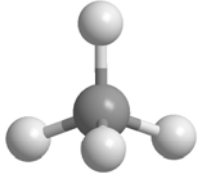


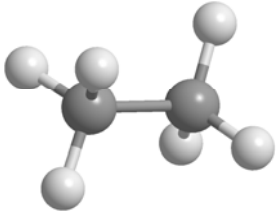
# HIDROCARBONETOS

**Alcanos:**  $C_nH_{(2n+2)}$

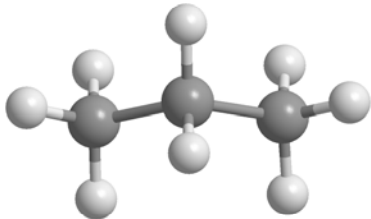
Metano:  $CH_4$



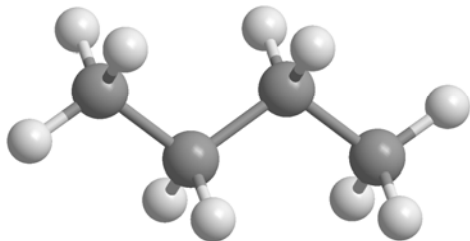
Etano:  $C_2H_6$



Propano:  $C_3H_8$

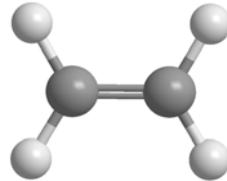


Butano:  $C_4H_{10}$

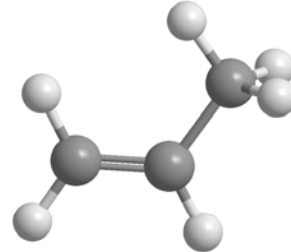


**Alcenos:**  $C_nH_{2n}$

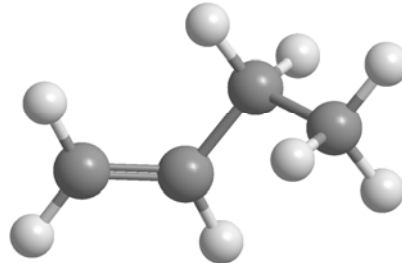
Eteno:  $C_2H_4$



Propeno:  $C_3H_6$

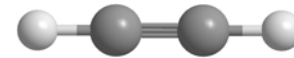


1-Buteno:  $C_4H_8$

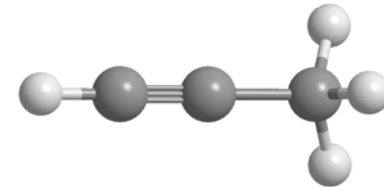


**Alcinos:**  $C_nH_{(2n-2)}$

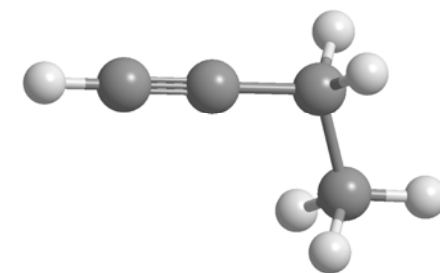
Etino:  $C_2H_2$



Propino:  $C_3H_4$

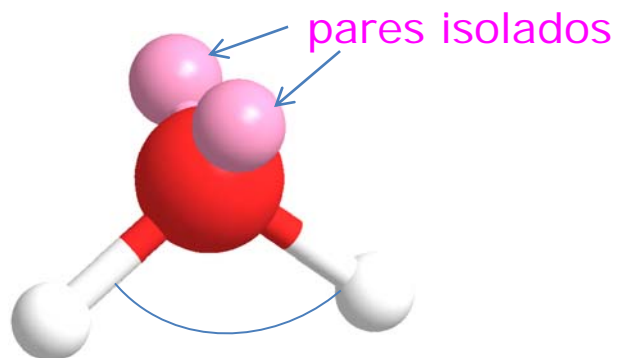


1-Butino:  $C_4H_6$



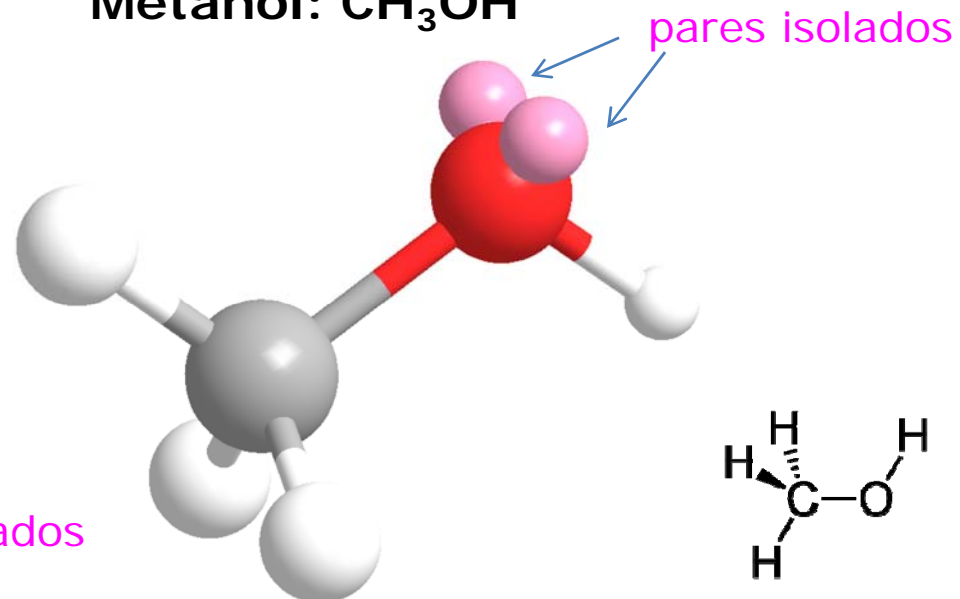
Oxigênio em hibridação  $sp_3$ :  $1s^2 2sp_3^2 2sp_3^2 2sp_3^1 2sp_3^1$

