

Química Orgânica – LCE 161

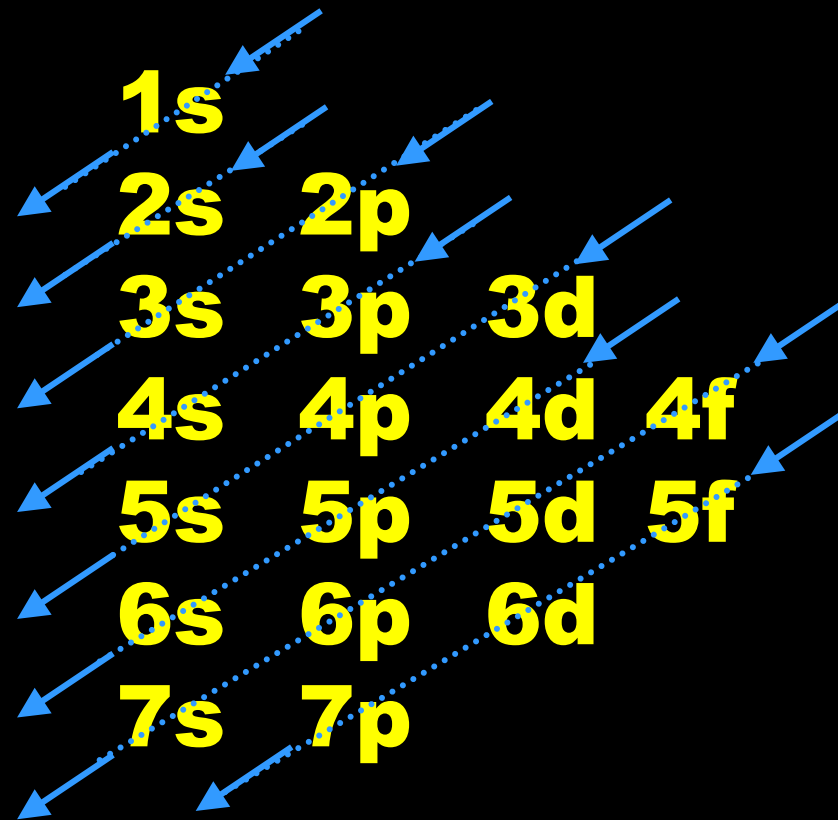
Prof. Dr. Marcos Yassuo Kamogawa

Material adaptado da página

<http://faculty.washington.edu/dwoodman/unitsHome.html>

DISTRIBUIÇÃO ELETRÔNICA

Aufbau



s 2e⁻

p 6e⁻

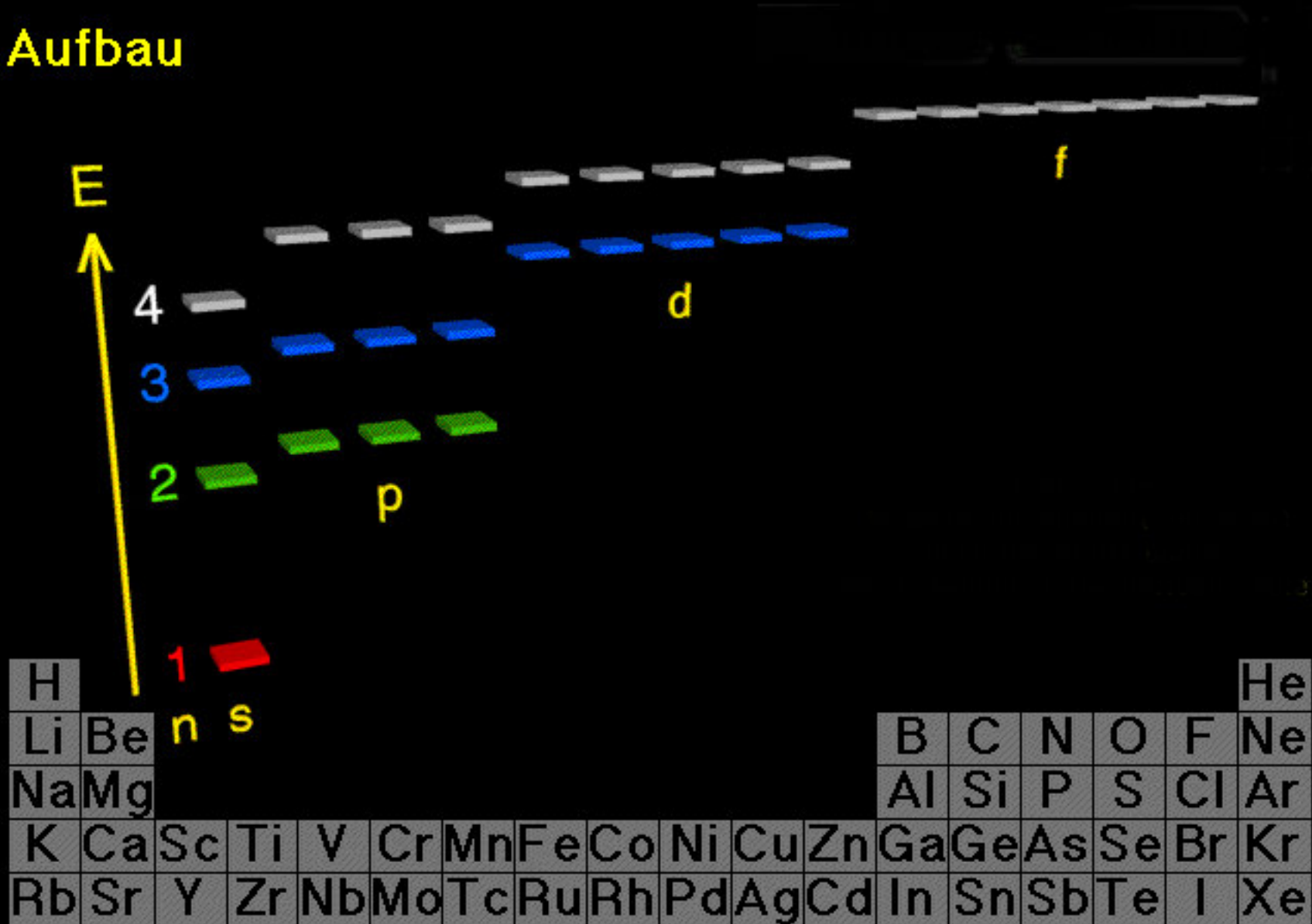
d 10e⁻

f 14e⁻

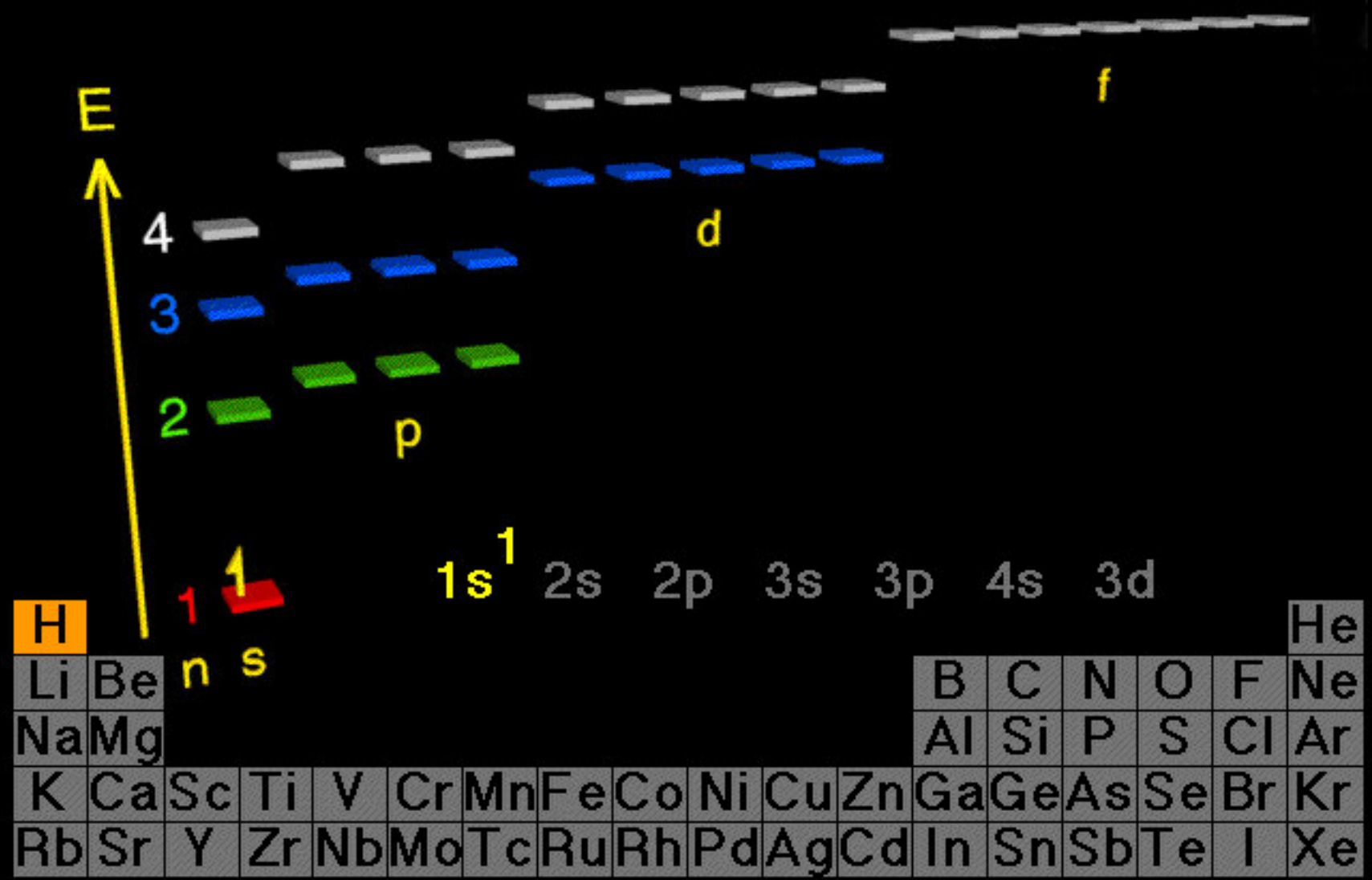
Aufbau

- 1) **Princípio da construção:** os e^- devem ocupar os orbitais de menor energia
- 2) **Princípio de exclusão de Pauli:** No máximo 2 e^- por orbital, com spins emparelhados
- 3) **Regra de Hund:** Em orbitais de mesma energia (p, d e f). Adicionamos um e^- a cada orbital até que cada um seja completado.

