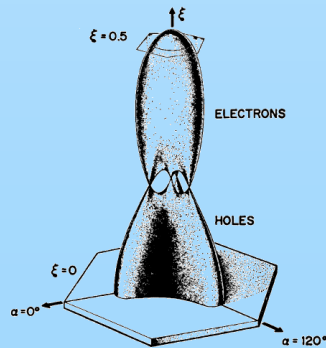
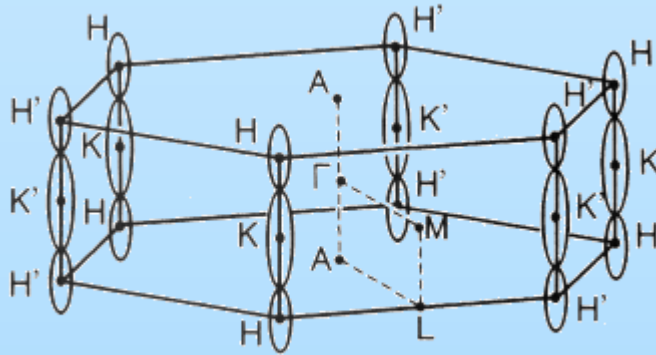
4 bande (tratteggiate)



$$\begin{aligned} \gamma_0 &= 3.16, \gamma_1 = 0.39, \\ \gamma_2 &= -0.020, \gamma_3 = 0.315, \gamma_4 \approx 0.044, \\ \gamma_5 &= 0.038; \Delta = -0.008 \text{ eV} \end{aligned}$$



Grafite: Superficie di Fermi



Dresselhaus 1964



Grafite: Superficie di Fermi