$H_2O$



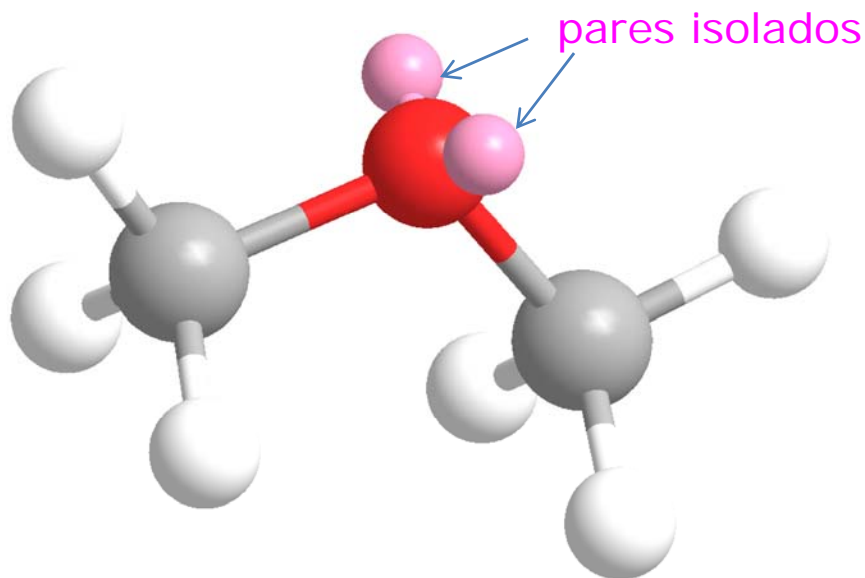
Álcoois:  $R_3C-OH$

Metanol:  $CH_3OH$



Éteres:  $R_3C-O-CR_3$

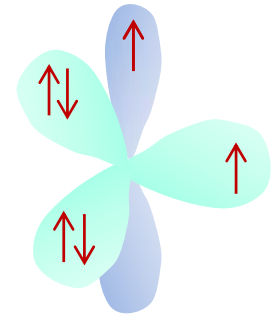
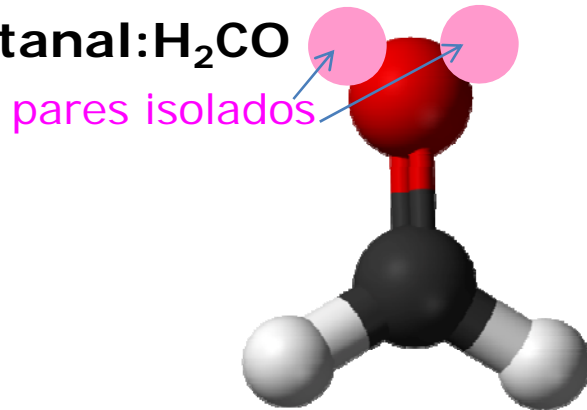
Dimetiléter:  $CH_3OCH_3$