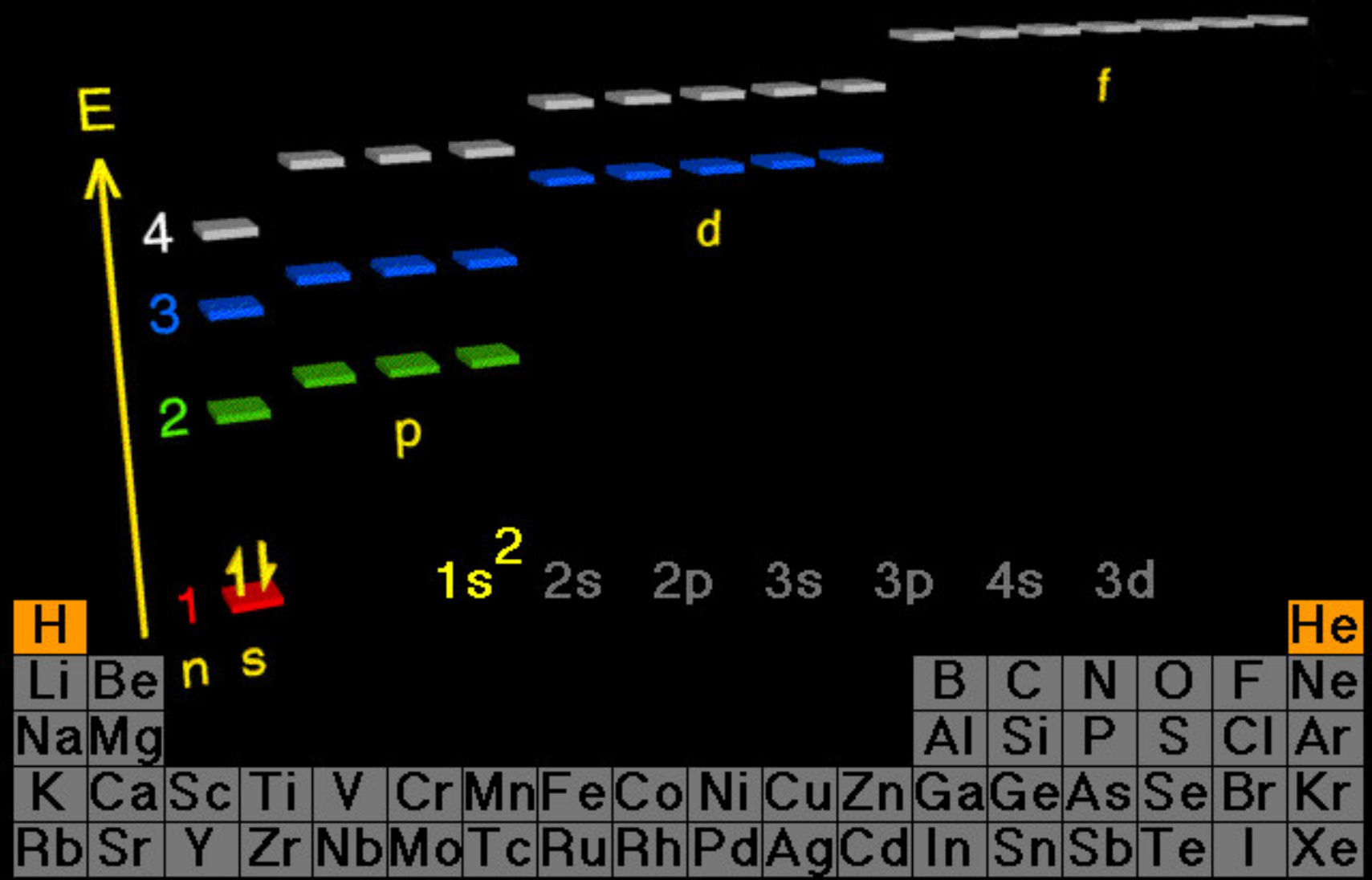
Aufbau



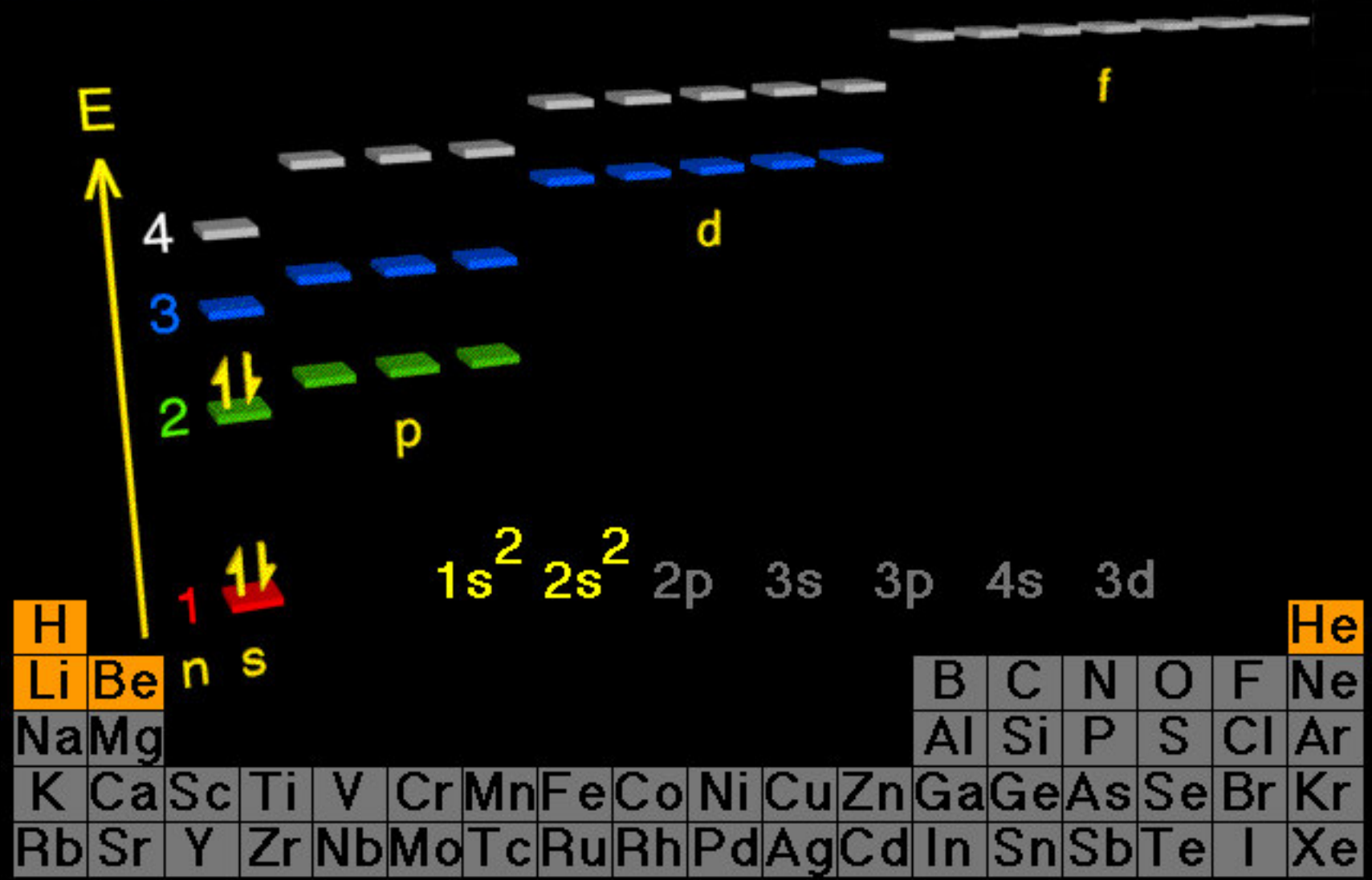
Aufbau



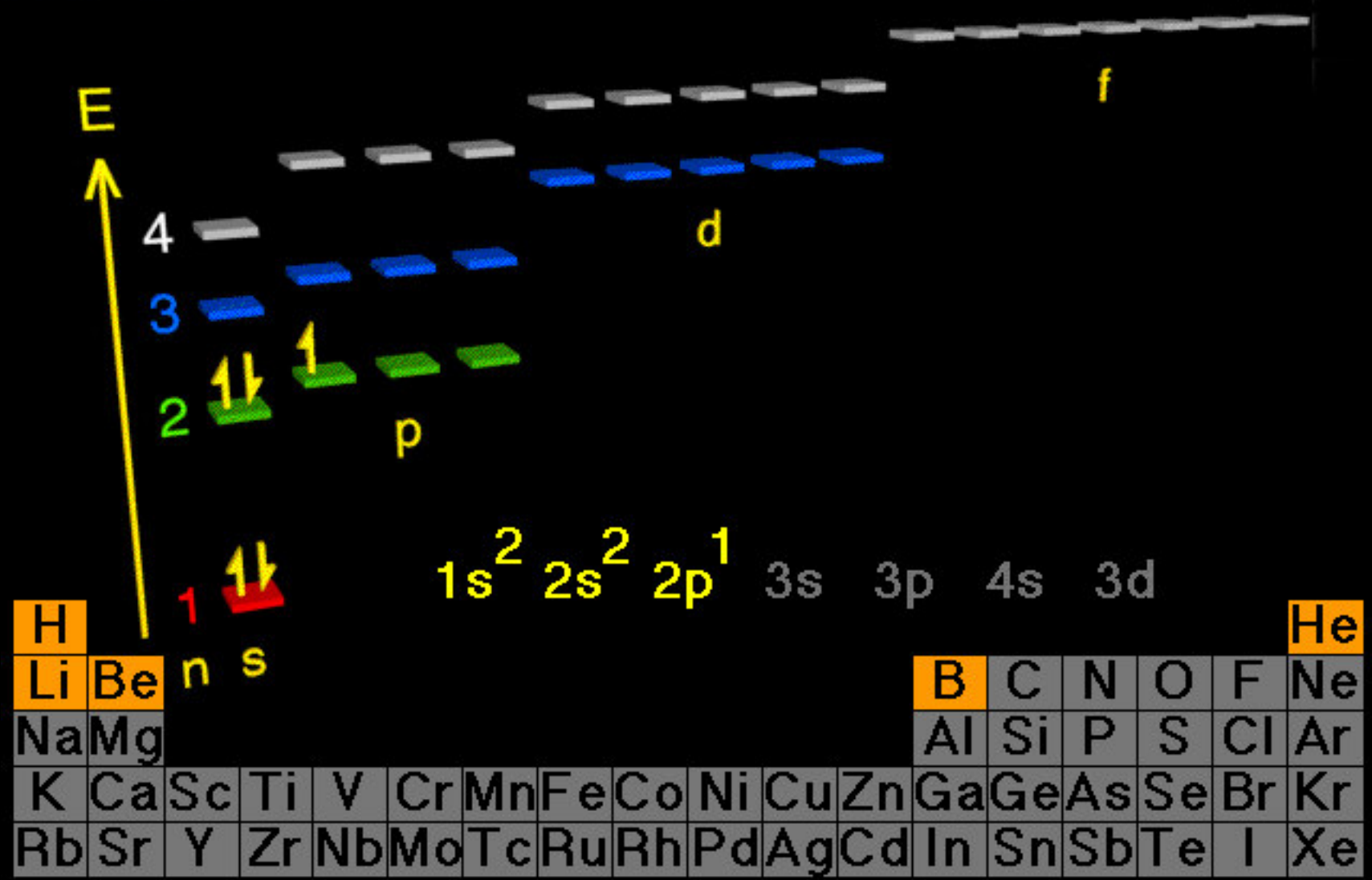
Aufbau



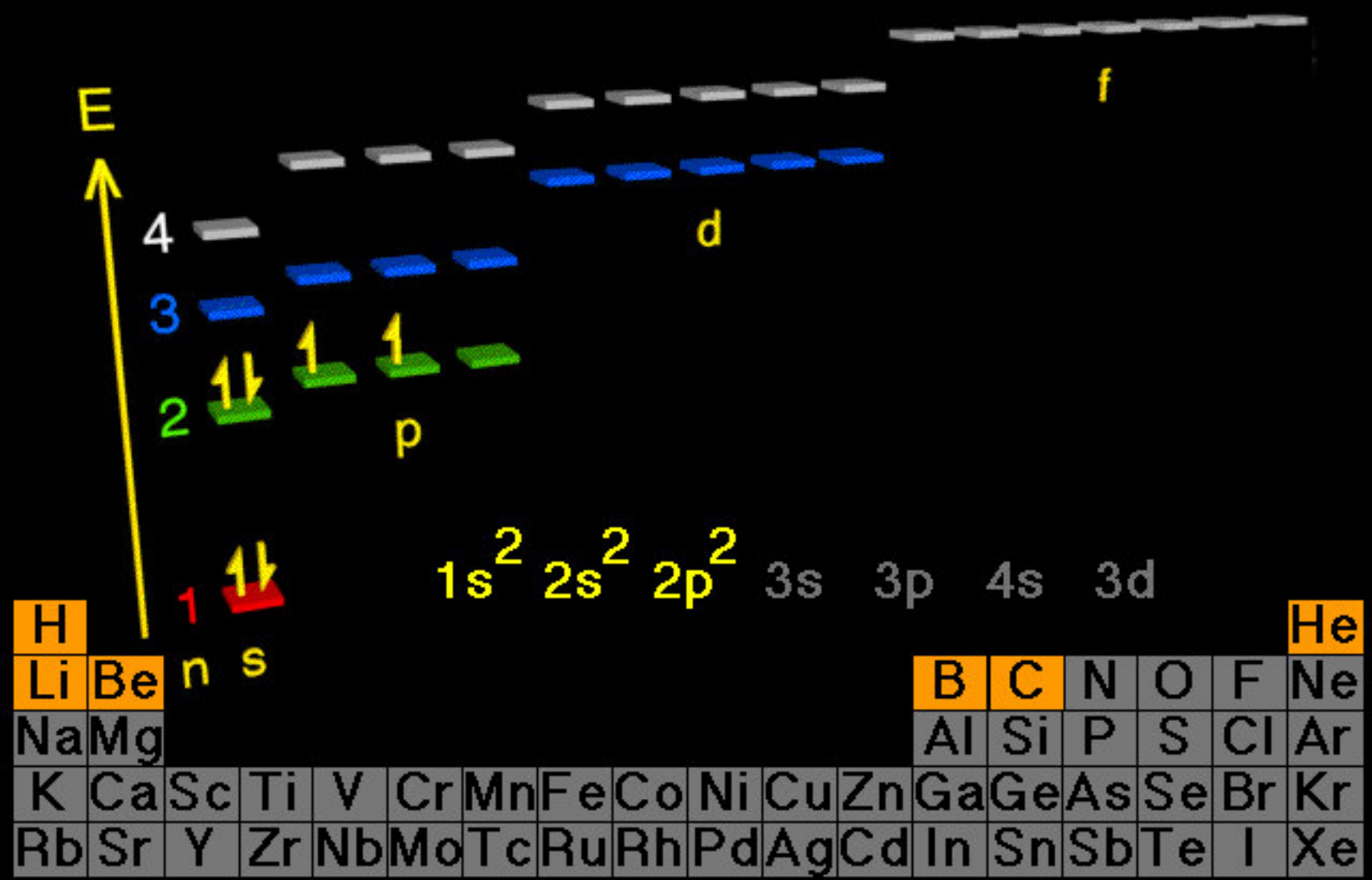
Aufbau



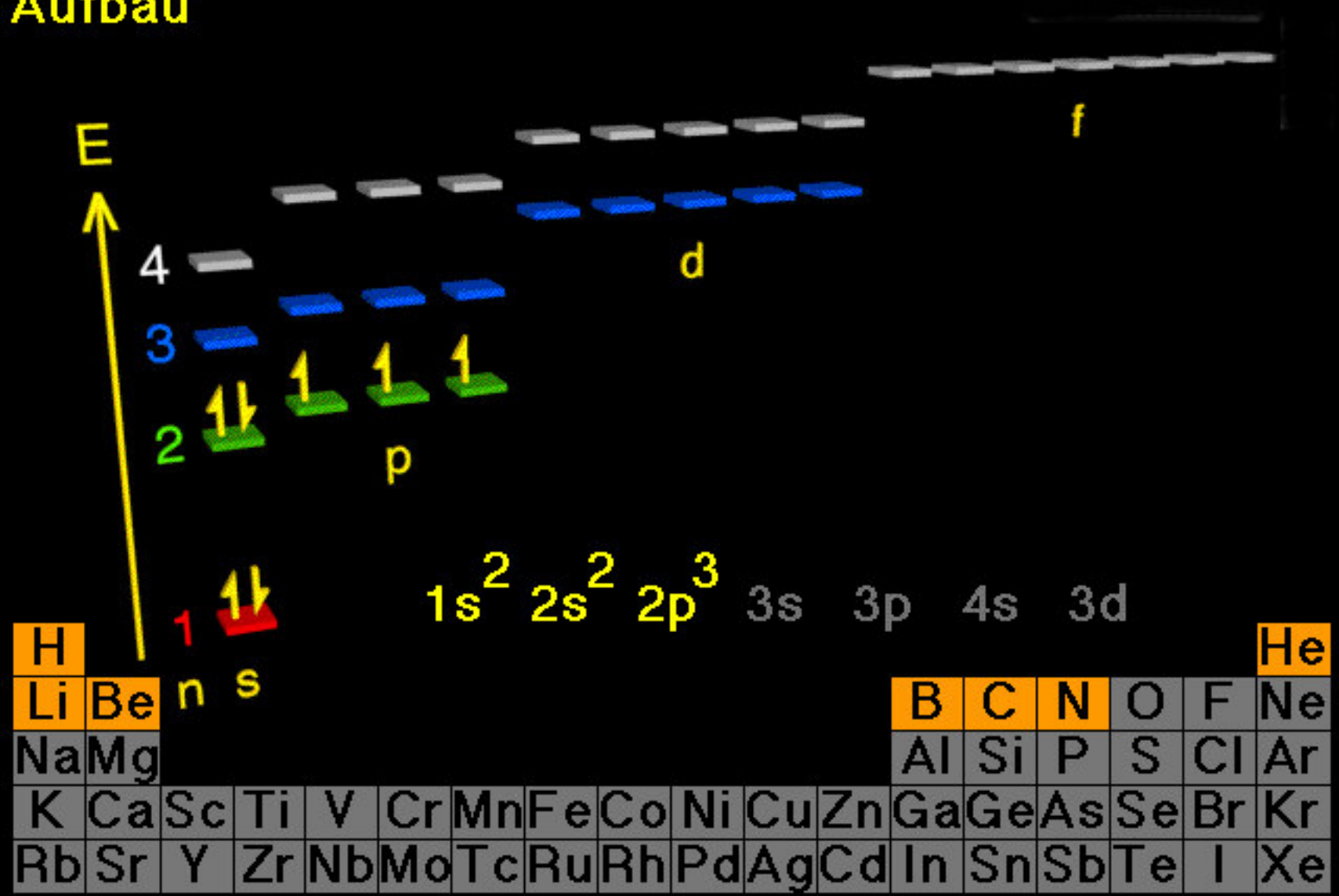
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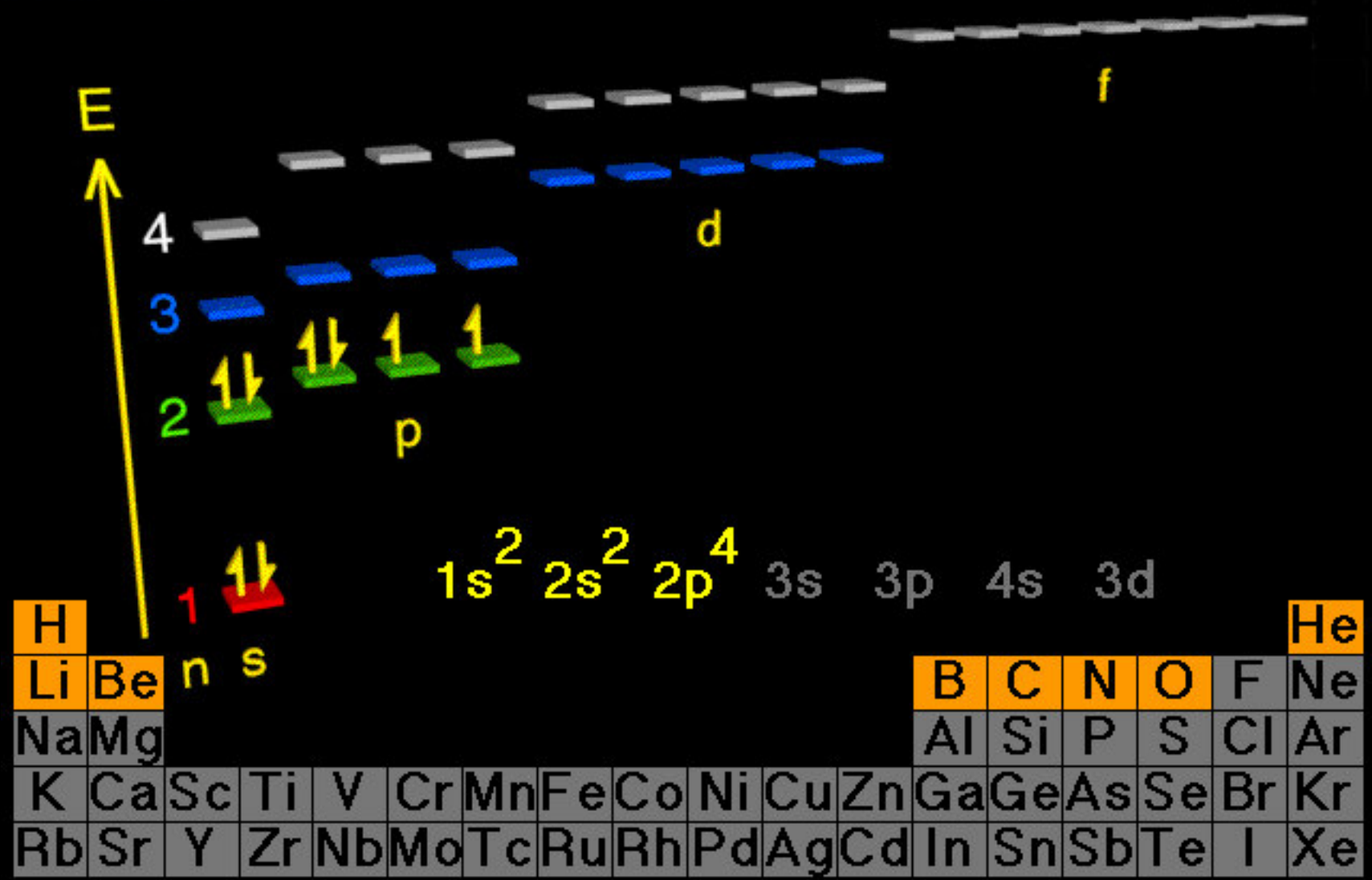
Aufbau



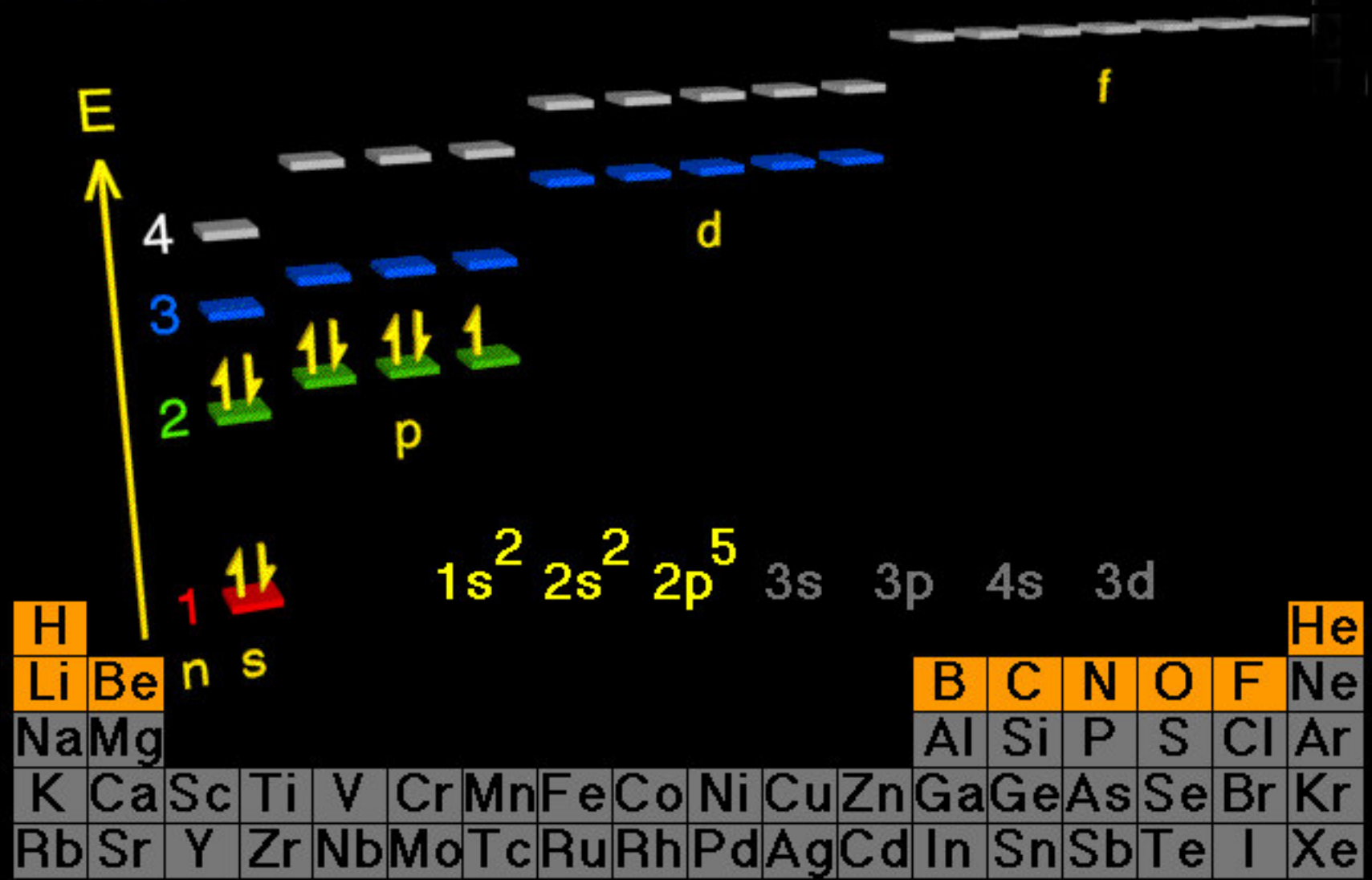
Aufbau



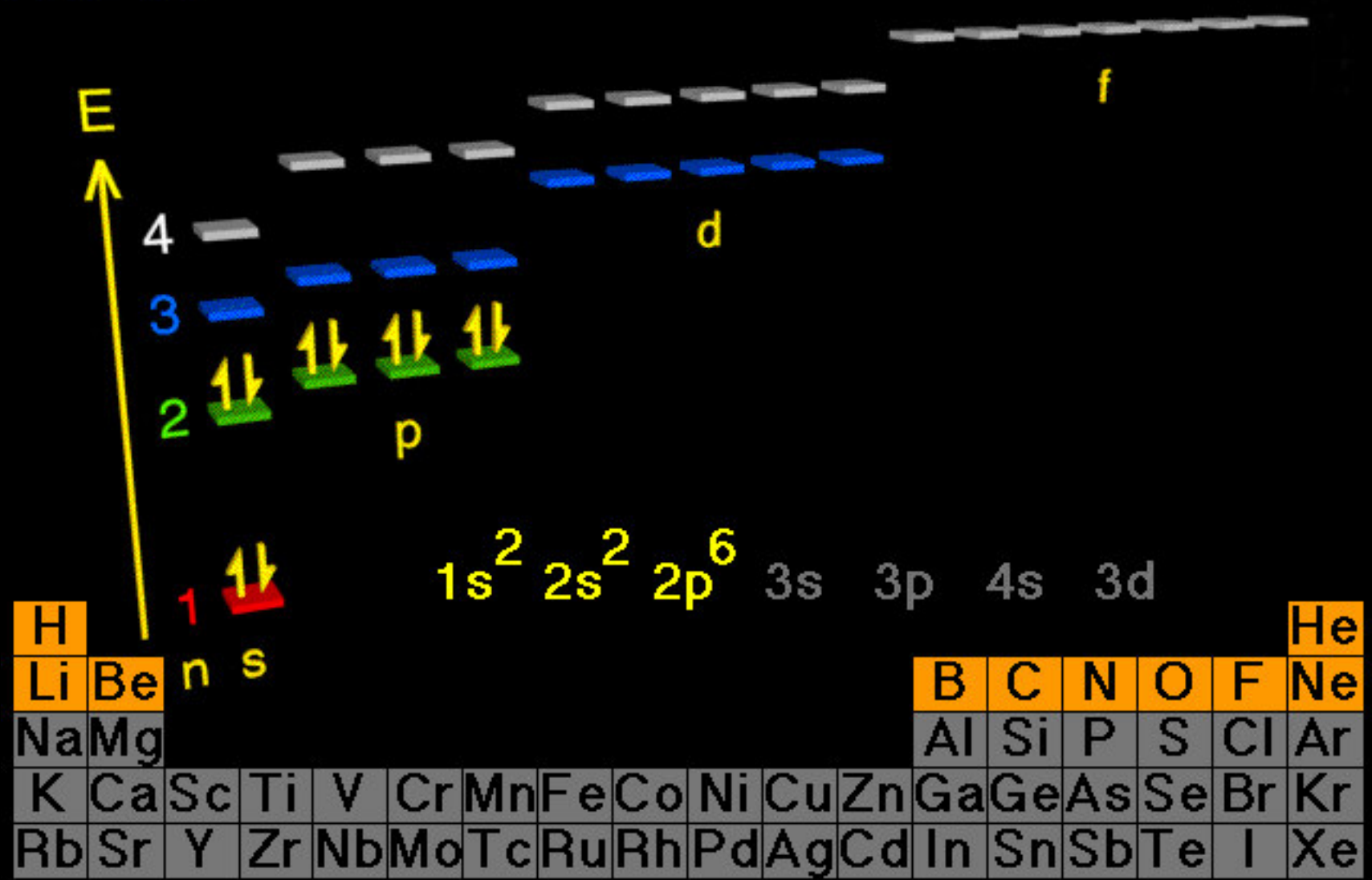
Aufbau



Aufbau

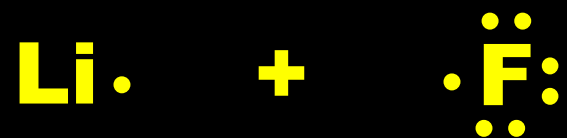
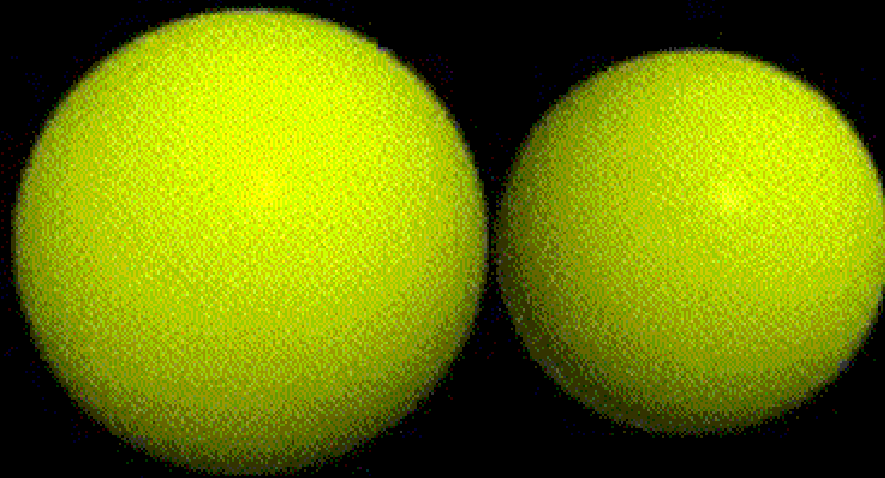


Aufbau

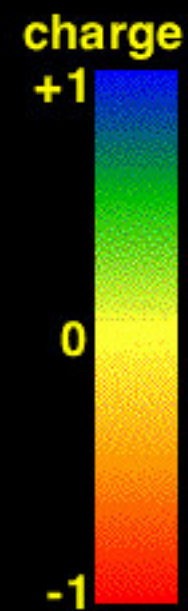
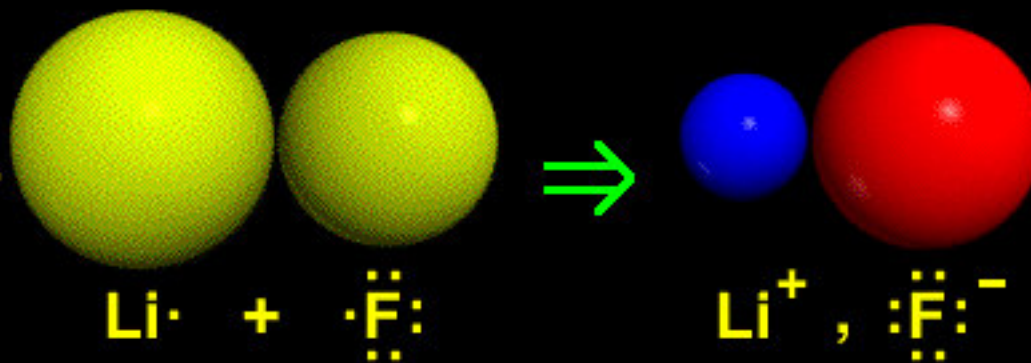


LIGAÇÕES QUÍMICA

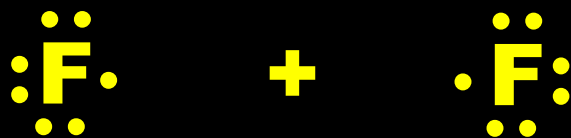
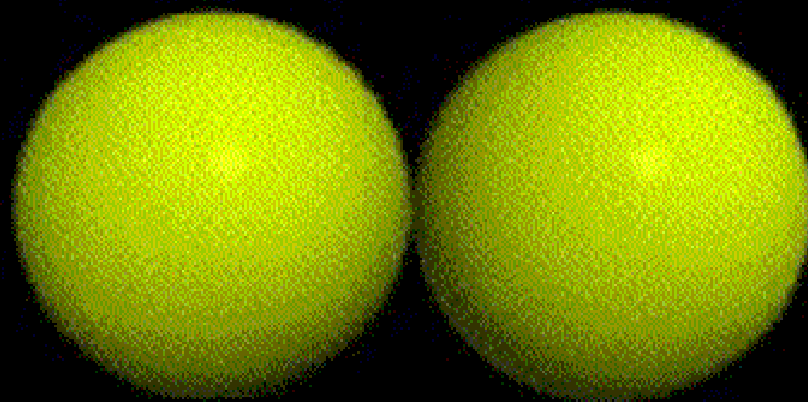
LIGAÇÃO IÔNICA



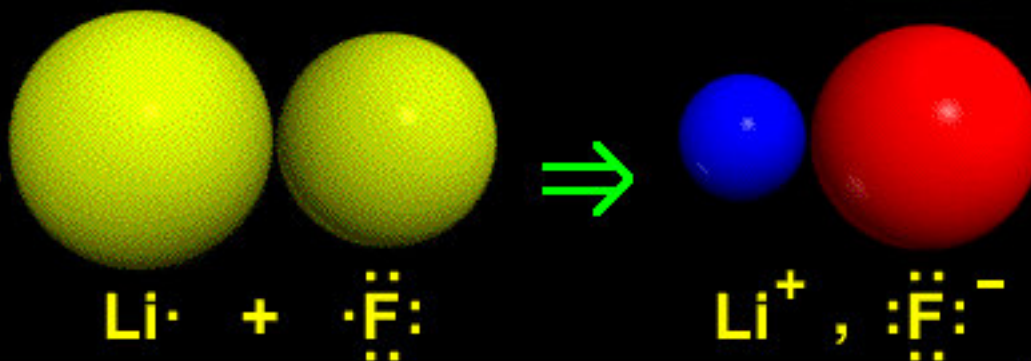
**Ionic Bond
Electron Transfer**



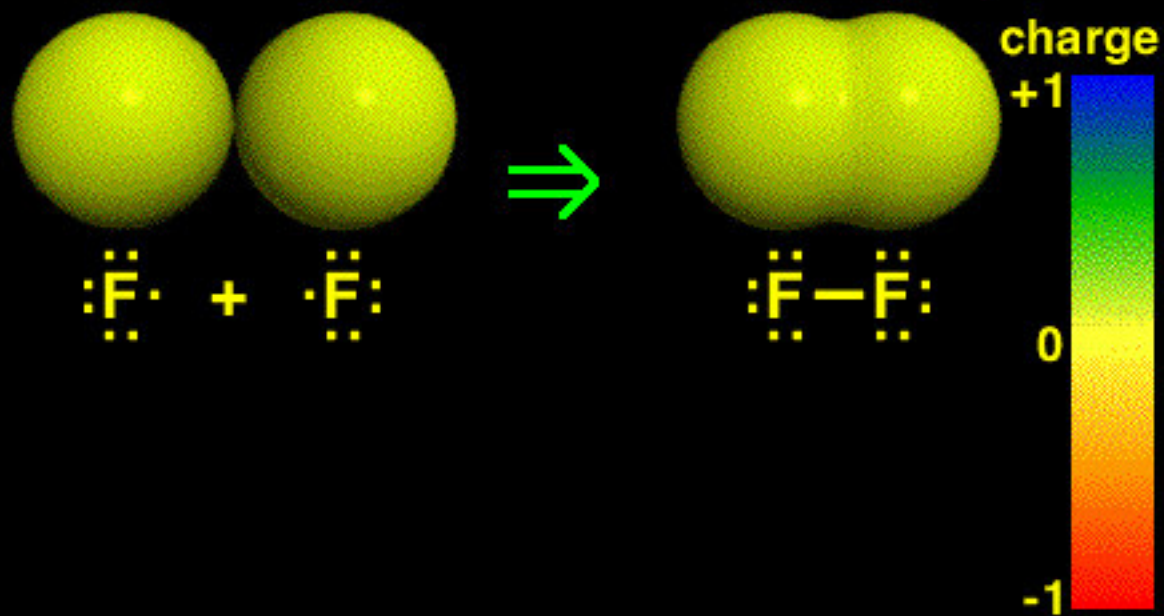
LIGAÇÃO COVALENTE



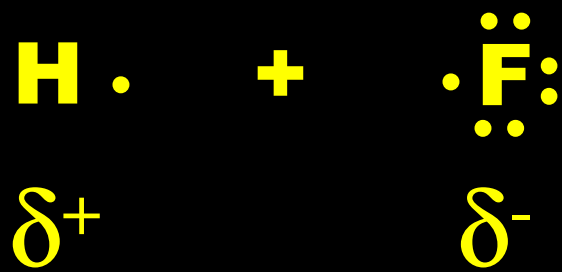
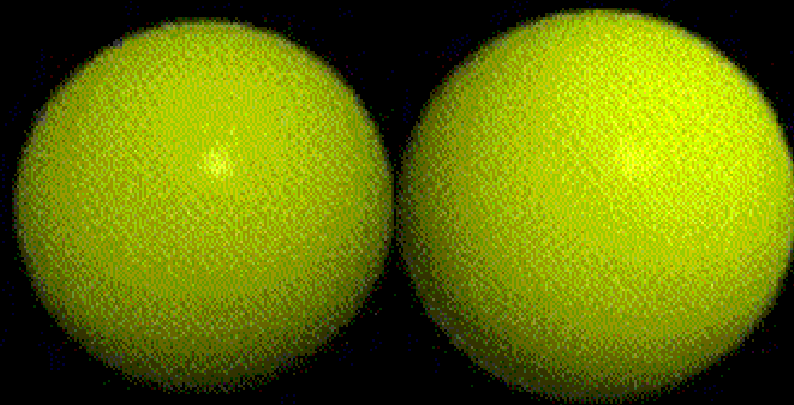
**Ionic Bond
Electron Transfer**