Oxigênio em hibridação  $sp_2$ :  $1s^2 2sp_2^2 2sp_2^2 2sp_2^1 2p_z^1$

*Aldeídos:  $R_2C-HO$*

Formaldeído  
ou metanal:  $H_2CO$

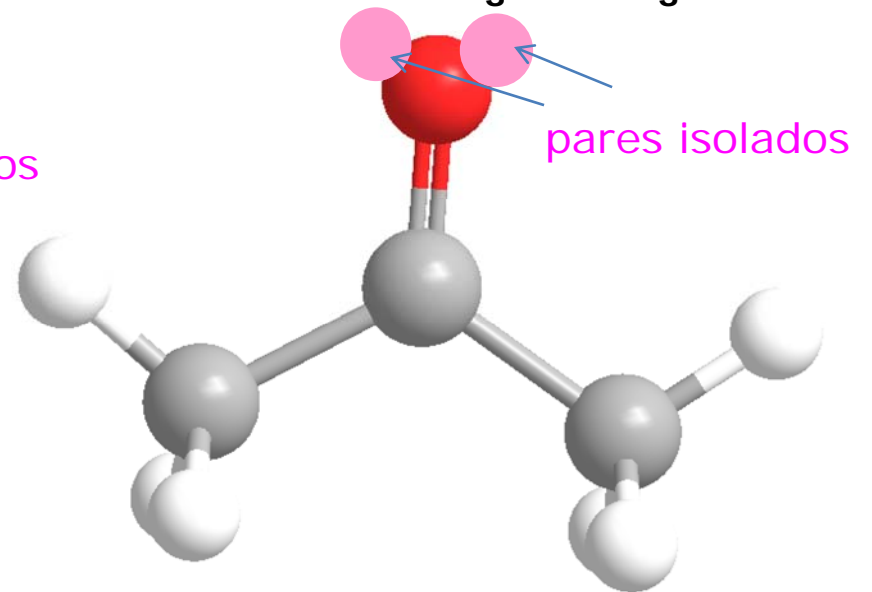
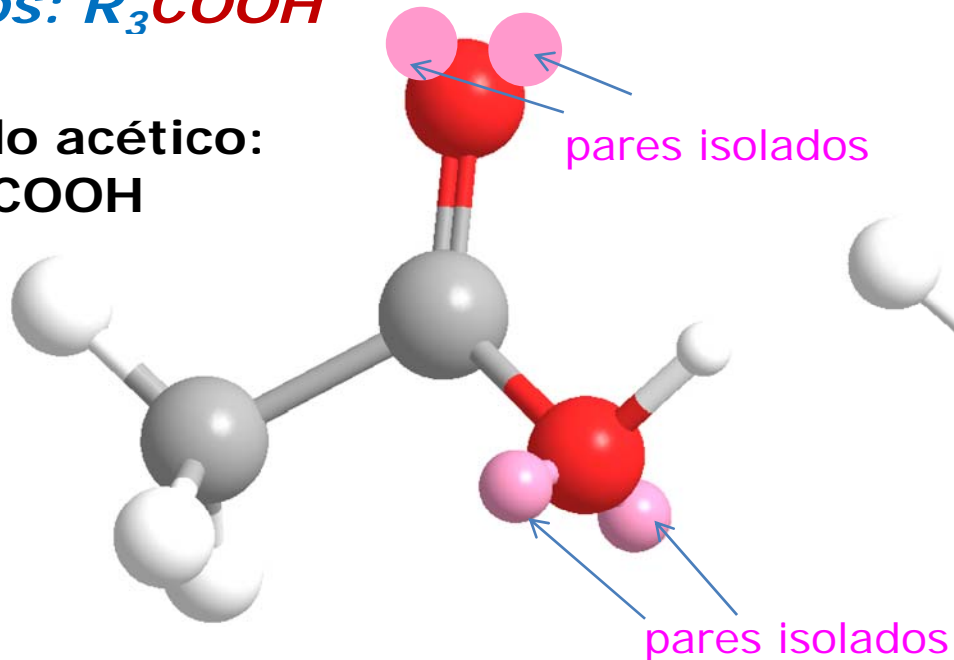