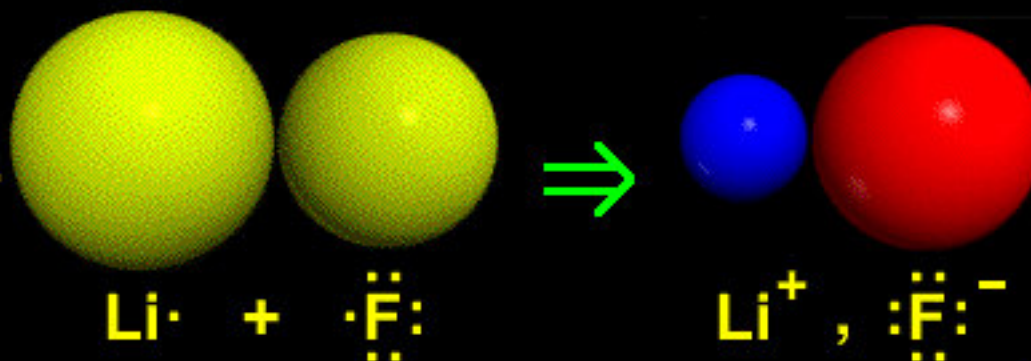
**Covalent Bond
Equal Sharing**



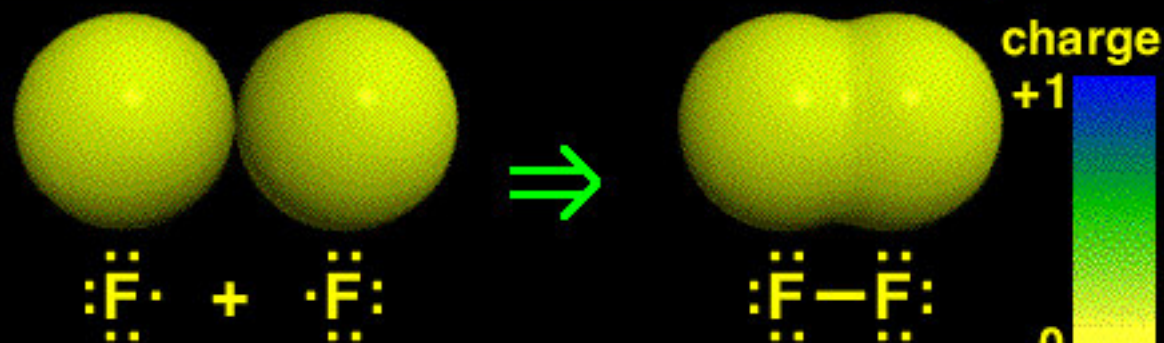
LIGAÇÃO COVALENTE



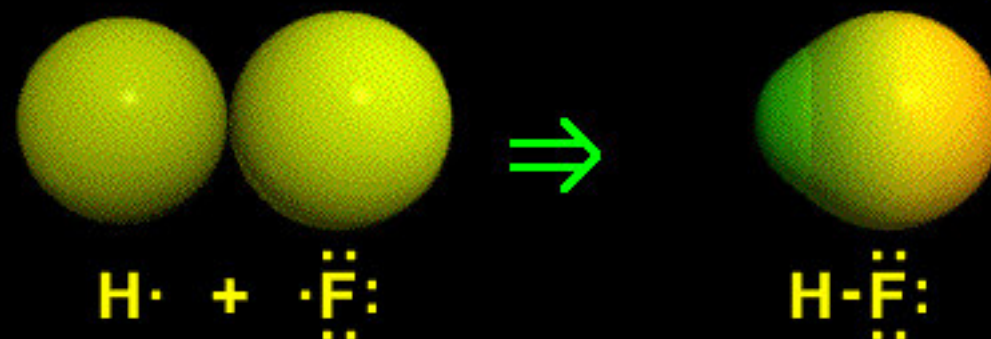
**Ionic Bond
Electron Transfer**



**Covalent Bond
Equal Sharing**

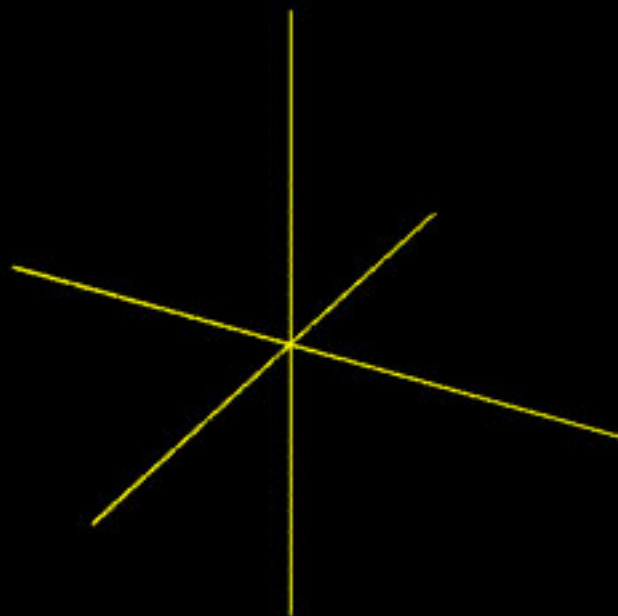


**Covalent Bond
Unequal Sharing**

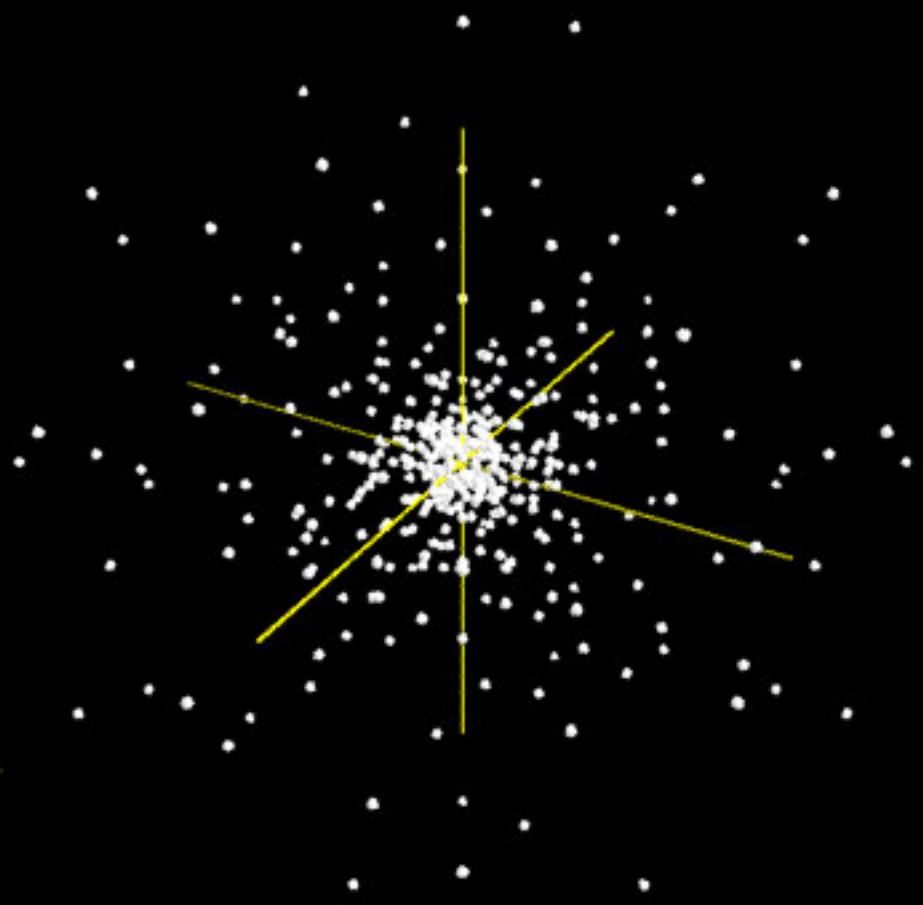


ORBITAL ATÔMICO

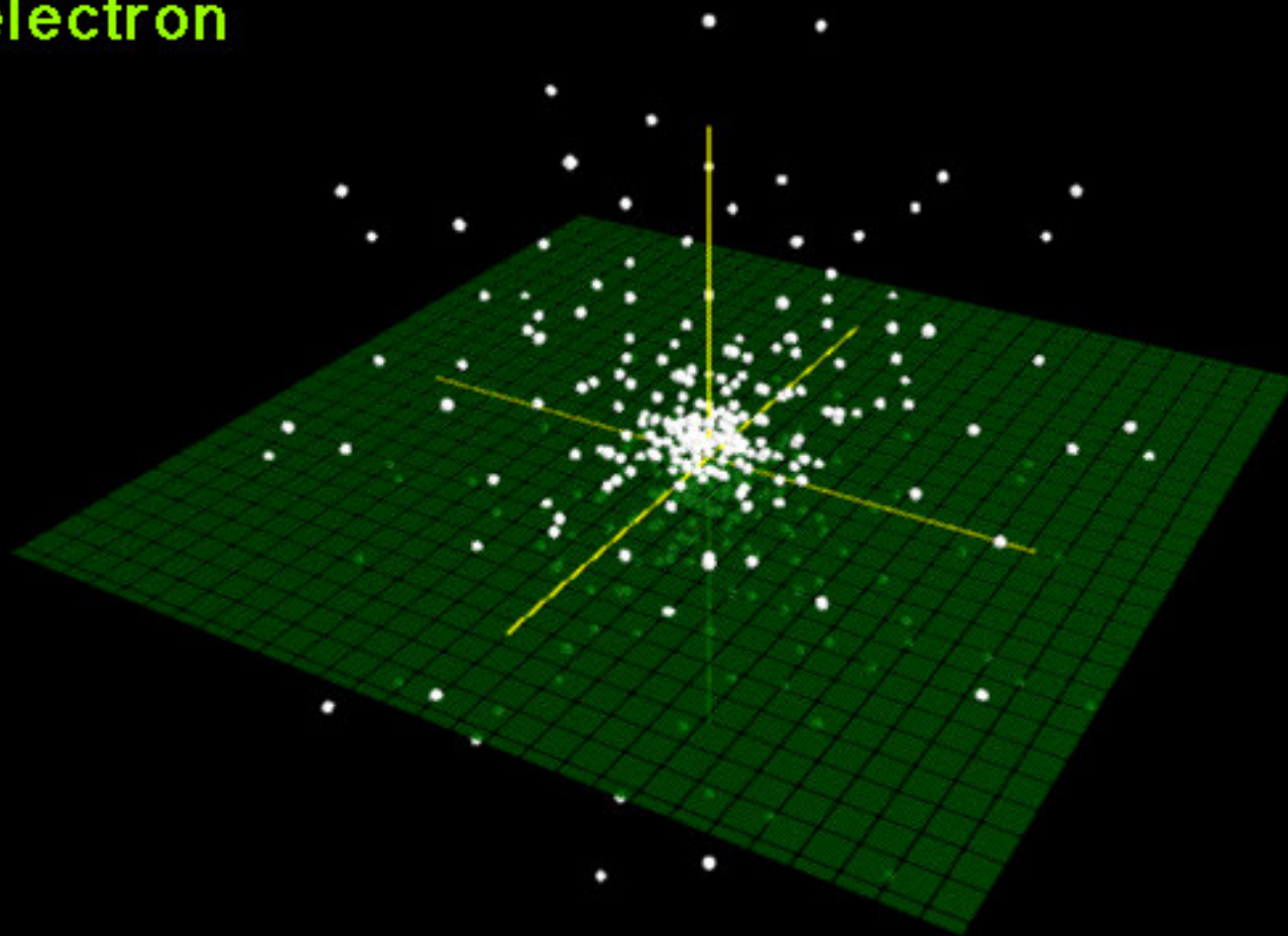
Probability Distribution 1s electron



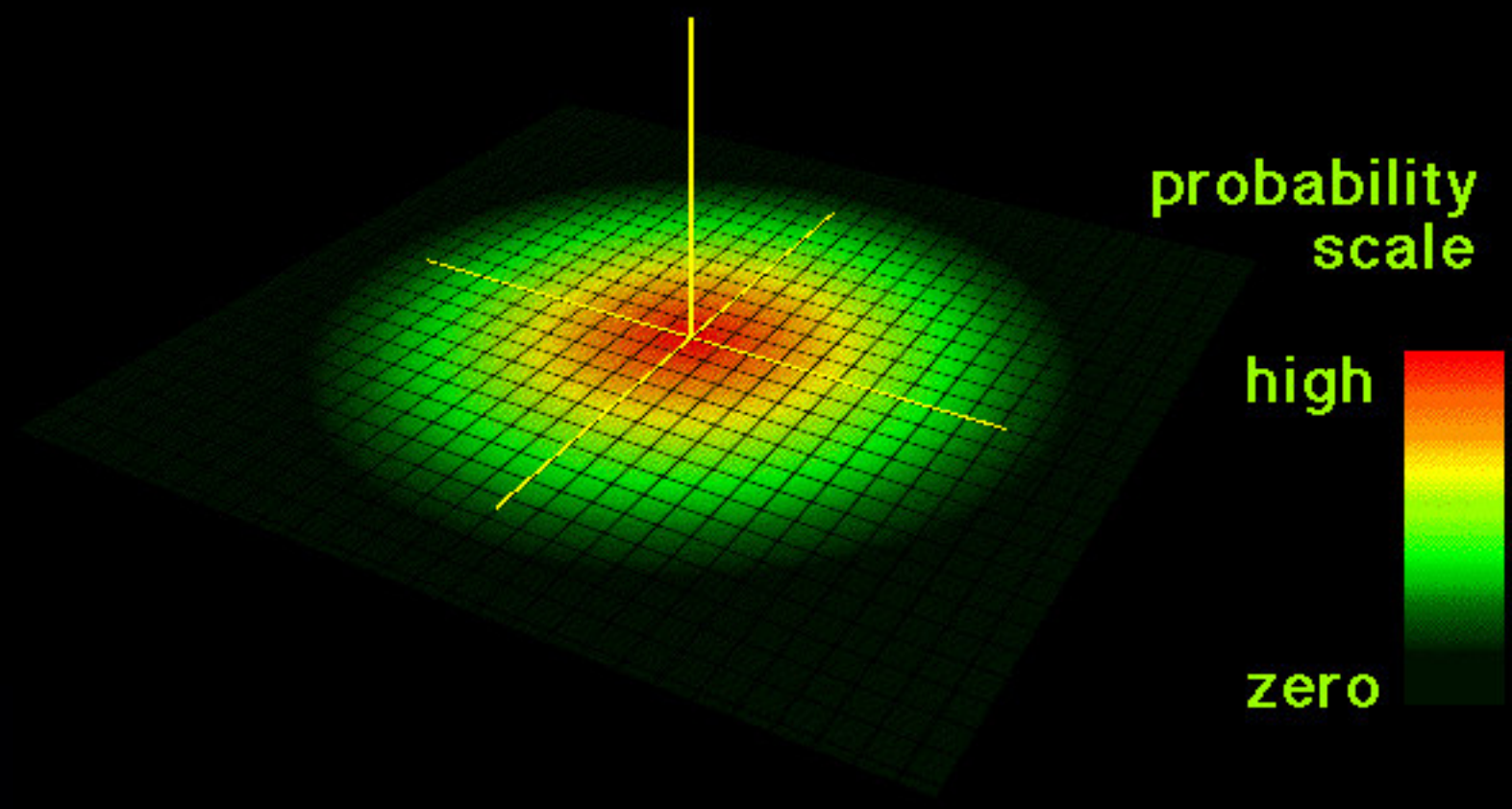
Probability Distribution 1s electron



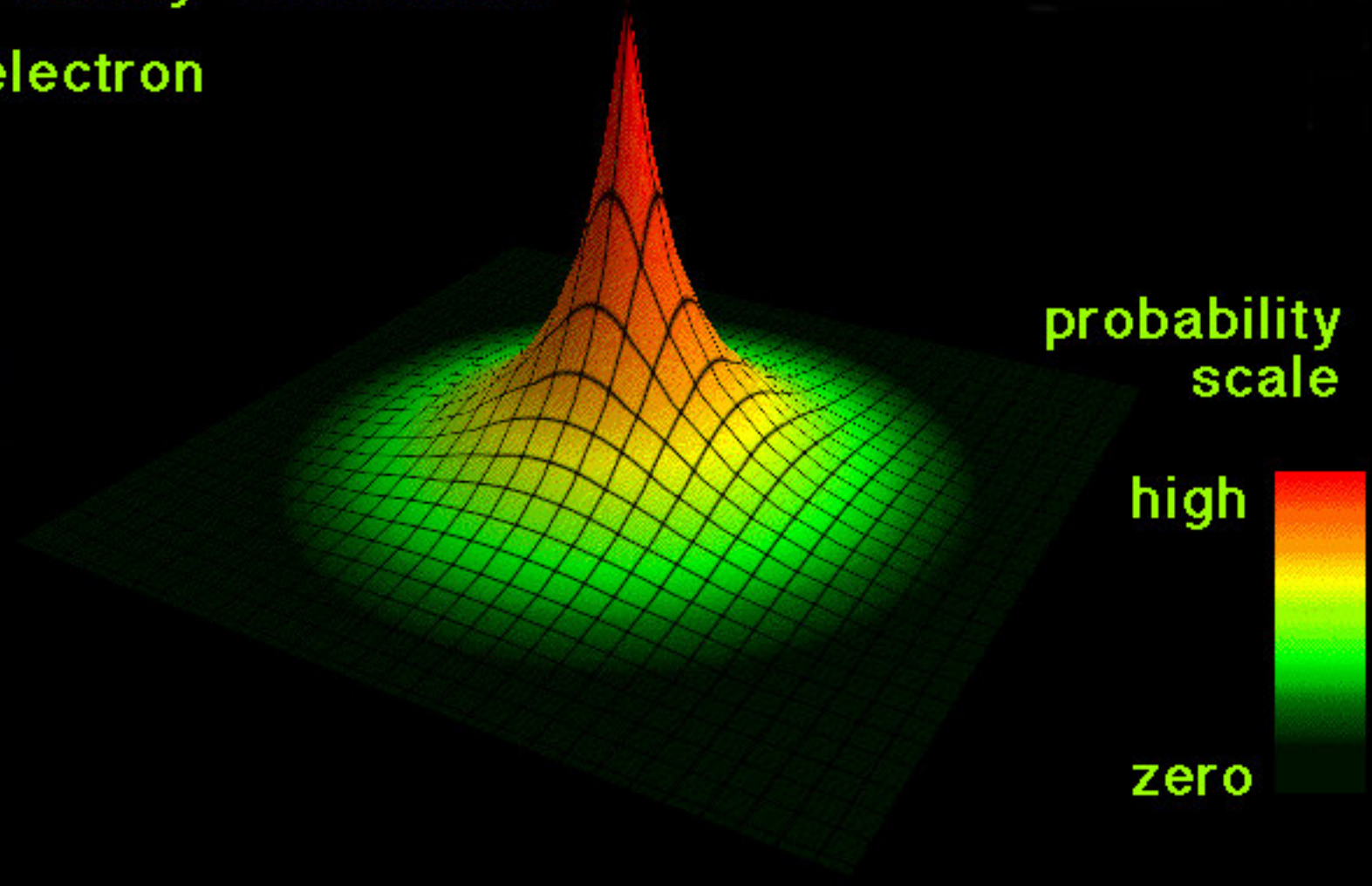
Probability Distribution 1s electron



Probability Distribution 1s electron

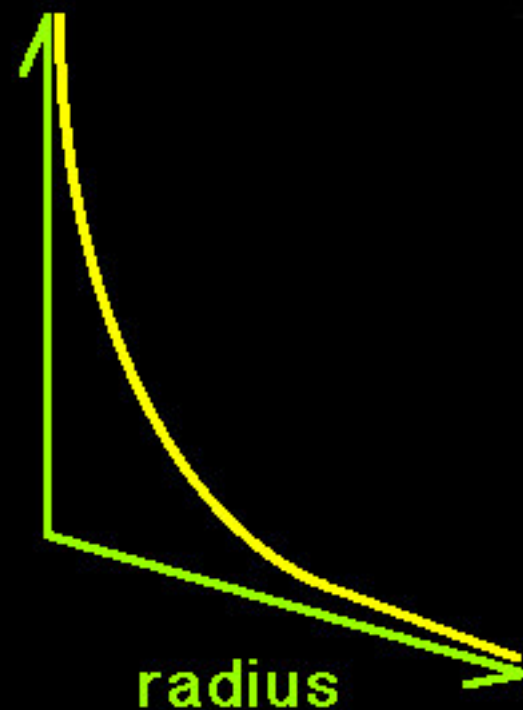


Probability Distribution 1s electron



Probability Distribution 1s electron

probability



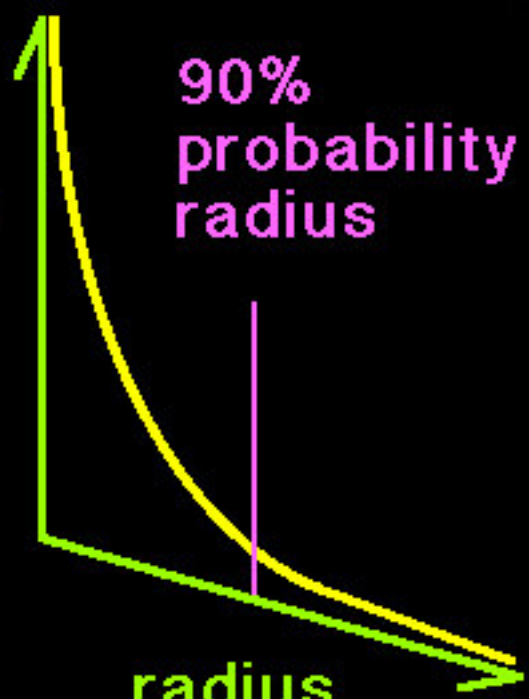
Probability Distribution

1s electron

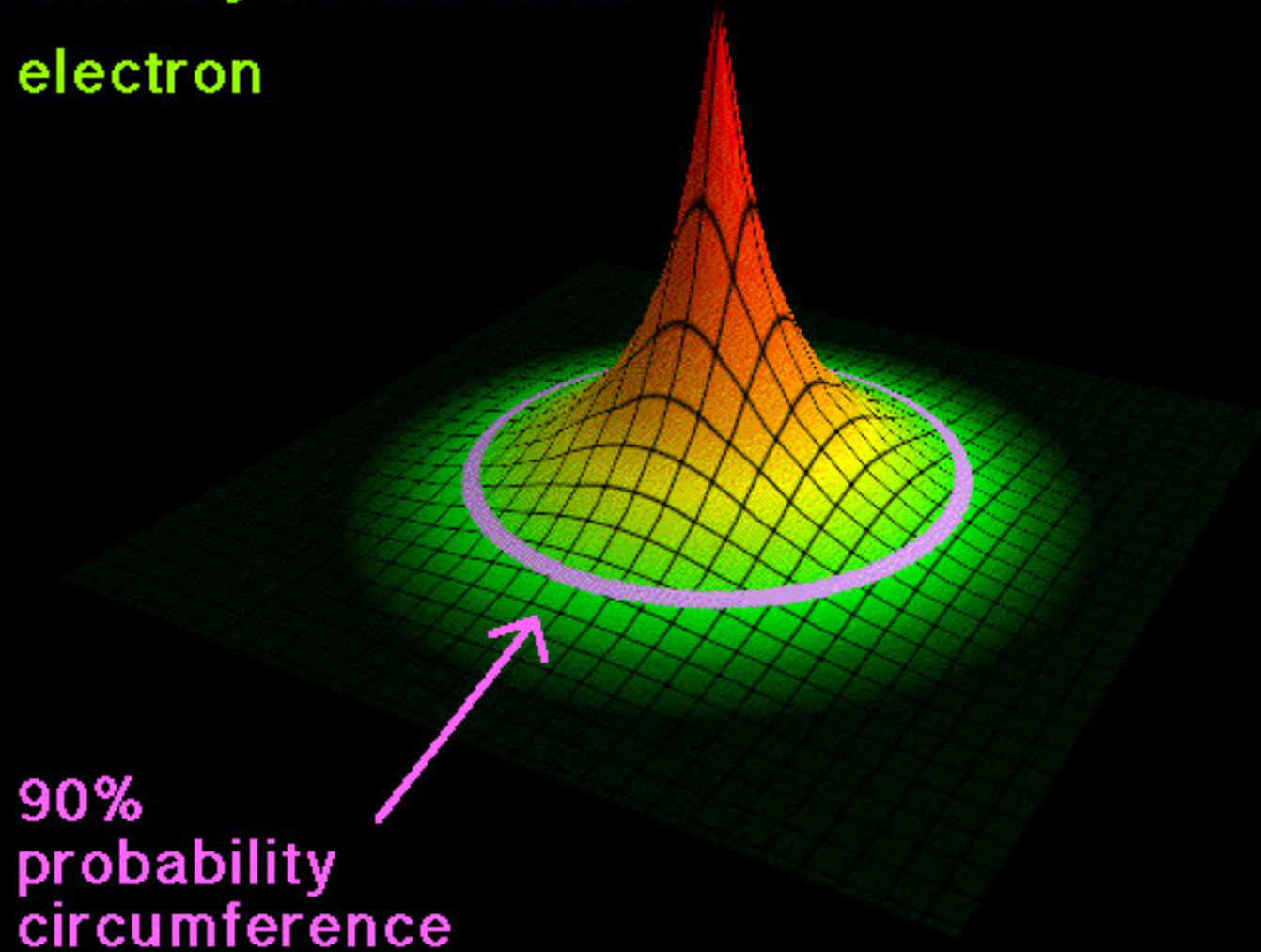
probability

90%
probability
radius

radius

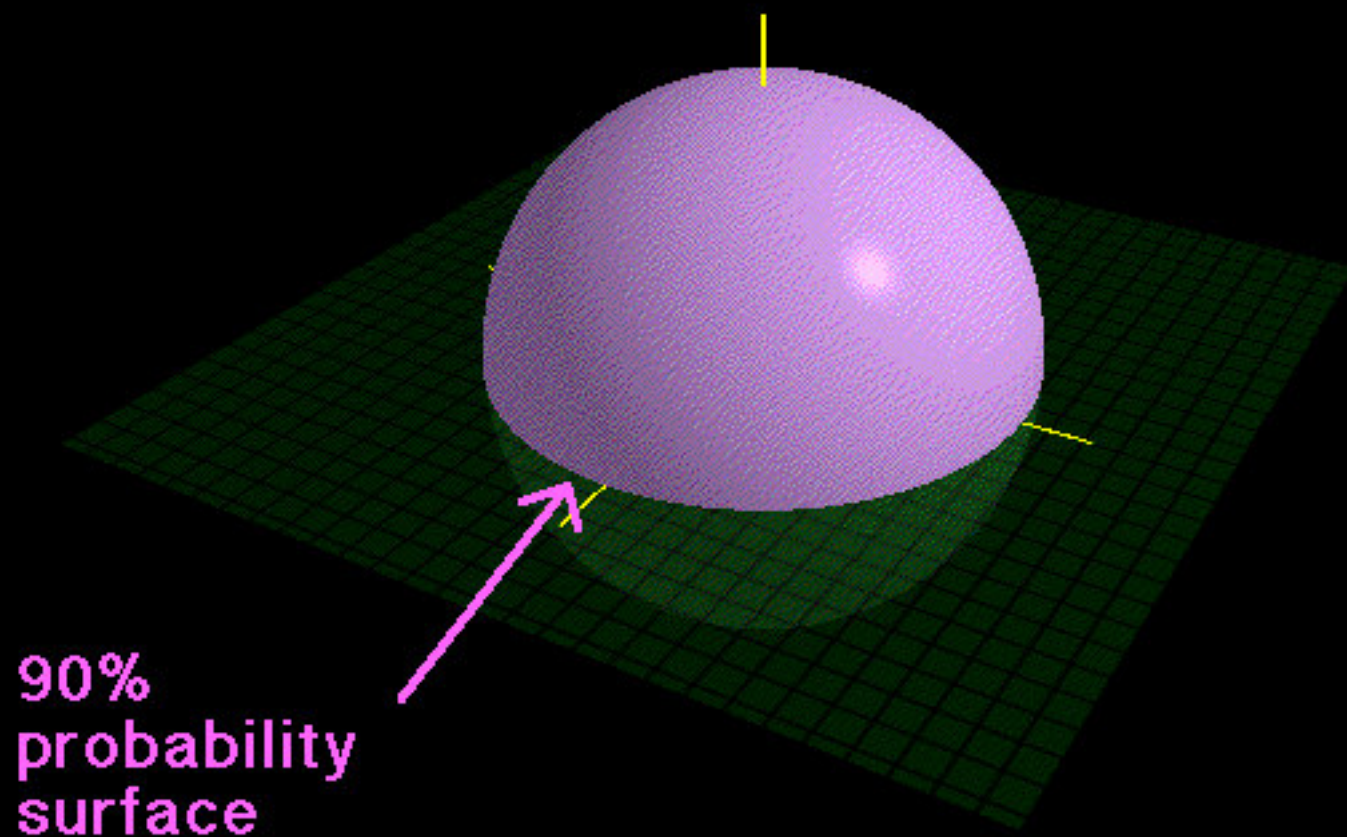


Probability Distribution 1s electron



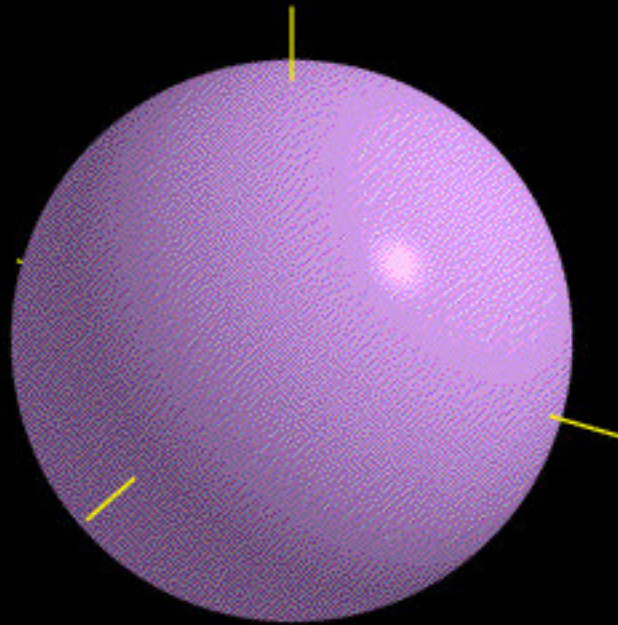
90%
probability
circumference

Probability Distribution 1s electron



Probability Distribution

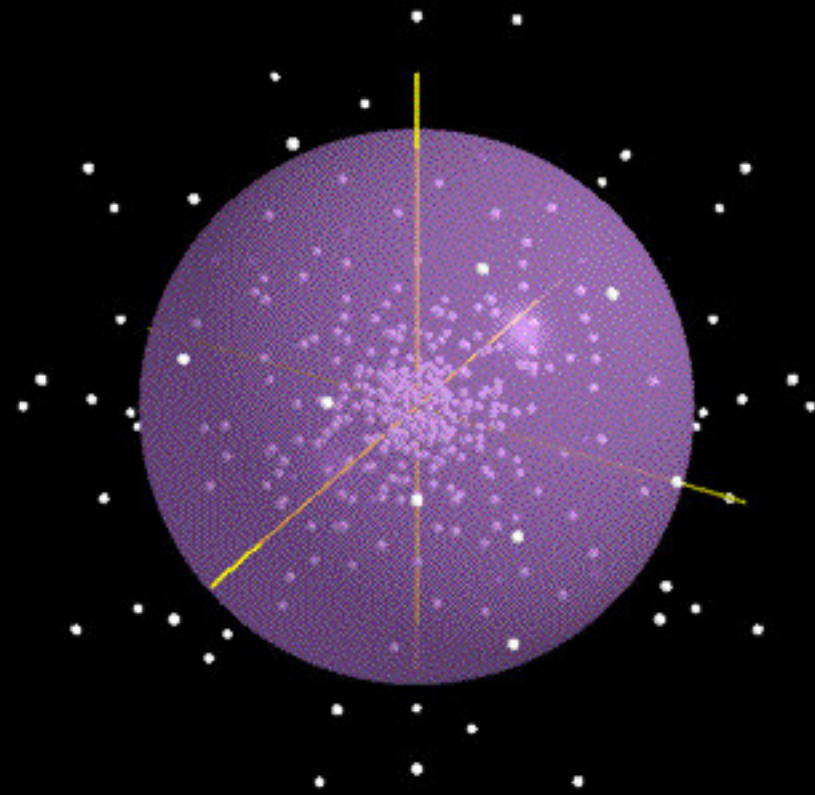
1s electron



orbital

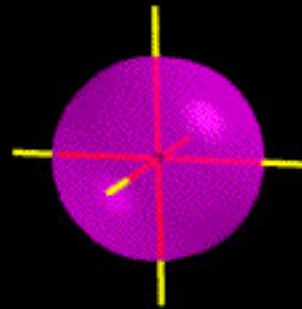
Probability Distribution

1s electron

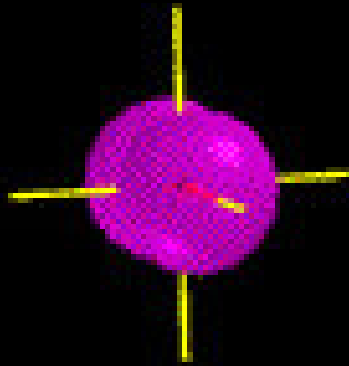


orbital

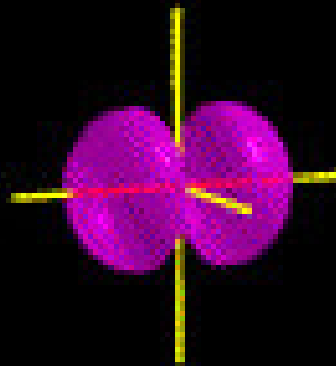
ORBITAIS MOLECULARES



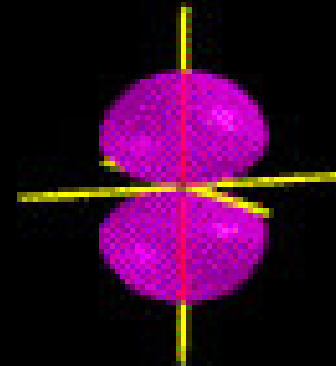
S



p_x

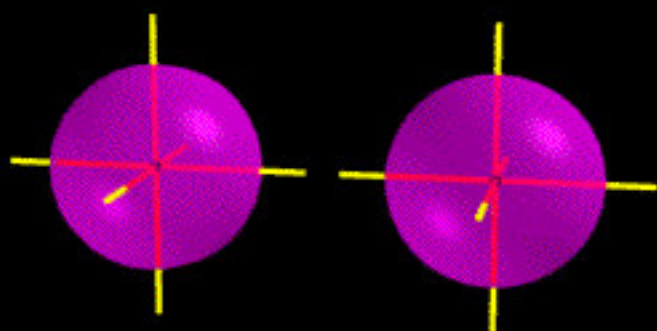


p_y



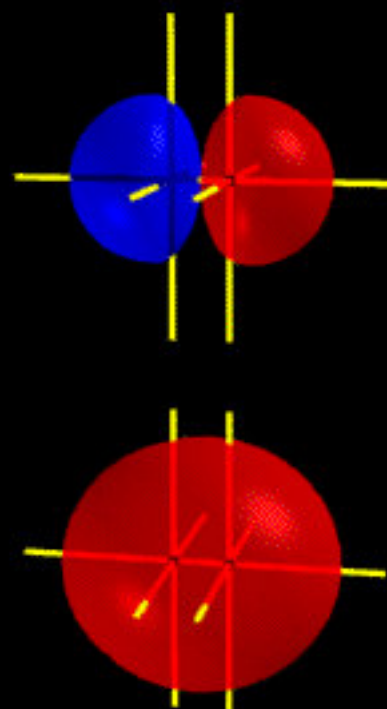
p_z

Molecular Orbitals s, s sigma orbitals



two atomic s orbitals \Rightarrow

E
↑



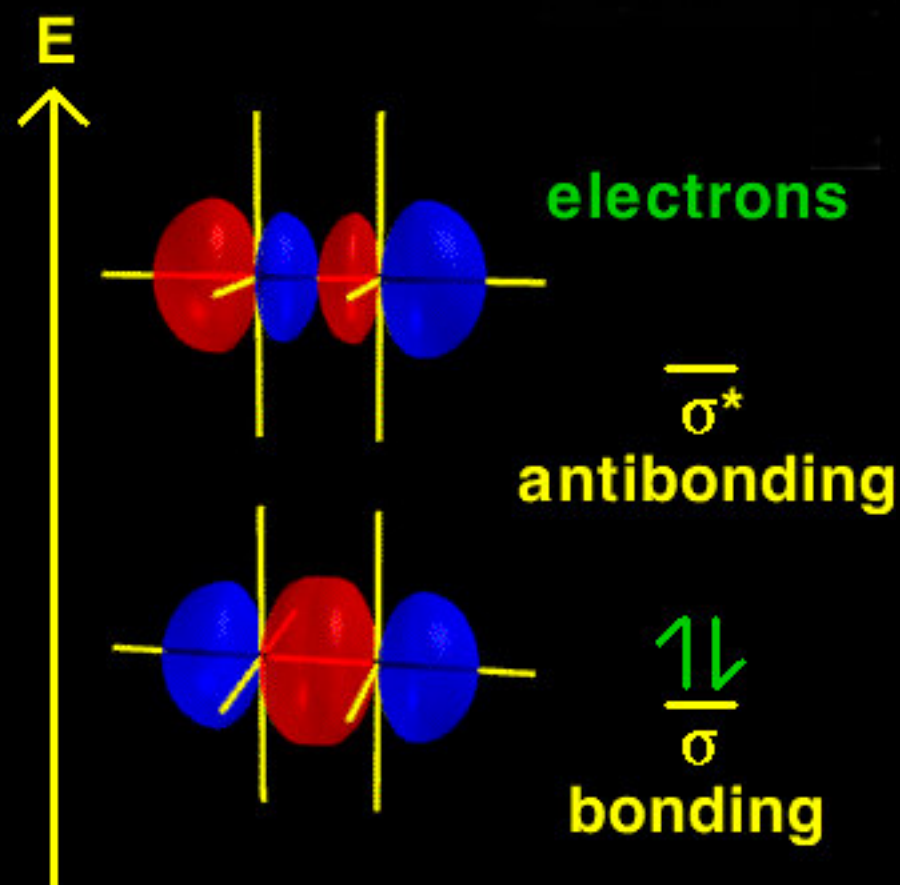
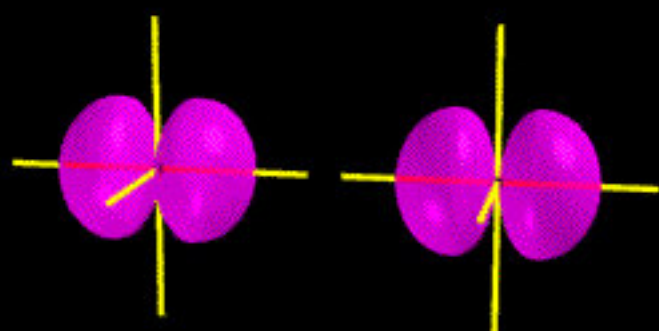
electrons

σ^*
antibonding

$\uparrow\downarrow$
 σ
bonding

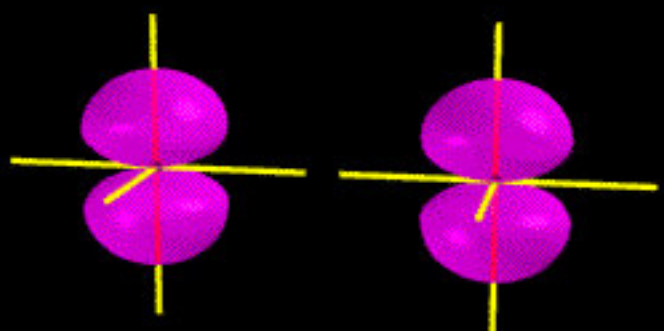
two molecular
sigma (σ) orbitals

Molecular Orbitals
p, p sigma orbitals



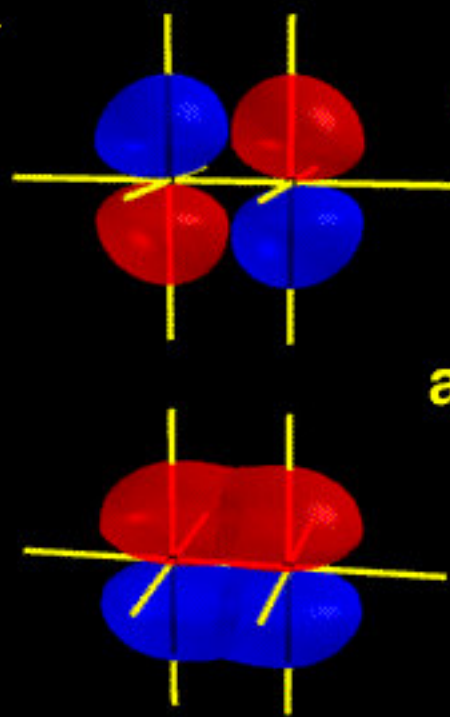
two atomic *p* orbitals \Rightarrow two molecular sigma (σ) orbitals