*Cetonas:  $R_3C-O-CR_3$*

Acetona  
ou dimetilcetona:  $CH_3COCH_3$

*Ácidos:  $R_3COOH$*

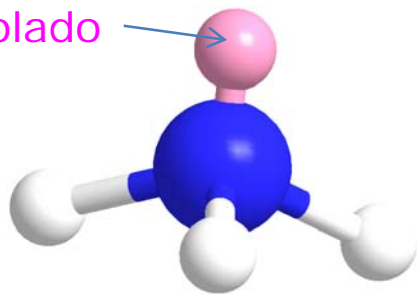
Ácido acético:  
 $CH_3COOH$



**Azoto em hibridação  $sp_3$ :  $1s^2 2sp_3^2 2sp_3^1 2sp_3^1 2sp_3^1$**



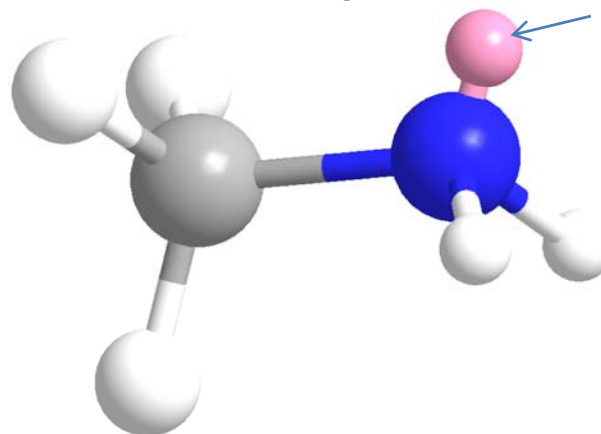
par isolado



**Aminas:  $R_3C-NH_2$**

**Metilamina: CH<sub>3</sub>NH<sub>2</sub>**

par isolado

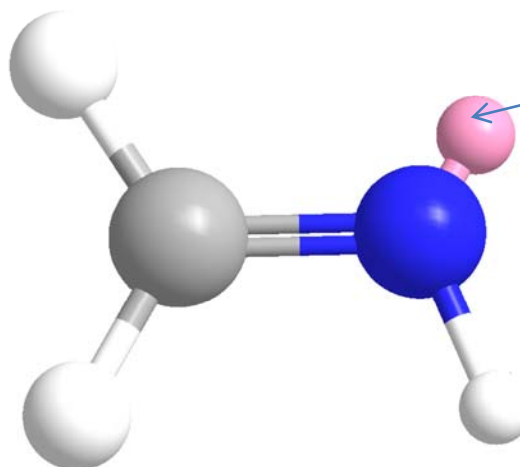


**Azoto em hibridação  $sp_2$ :  $1s^2 2sp_2^2 2sp_2^1 2sp_2^1 2p_z^1$**

**Iminas:  $R_2C-NH$**

**Metanimina: CH<sub>2</sub>NH**

par isolado



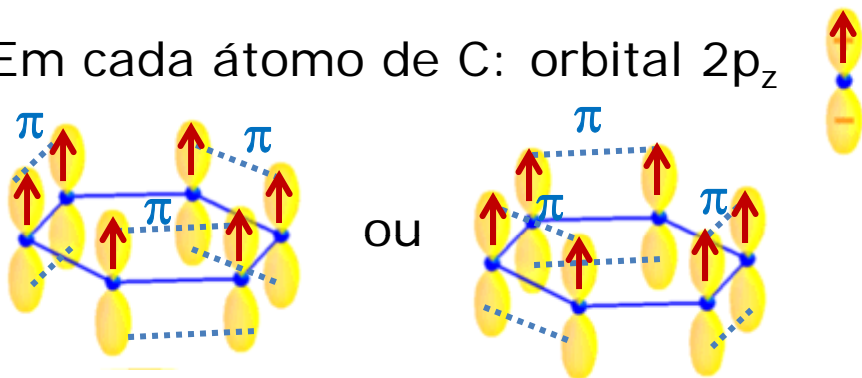
# Ligações deslocalizadas

## Benzeno: $C_6H_6$

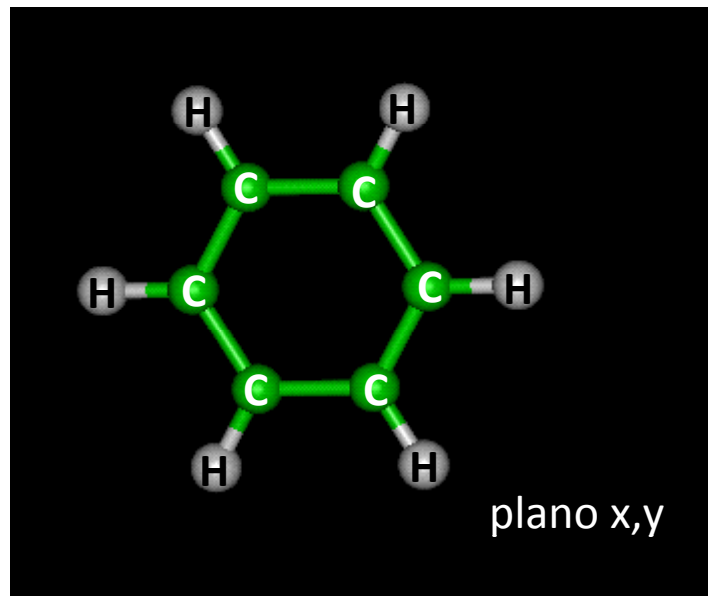
Carbono em hibridação  $sp_2$

${}^6C$ :  $1s^2 2sp_2^1 2sp_2^1 2sp_2^1 2p_z^1$

Em cada átomo de C: orbital  $2p_z$

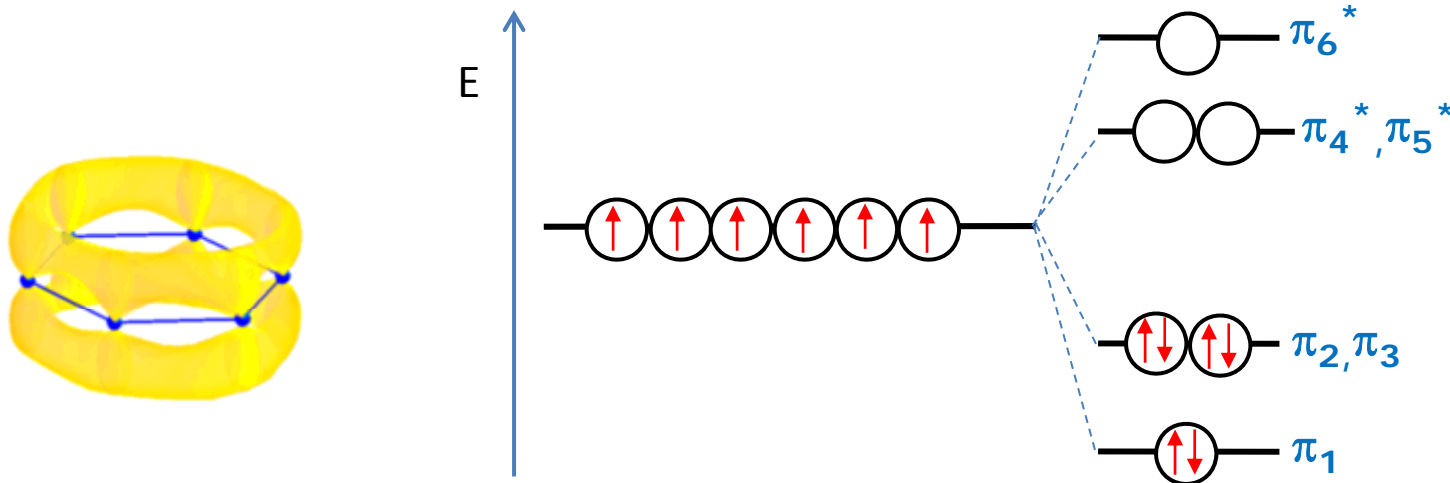


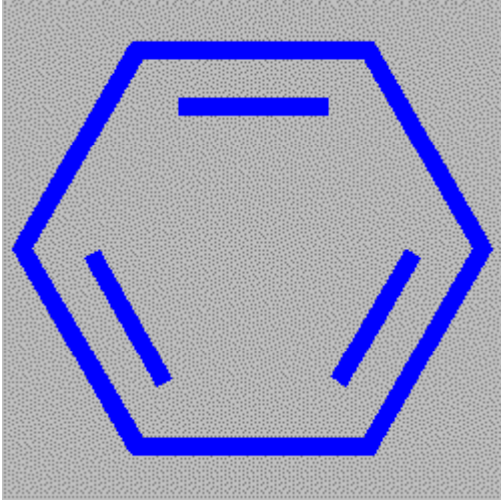
ou ainda outras hipóteses... **ressonância**



Esqueleto da molécula: **ligações  $\sigma$**

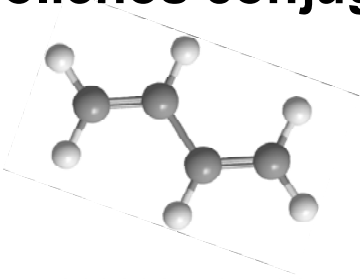
**TOM:** 6 orbitais moleculares  $\pi$  estendidas a toda a molécula



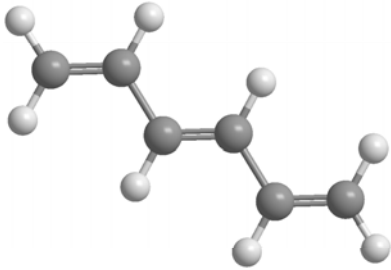


# Polienos conjugados

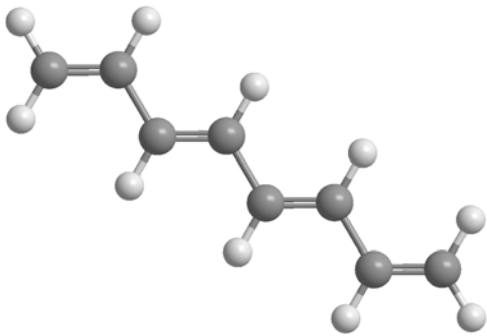
# Ligações deslocalizadas



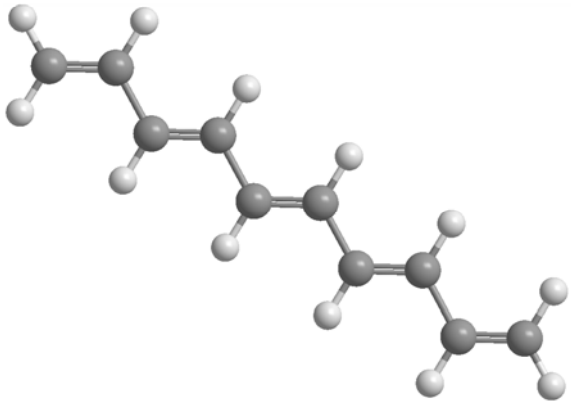
1,3-butadieno



1,3,5-hexatrieno



1,3,5,7-octatetraeno

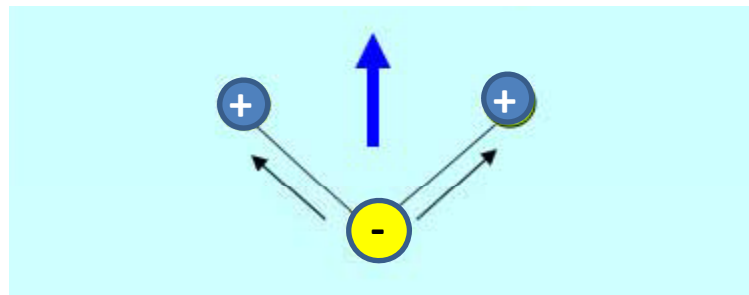


1,3,5,7,9-decapentaeno

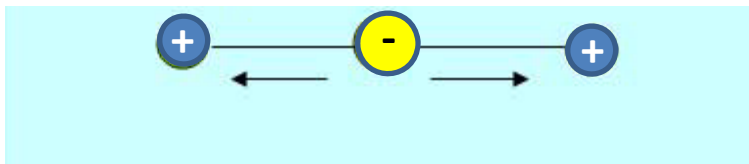
C em hibridação  $sp_2$ :  
*deslocalização dos e-s  $\pi$  a todos os átomos de C em hibridação  $sp_2$*

## Momento Dipolar de Moléculas Poliatômicas

Resultante da soma vectorial dos dipolos das ligações:



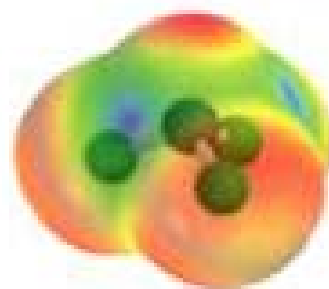
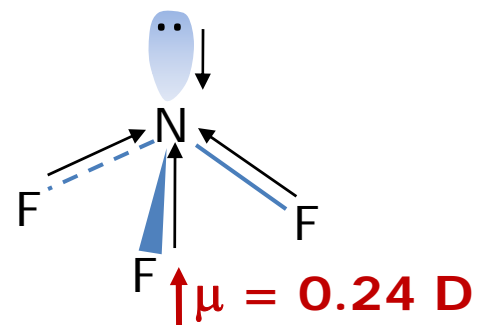
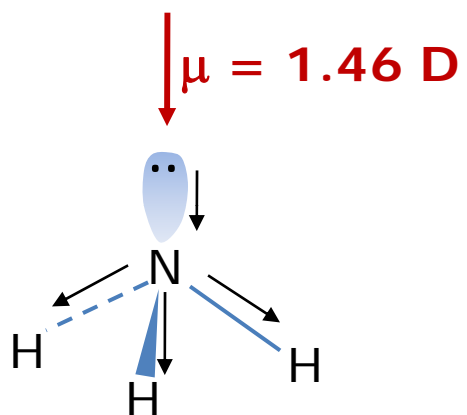
$$\mu \neq 0$$