Molecular Orbitals
p, p pi orbitals



two atomic *p* orbitals \Rightarrow

E
↑



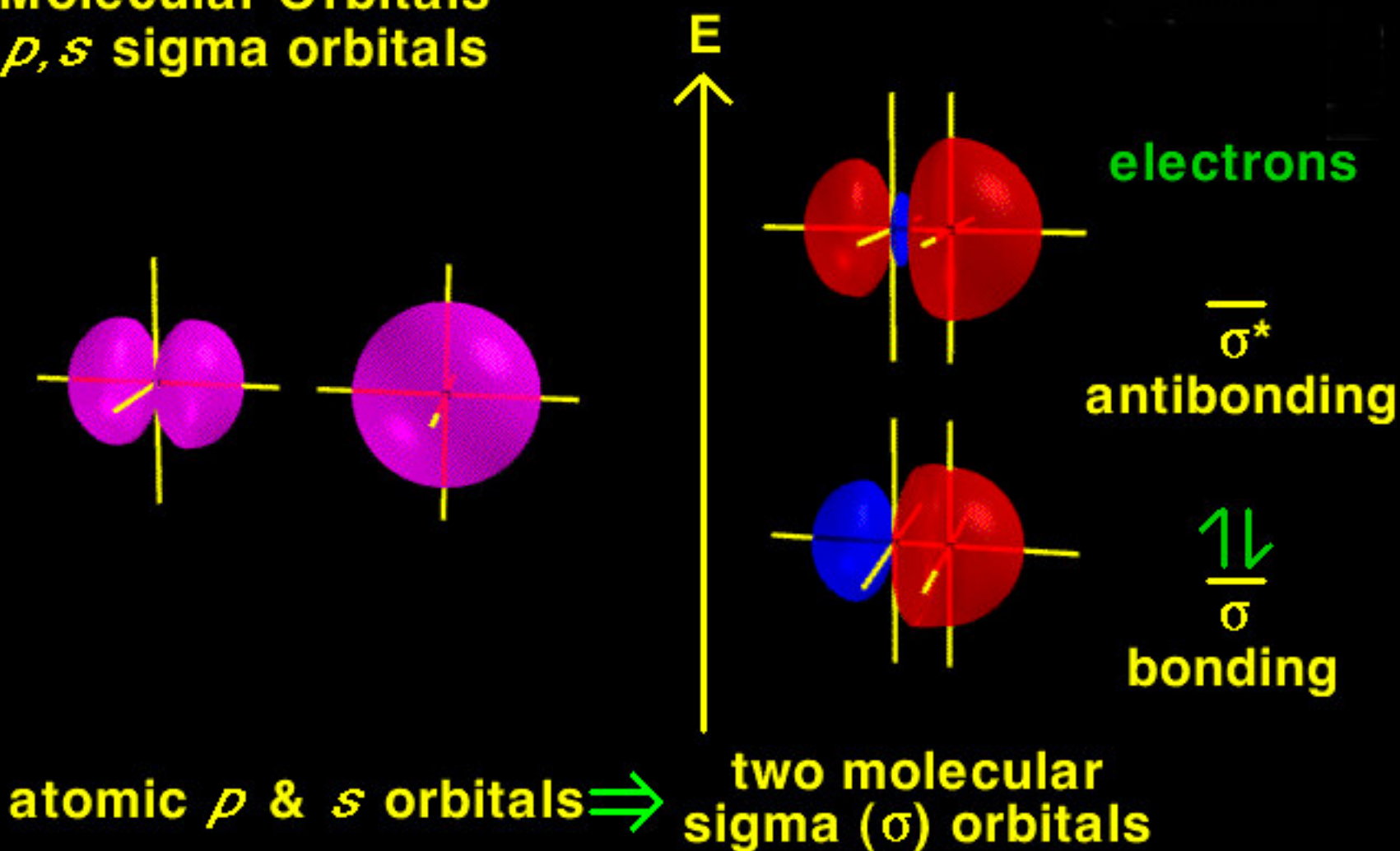
electrons

π^*
antibonding

$\uparrow\downarrow$
 π
bonding

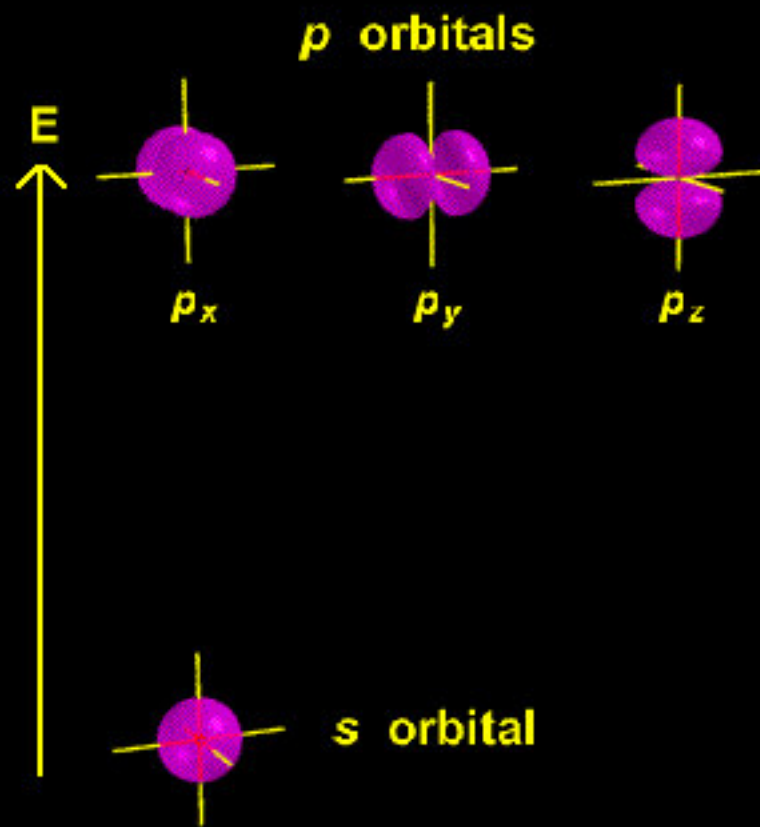
two molecular
pi (π) orbitals

Molecular Orbitals p, s sigma orbitals

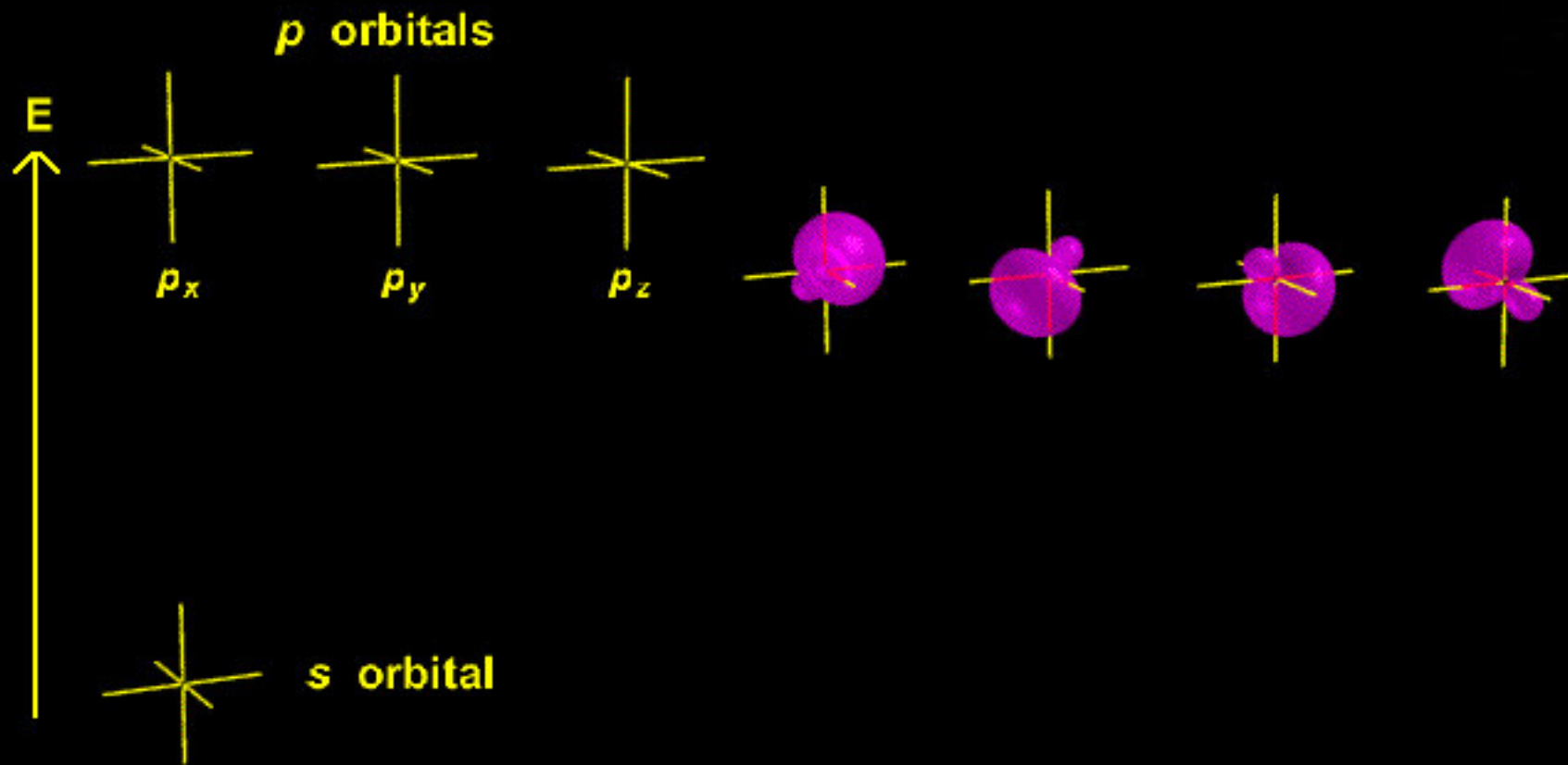


HIBRIDIZAÇÃO sp^3

sp^3 Hybridization



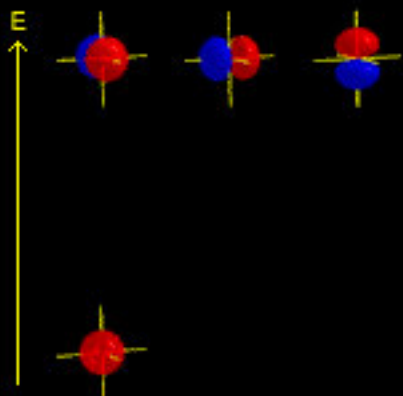
sp^3 Hybridization



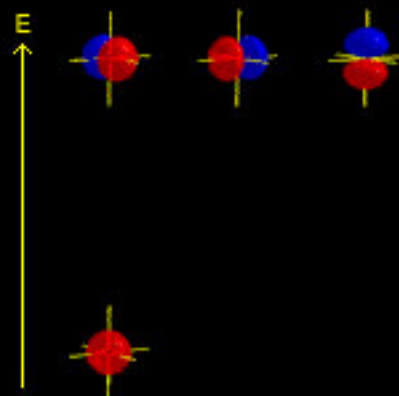
sp^3 Hybridization

four combinations

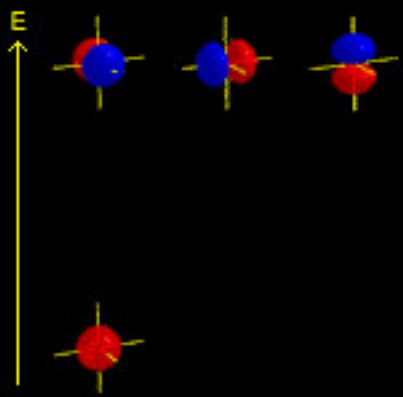
$$[(s) + (p_x) + (p_y) + (p_z)]/2$$



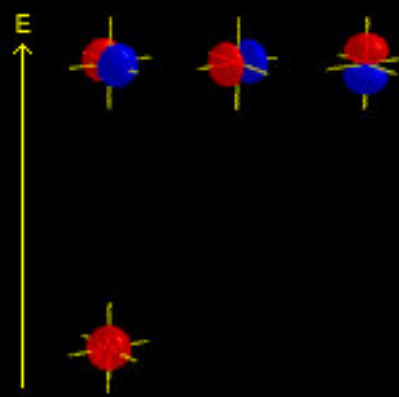
$$[(s) + (p_x) - (p_y) - (p_z)]/2$$



$$[(s) - (p_x) + (p_y) - (p_z)]/2$$



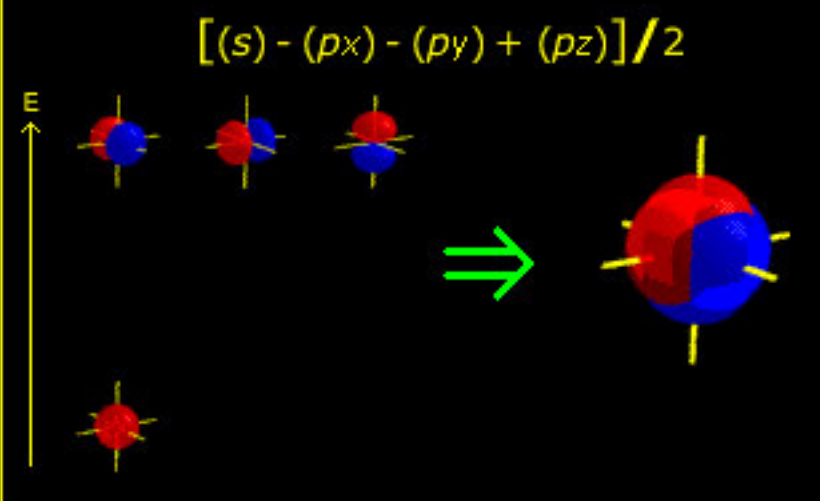
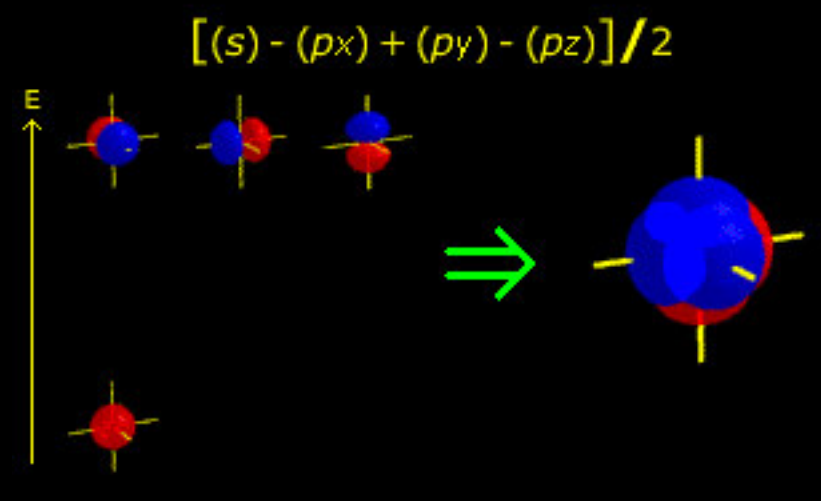
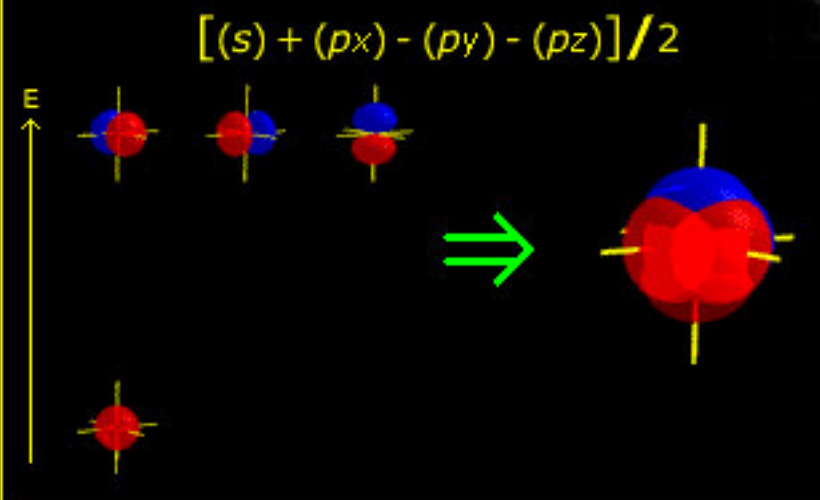
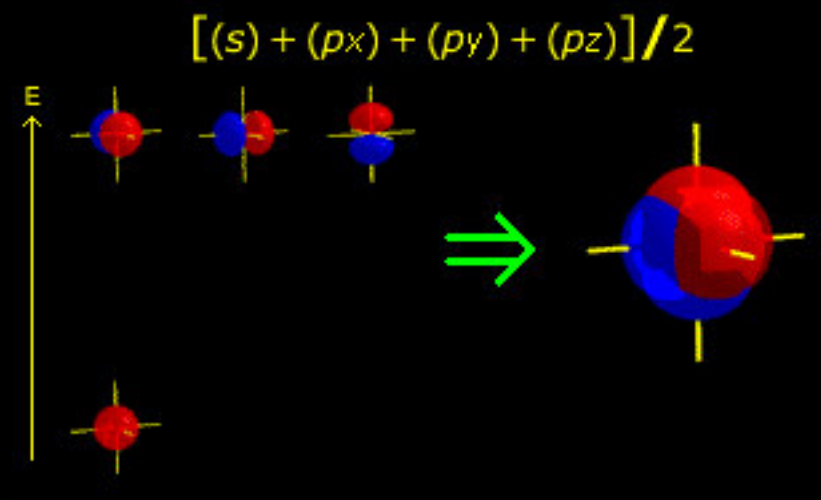
$$[(s) - (p_x) - (p_y) + (p_z)]/2$$



red and blue shows orbital phase

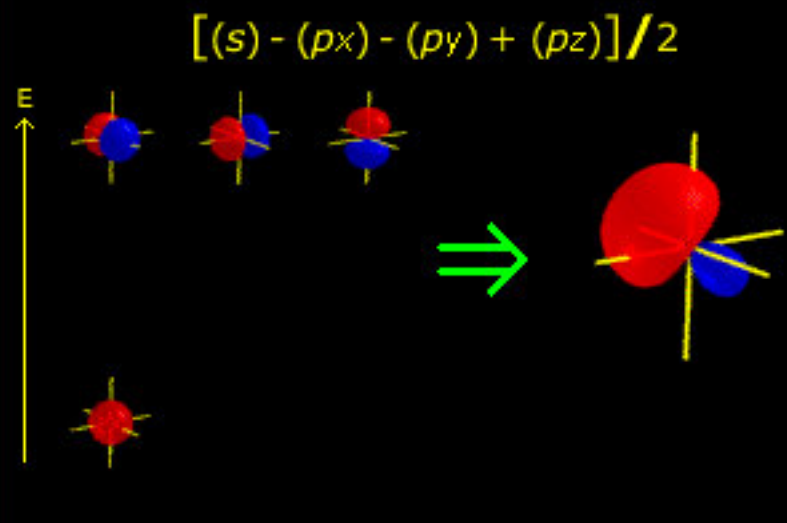
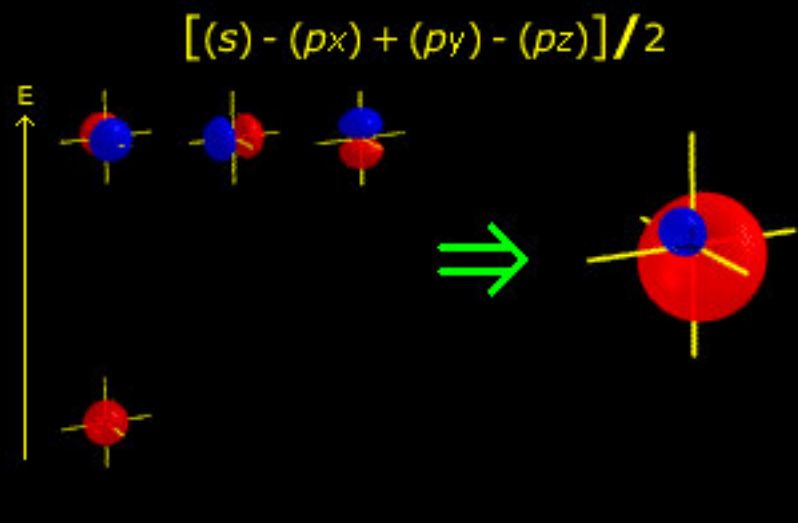
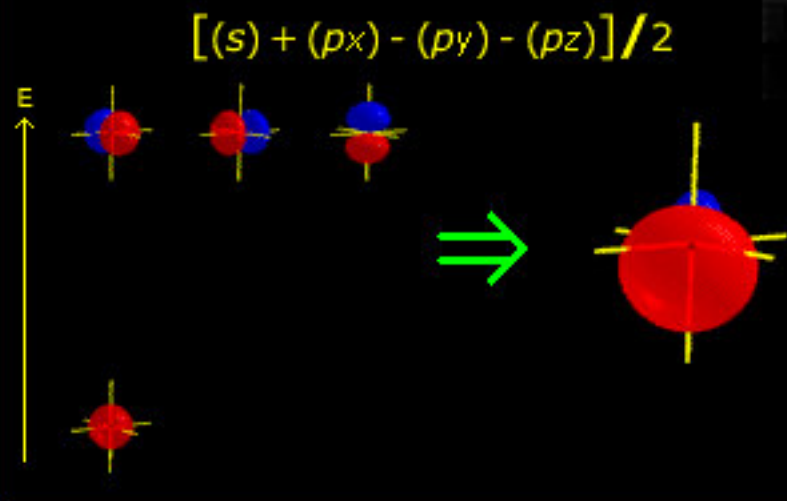
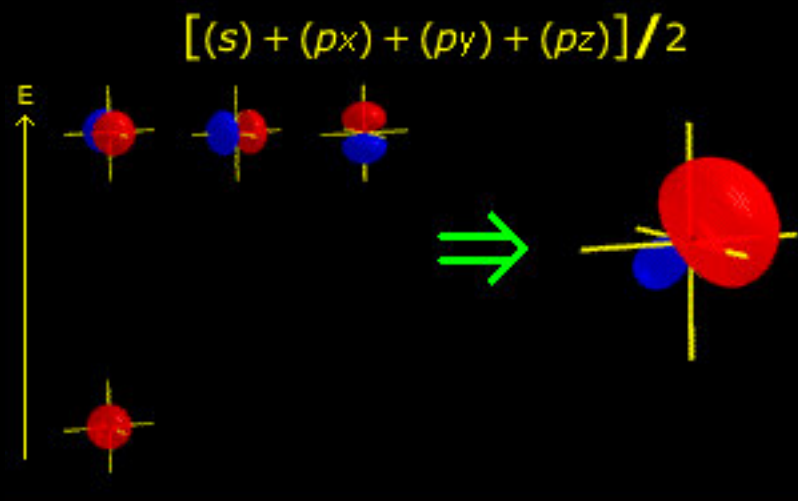
sp³ Hybridization

four combinations



sp^3 Hybridization

four sp^3 hybrids

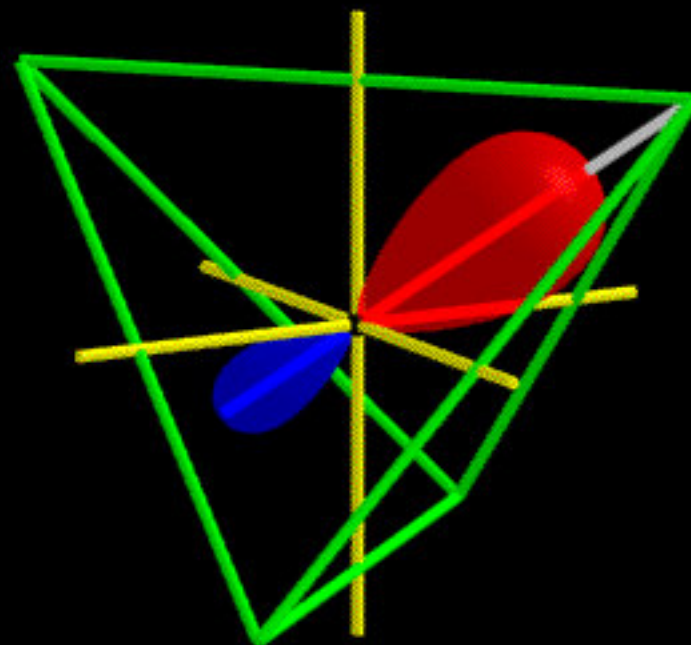
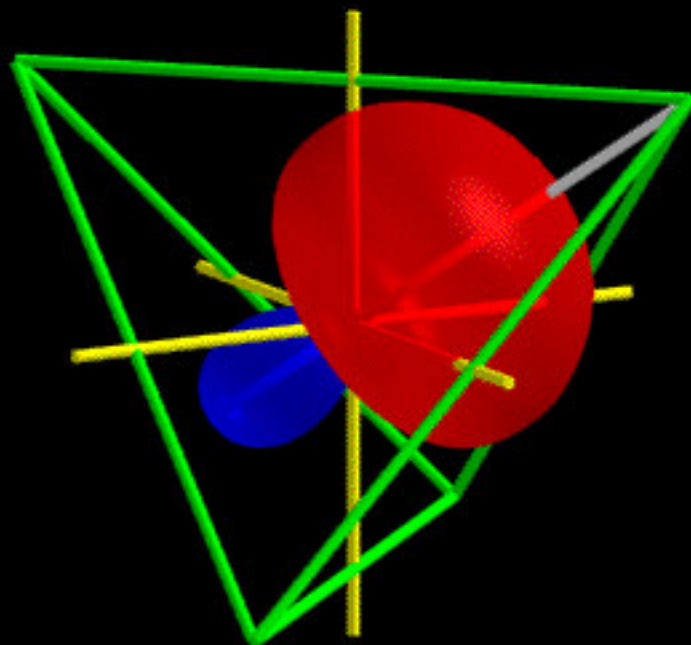


sp^3 Hybridization

accurate orbital shapes

schematic orbital shapes

one sp^3 hybrid



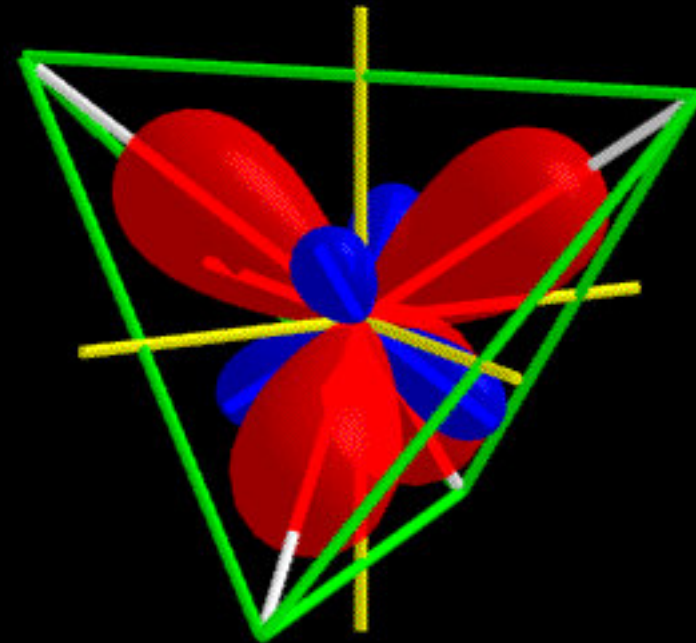
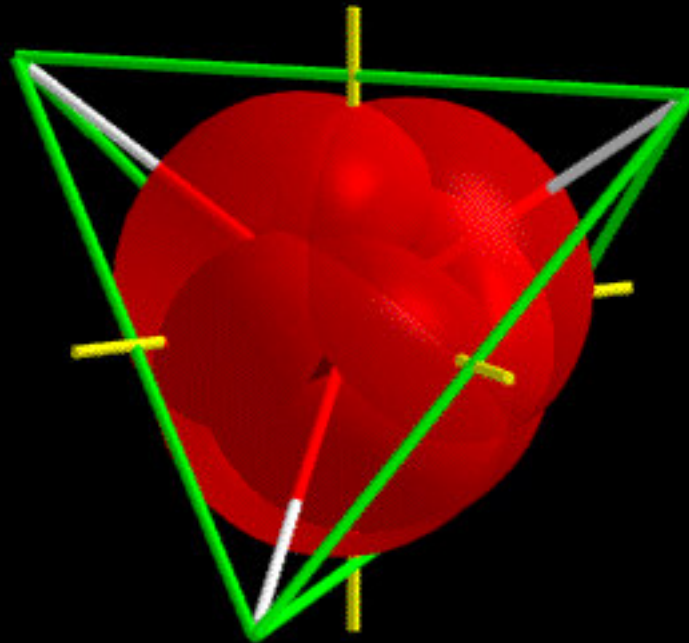
tetrahedral
 sp^3 hybridized atom

sp^3 Hybridization

accurate orbital shapes

schematic orbital shapes

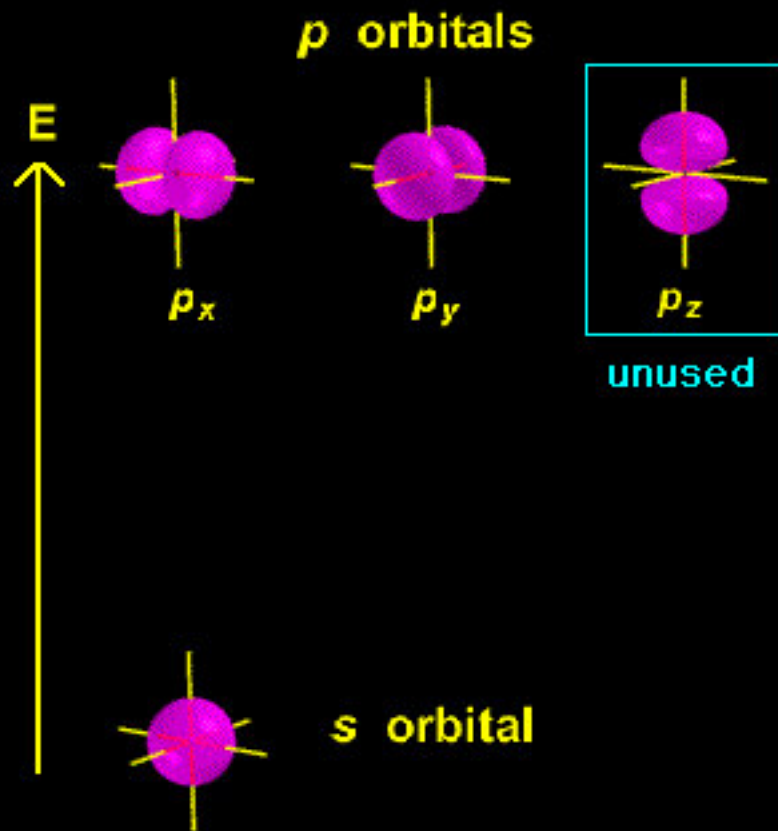
all sp^3 hybrids



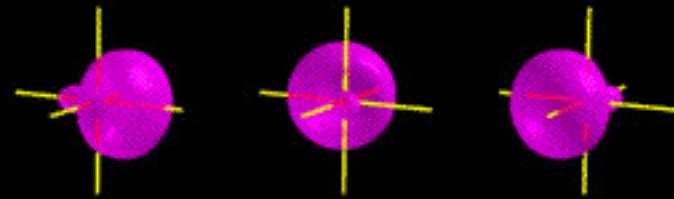
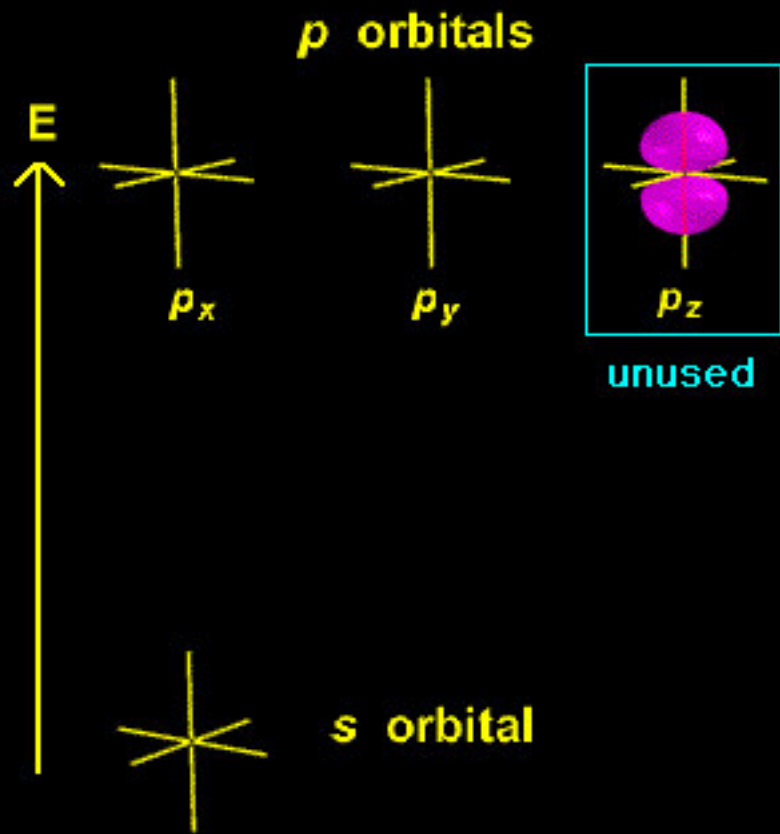
tetrahedral
 sp^3 hybridized atom