$$\mu = 0$$



## Momento dipolar de moléculas poliatómicas

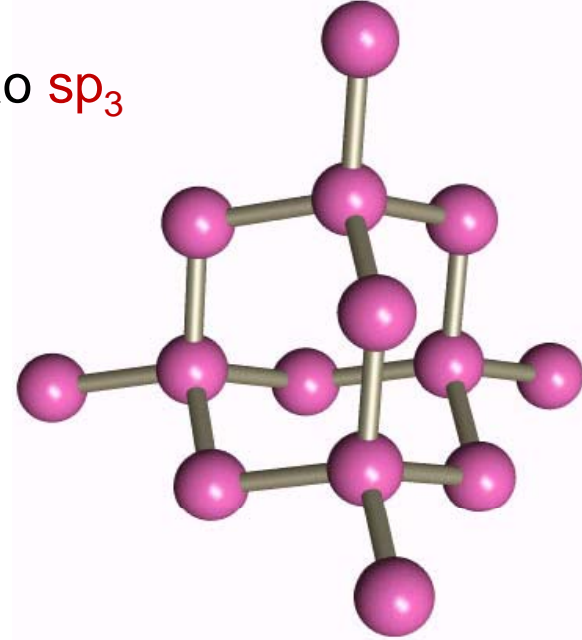
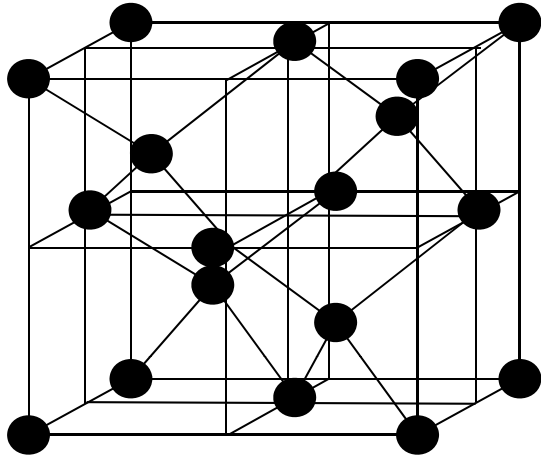


## Momentos Dipolares de Algumas Moléculas

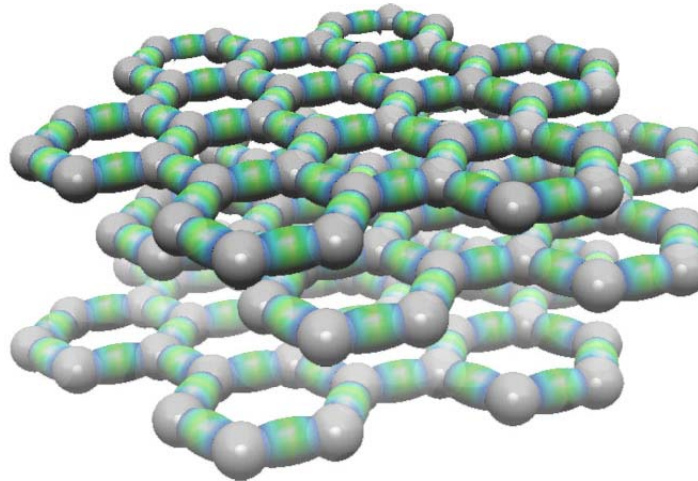
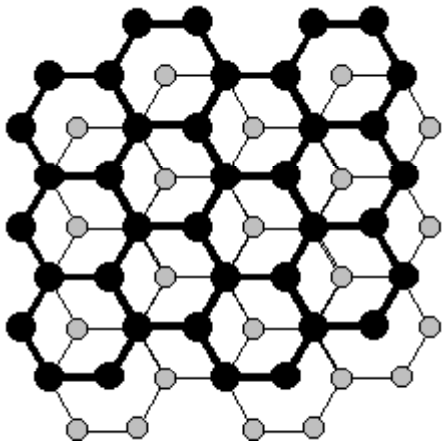
| <b>Composto</b>                                     | <b><math>\mu</math> / D</b> |
|---|-----------------------------|
| Metano (CH <sub>4</sub> )                           | 0                           |
| Etano (C <sub>2</sub> H <sub>6</sub> )              | 0                           |
| Propano (C <sub>3</sub> H <sub>8</sub> )            | 0.084                       |
| Etanol (C <sub>2</sub> H <sub>5</sub> OH)           | 1.69                        |
| 1-Propanol (C <sub>3</sub> H <sub>7</sub> OH)       | 1.68                        |
| Éter dimetílico (CH <sub>3</sub> OCH <sub>3</sub> ) | 1.30                        |
| Metilamina (CH <sub>3</sub> NH <sub>2</sub> )       | 1.31                        |
| Etanal (CH <sub>3</sub> CHO)                        | 2.69                        |
| Propanal (CH <sub>3</sub> CH <sub>2</sub> CHO)      | 2.52                        |
| Ácido Etanóico (CH <sub>3</sub> COOH)               | 1.74                        |
| Fluorometano (CH <sub>3</sub> F)                    | 1.85                        |

# Cristais Covalentes

**Diamante:** cristal formado por C em hibridação  $sp_3$



**Grafite:** planos formados por C em hibridação  $sp_2$



## **C<sub>60</sub> (fulereno ou futebuleno):**

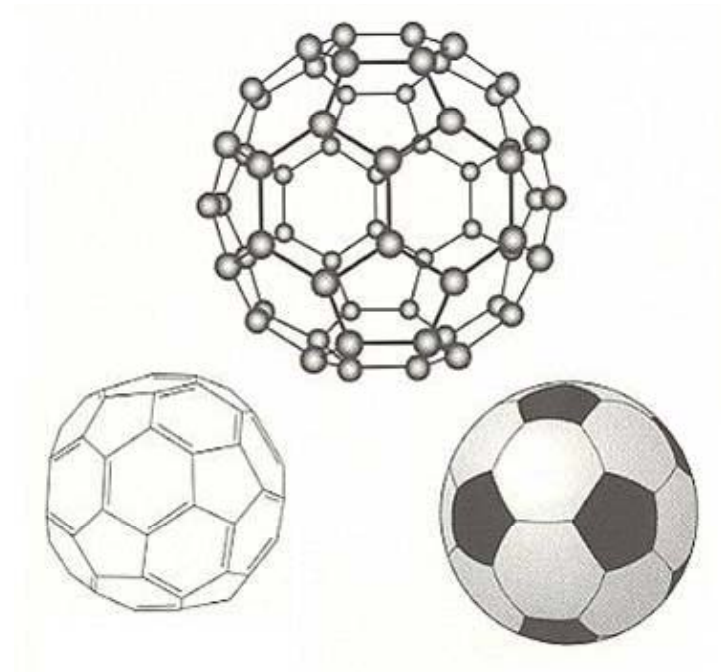
superfície esférica formada por C em hibridação **sp<sub>2</sub>**



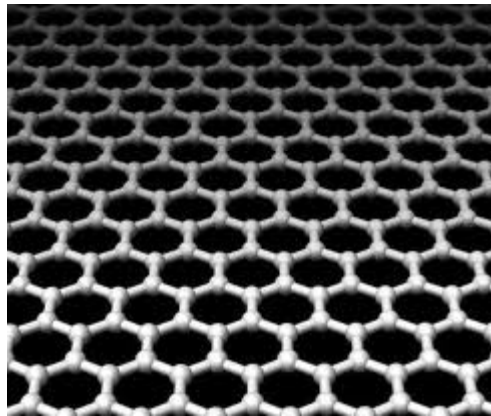
Pavilhão dos Estados Unidos da América  
Exposição Mundial de 1967 (Montreal, Canada)

*Arquitecto: Buckminster Fuller (Bucky)*

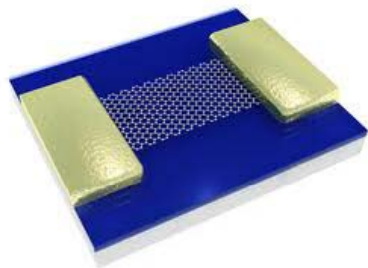
**1985: Harold Kroto, Richard Smalley, Robert Curl**  
*(Nobel da Química em 1996)*



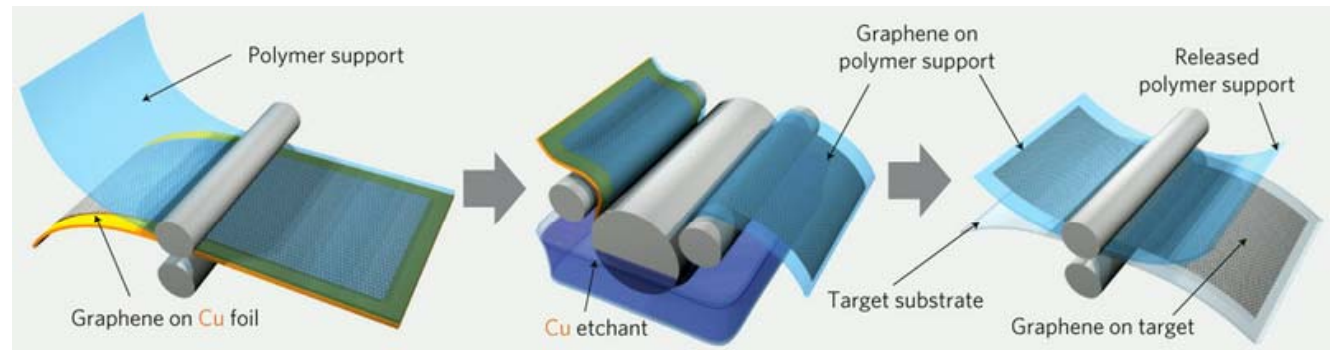
**Grafeno:** material bidimensional formado por uma camada de átomos de C em hibridação  $sp_2$