HIBRIDIZAÇÃO sp^2

sp^2 Hybridization



sp^2 Hybridization



11

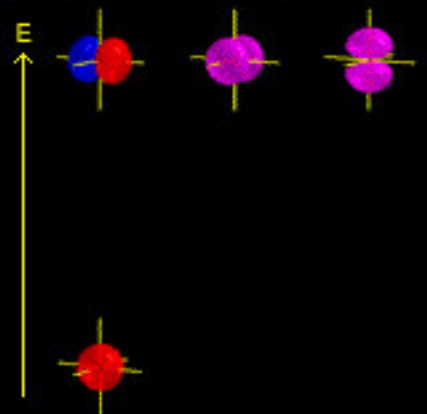
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13

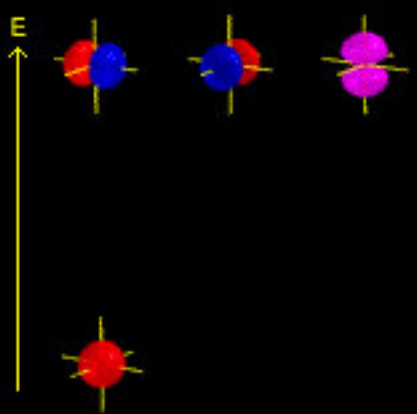
sp² Hybridization

three combinations

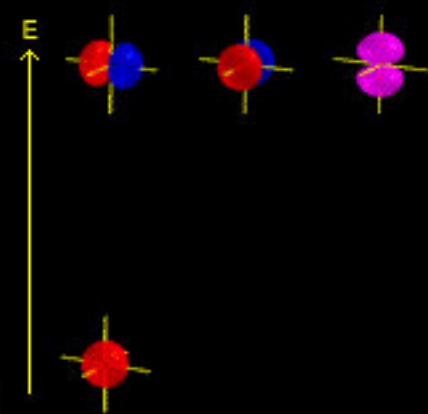
$$[(s) + \sqrt{2}(p_x)] / \sqrt{3}$$



$$[\sqrt{2}(s) - (p_x) + \sqrt{3}(p_y)] / \sqrt{6}$$



$$[\sqrt{2}(s) - (p_x) - \sqrt{3}(p_y)] / \sqrt{6}$$

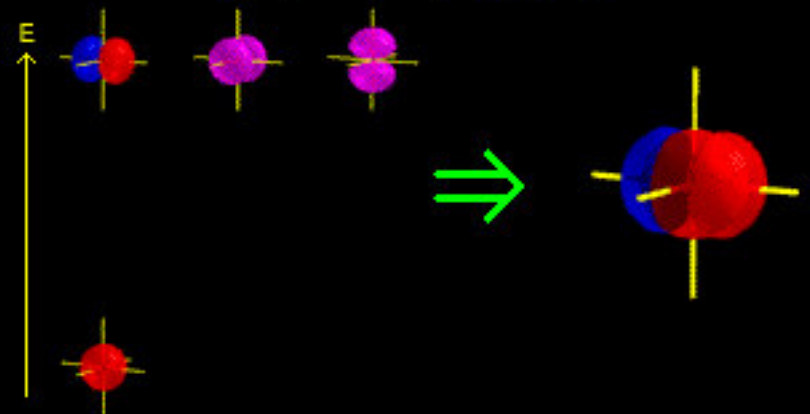


red and blue shows orbital phase

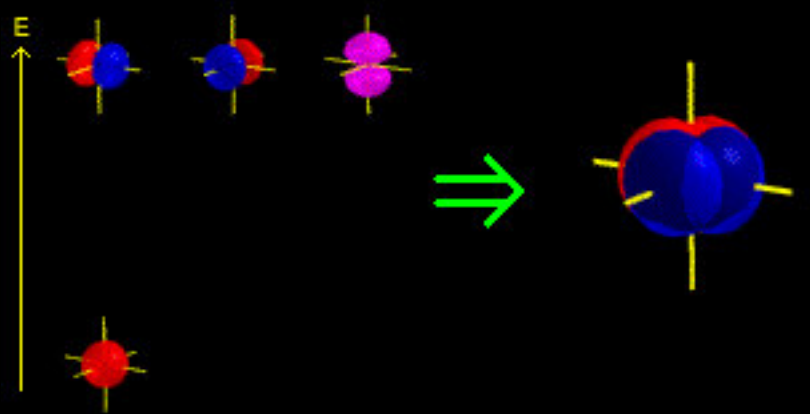
sp² Hybridization

three combinations

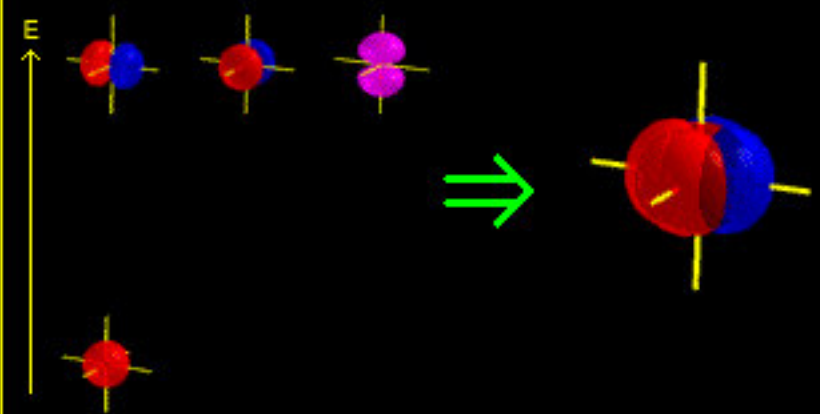
$$[(s) + \sqrt{2}(p_x)] / \sqrt{3}$$



$$[\sqrt{2}(s) - (p_x) + \sqrt{3}(p_y)] / \sqrt{6}$$



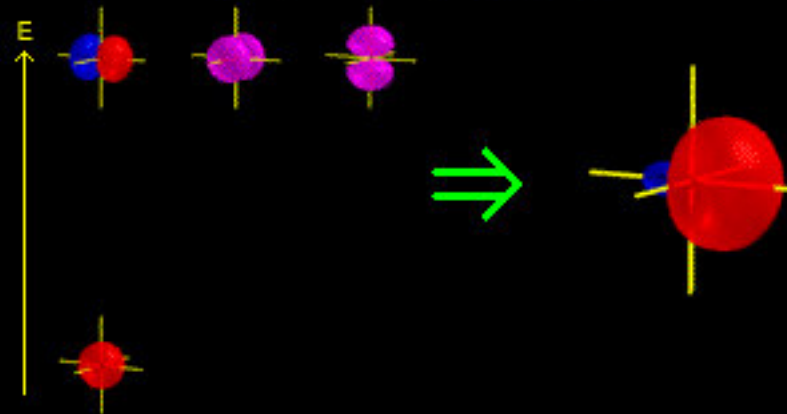
$$[\sqrt{2}(s) - (p_x) - \sqrt{3}(p_y)] / \sqrt{6}$$



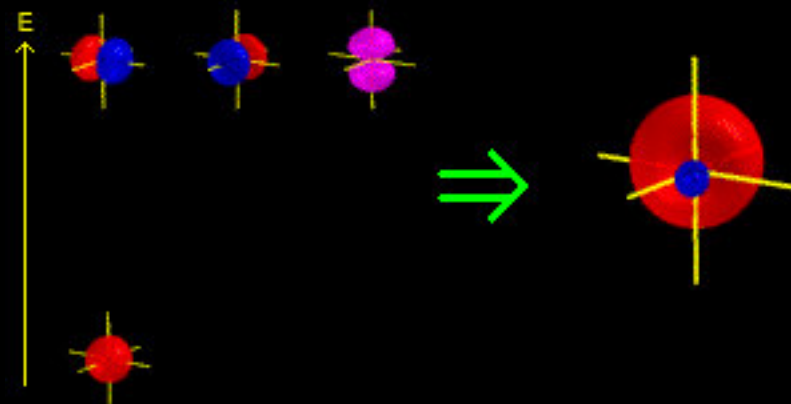
sp^2 Hybridization

three sp^2 hybrids

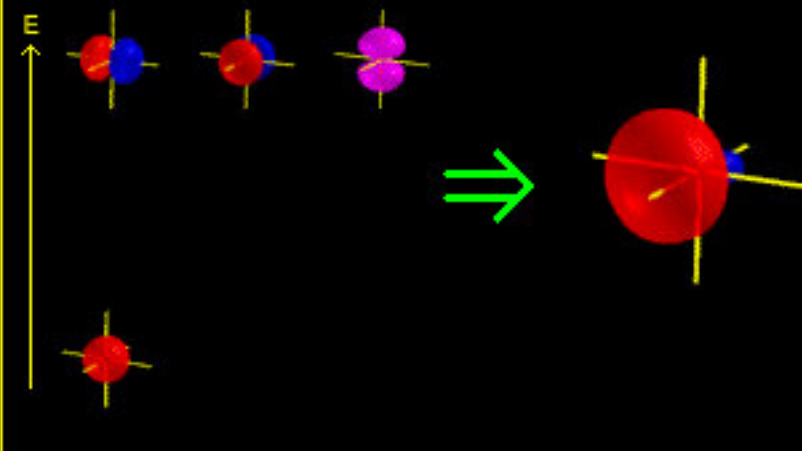
$$[(s) + \sqrt{2}(p_x)] / \sqrt{3}$$



$$[\sqrt{2}(s) - (p_x) + \sqrt{3}(p_y)] / \sqrt{6}$$



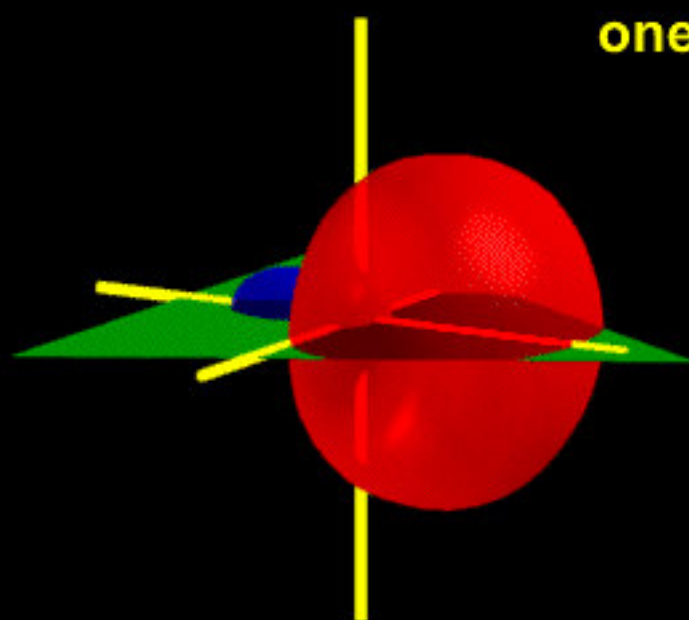
$$[\sqrt{2}(s) - (p_x) - \sqrt{3}(p_y)] / \sqrt{6}$$



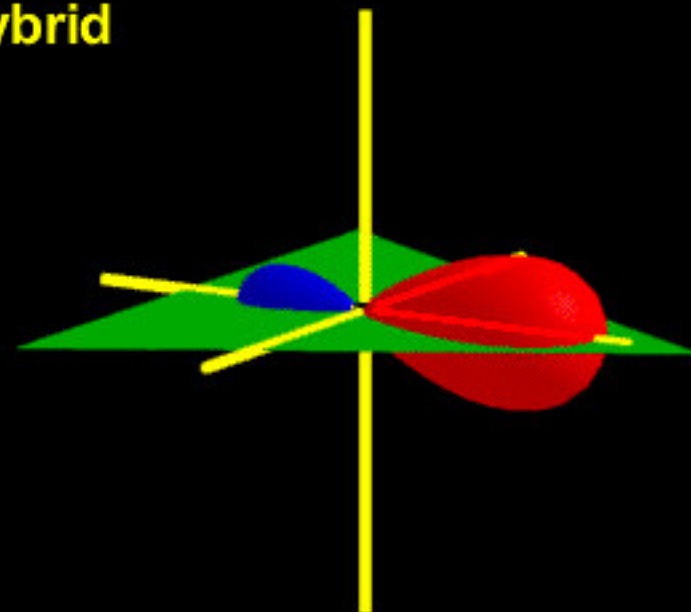
sp^2 Hybridization

accurate orbital shapes

schematic orbital shapes



one sp^2 hybrid



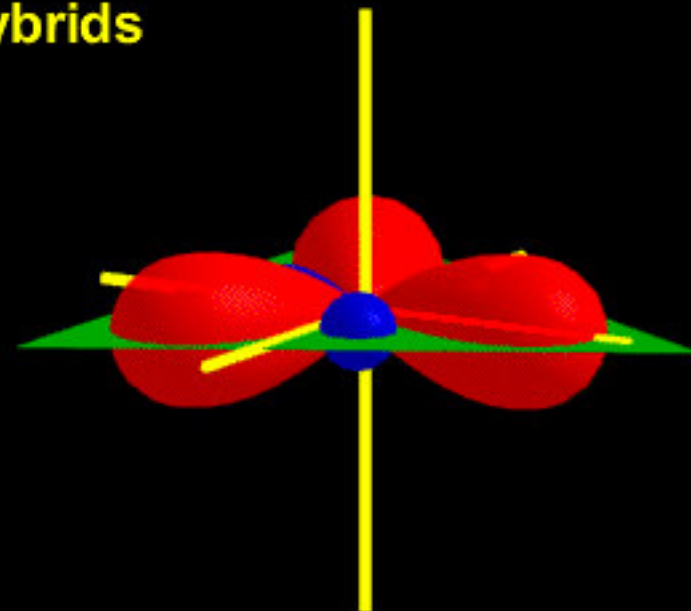
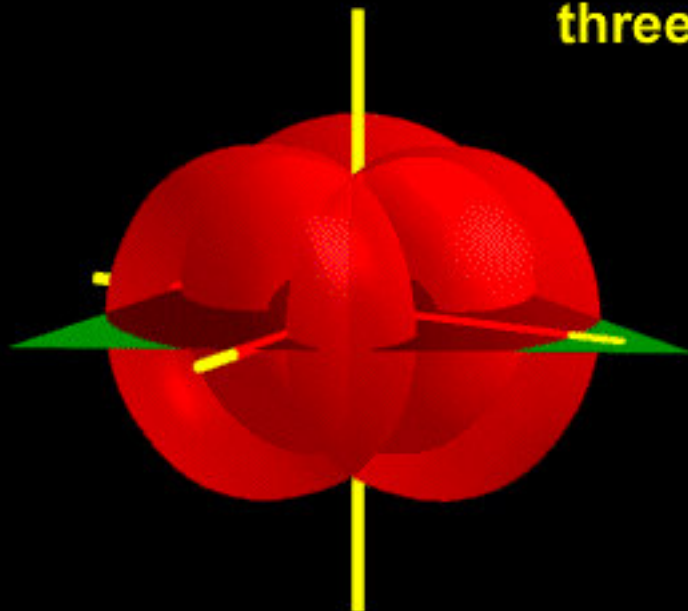
planar trigonal
 sp^2 hybridized atom

sp^2 Hybridization

accurate orbital shapes

schematic orbital shapes

three sp^2 hybrids



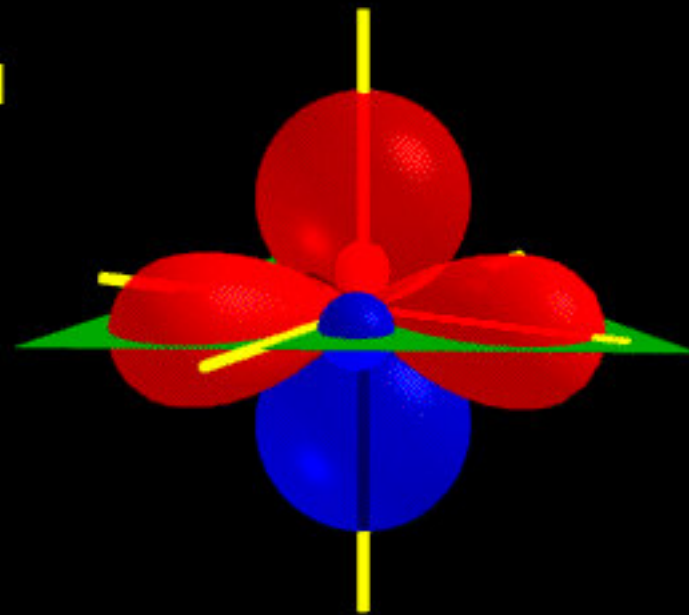
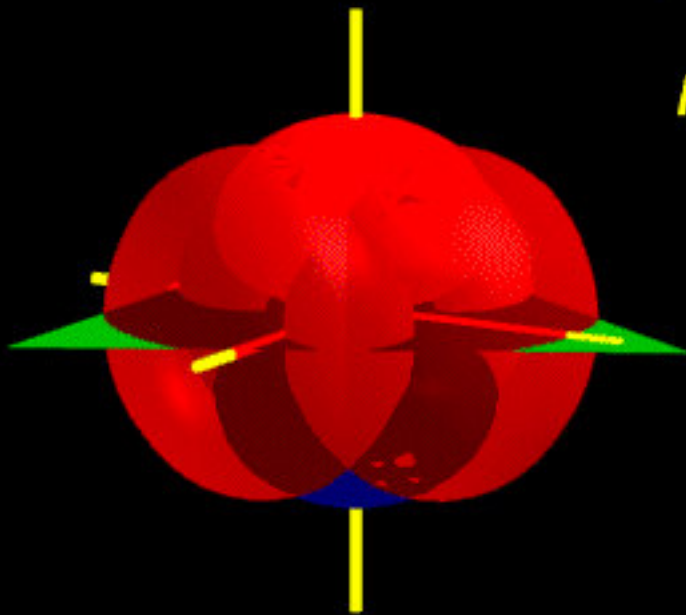
planar trigonal
 sp^2 hybridized atom

sp^2 Hybridization

accurate orbital shapes

schematic orbital shapes

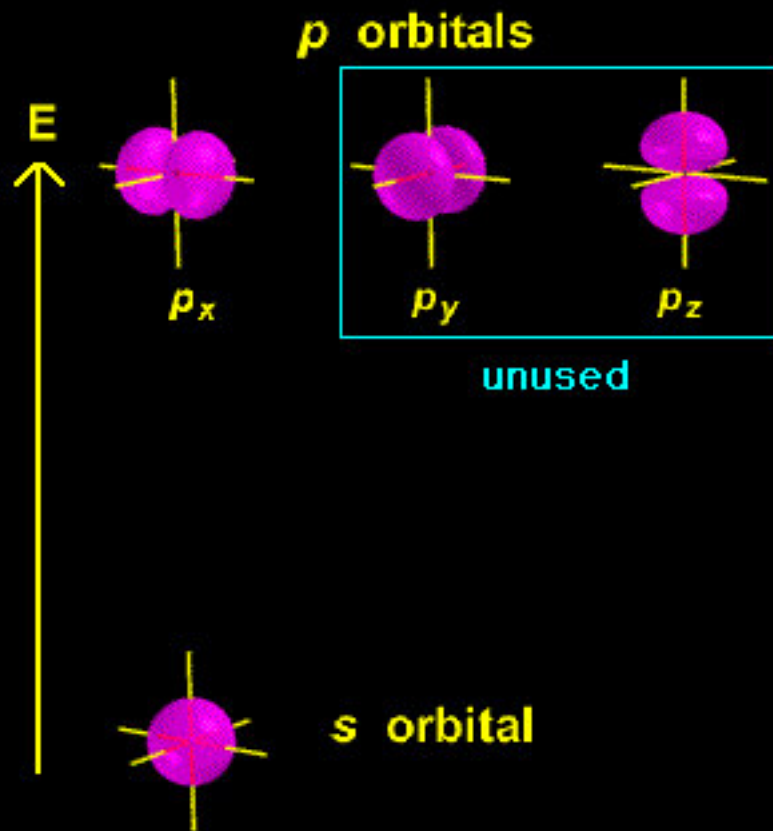
sp^2 hybrids
+
 p orbital



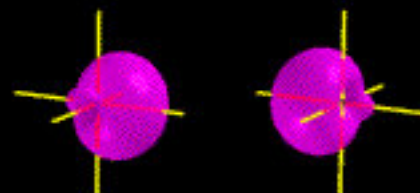
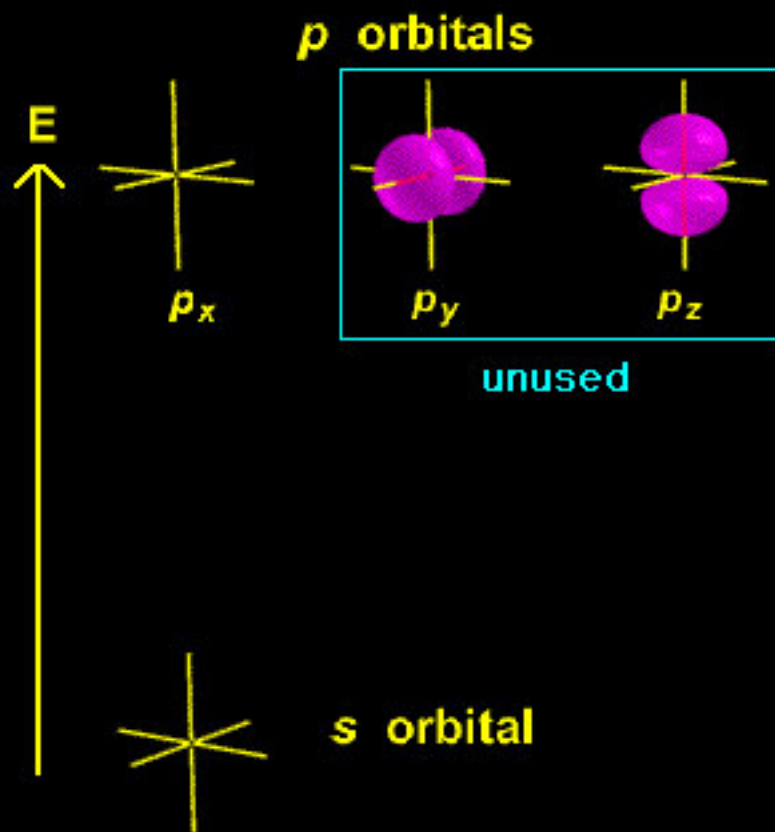
planar trigonal
 sp^2 hybridized atom

HIBRIDIZAÇÃO sp

sp Hybridization



sp Hybridization

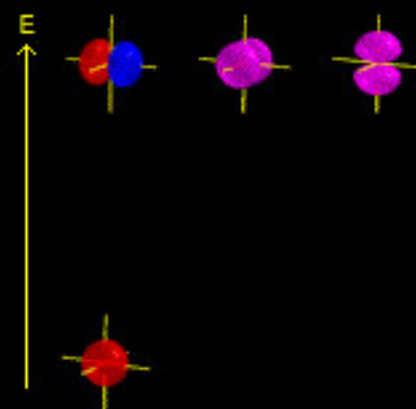
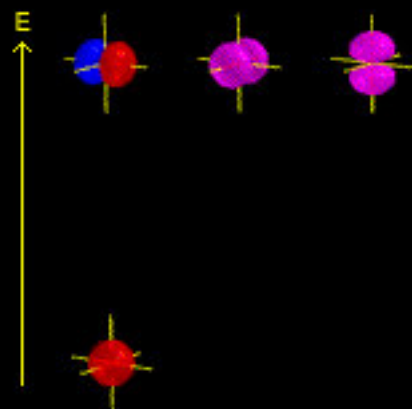


sp Hybridization

two combinations

$$[(s) + (p_x)] / \sqrt{2}$$

$$[(s) - (p_x)] / \sqrt{2}$$



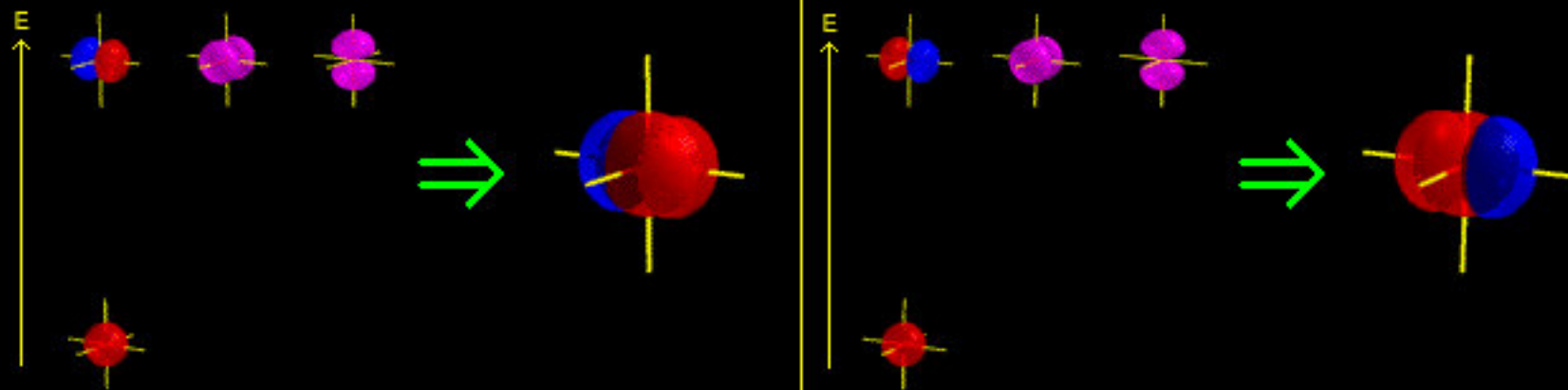
red and blue
shows orbital phase

sp Hybridization

two combinations

$$[(s) + (p_x)] / \sqrt{2}$$

$$[(s) - (p_x)] / \sqrt{2}$$



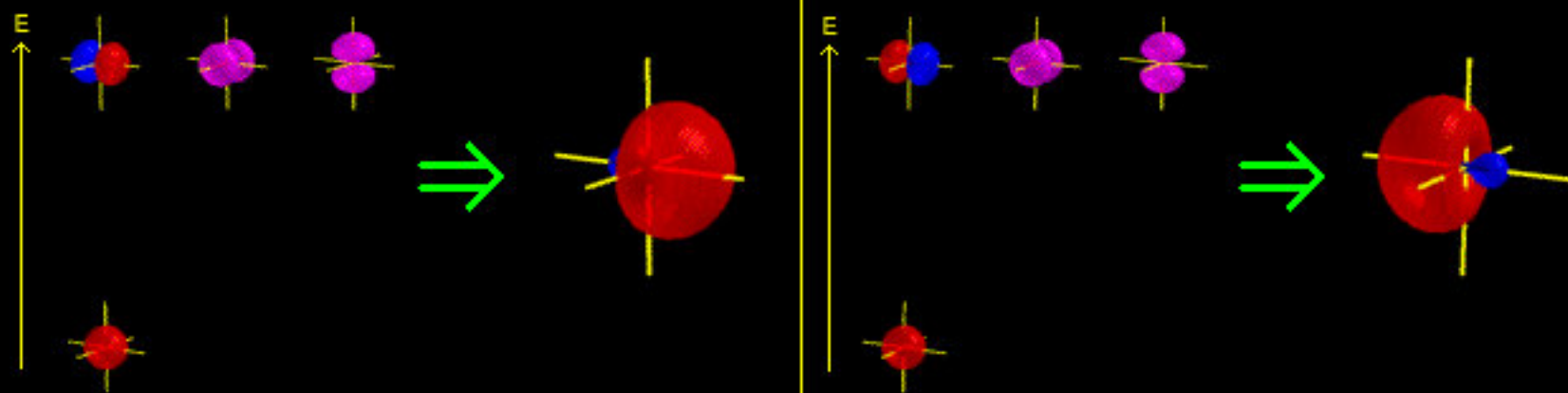
red and blue
shows orbital phase

sp Hybridization

two *sp* hybrids

$$[(s) + (p_x)] / \sqrt{2}$$

$$[(s) - (p_x)] / \sqrt{2}$$



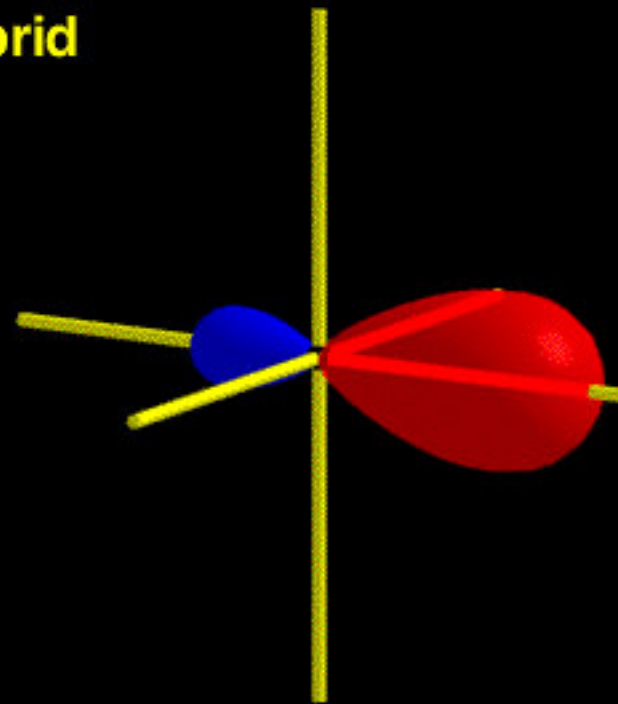
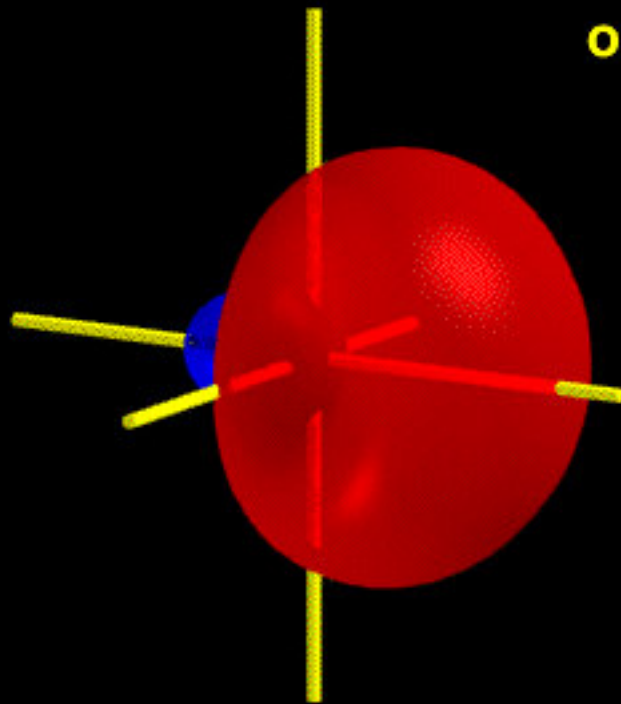
red and blue
shows orbital phase

sp Hybridization

accurate orbital shapes

schematic orbital shapes

one *sp* hybrid



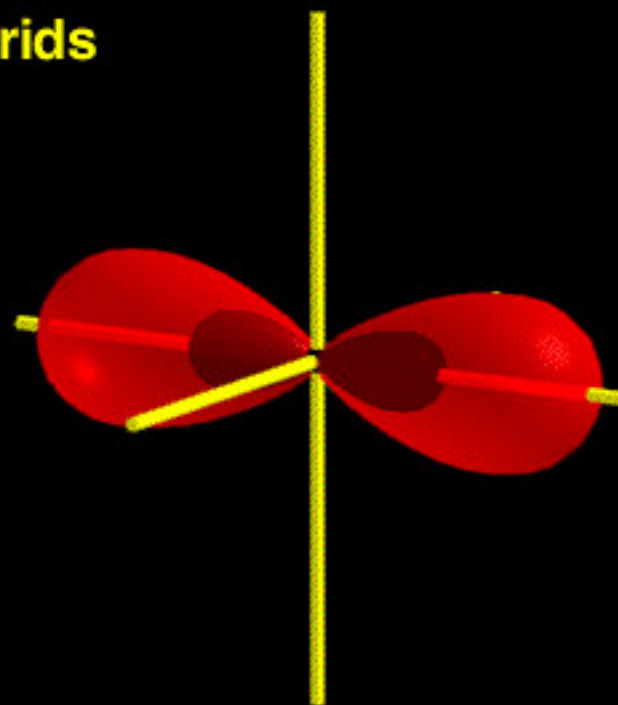
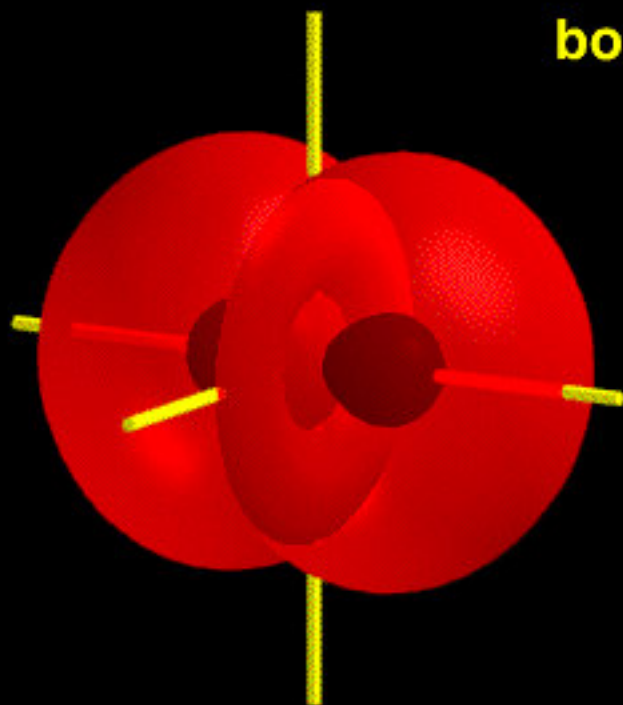
linear *sp* hybridized atom

sp Hybridization

accurate orbital shapes

schematic orbital shapes

both *sp* hybrids



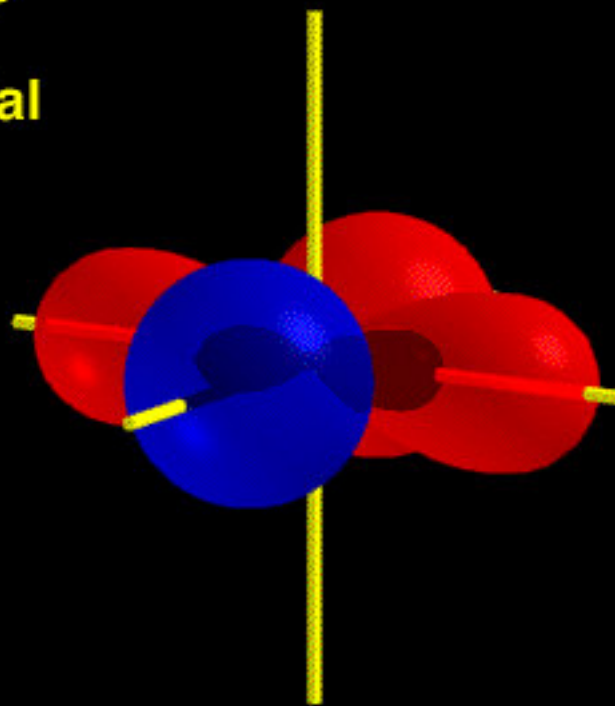
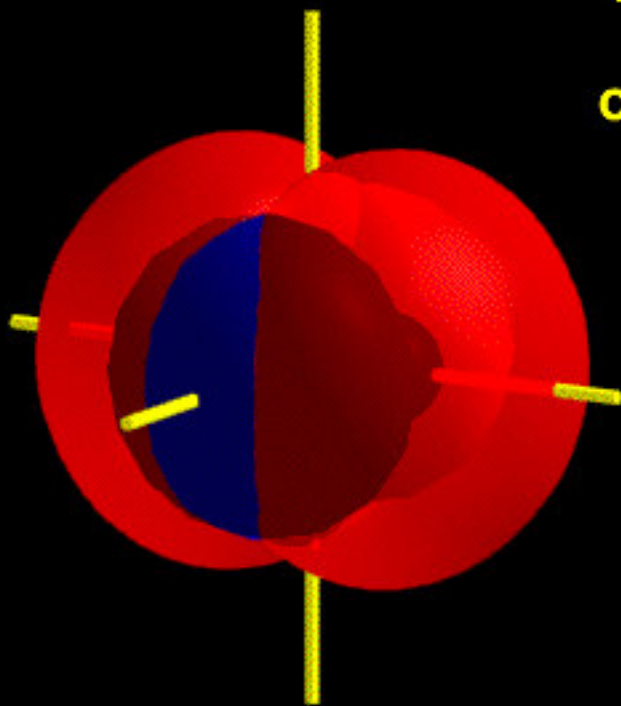
linear *sp* hybridized atom

sp Hybridization

accurate orbital shapes

schematic orbital shapes

sp hybrids
+
one *p* orbital



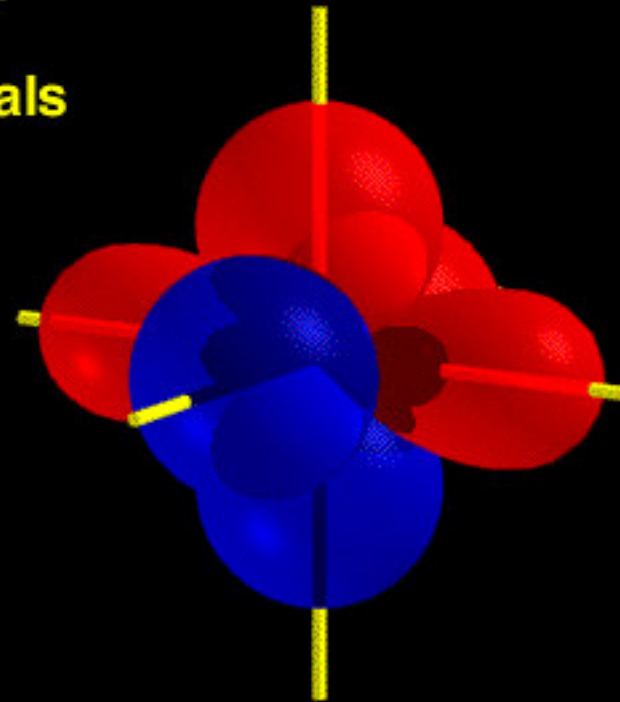
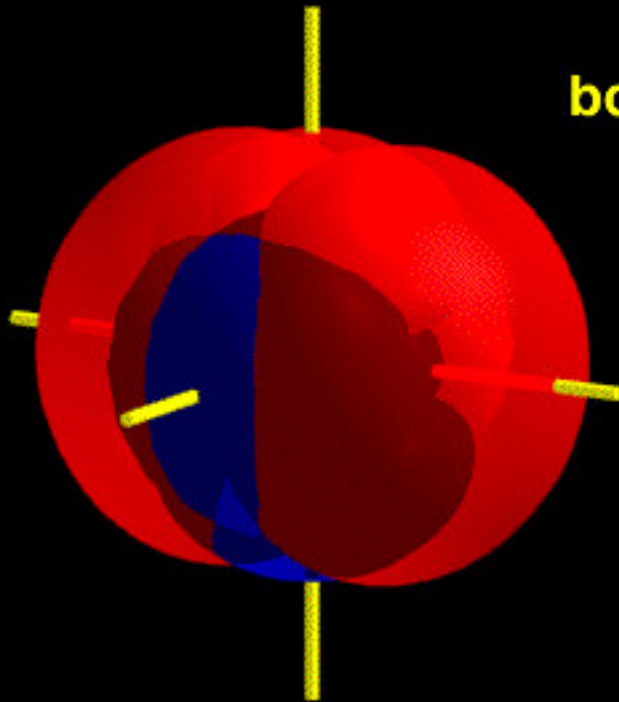
linear *sp* hybridized atom

sp Hybridization

accurate orbital shapes

schematic orbital shapes

sp hybrids
+
both *p* orbitals



linear *sp* hybridized atom