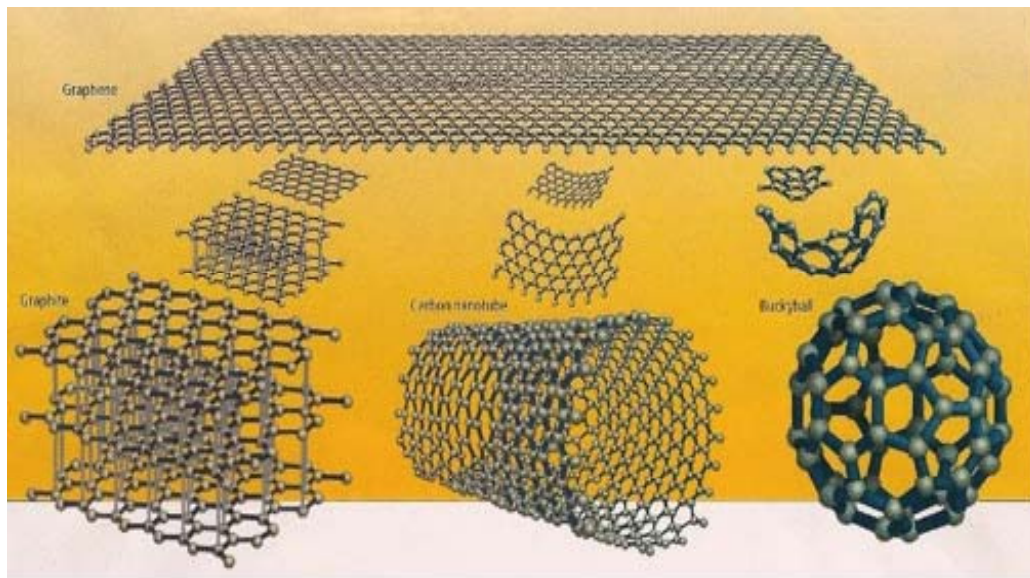
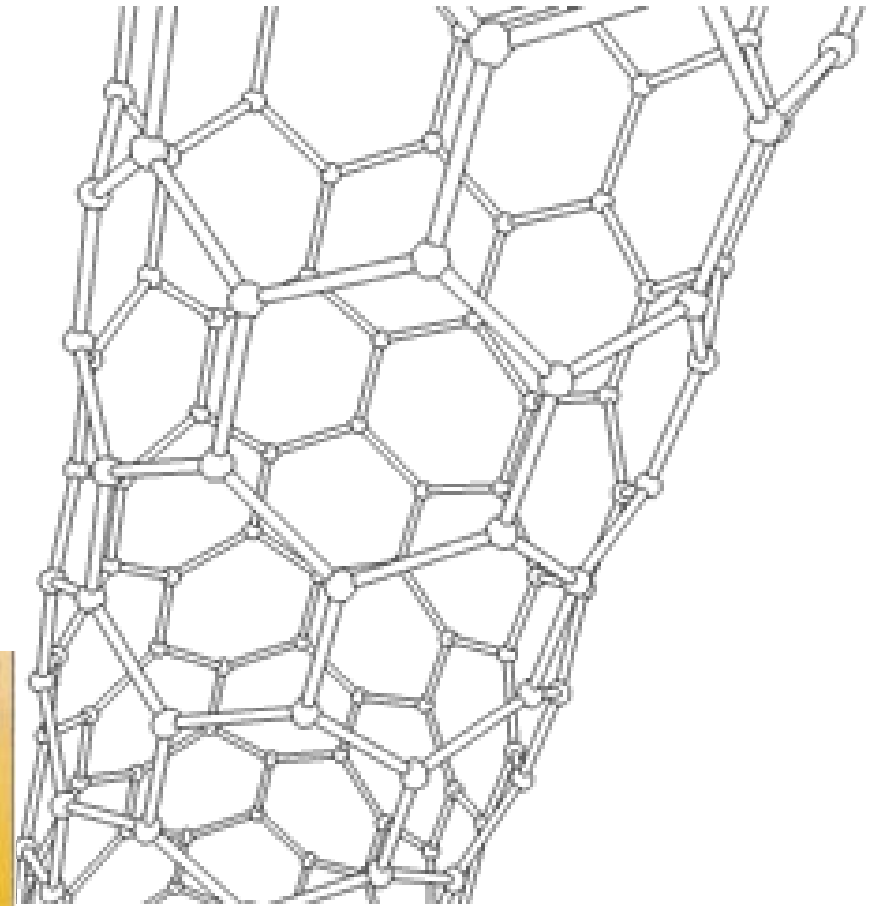
O prémio Nobel da Física em 2010 foi atribuído a **Andre Geim** e **Konstantin Novoselov** por trabalhos pioneiros com inovadoras com o material bi-dimensional grafeno



Aplicável em nanoelectrónica



# Grafenos





# Sumário 8

## Ligação Química

- **Teoria das Orbitais Moleculares (TOM)**
  - **II. Método do Enlace de Valência**
    - **Moléculas Poliatômicas**
      - Álcoois; Éteres
      - Cetonas; Ácidos
      - Aminas; Imina
      - Outras Moléculas Envolvendo Átomos do 2º Período: Be e B
      - Moléculas onde falha a Aproximação das Ligações Localizadas:  
Benzeno; Polienos conjugados
      - Moléculas envolvendo Átomos do 3º Período
    - **Momentos Dipolares de Moléculas Poliatômicas.**
    - **Cristais Covalentes:** Diamante; Grafite; Fullerenos; Grafenos