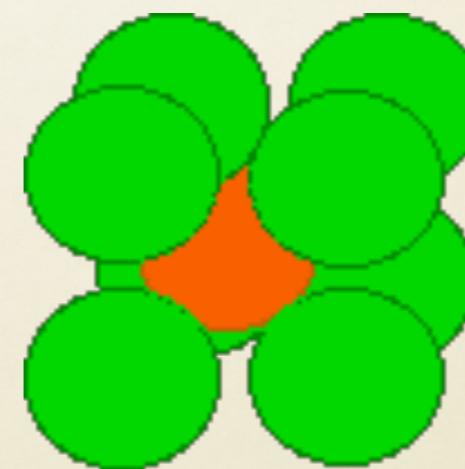
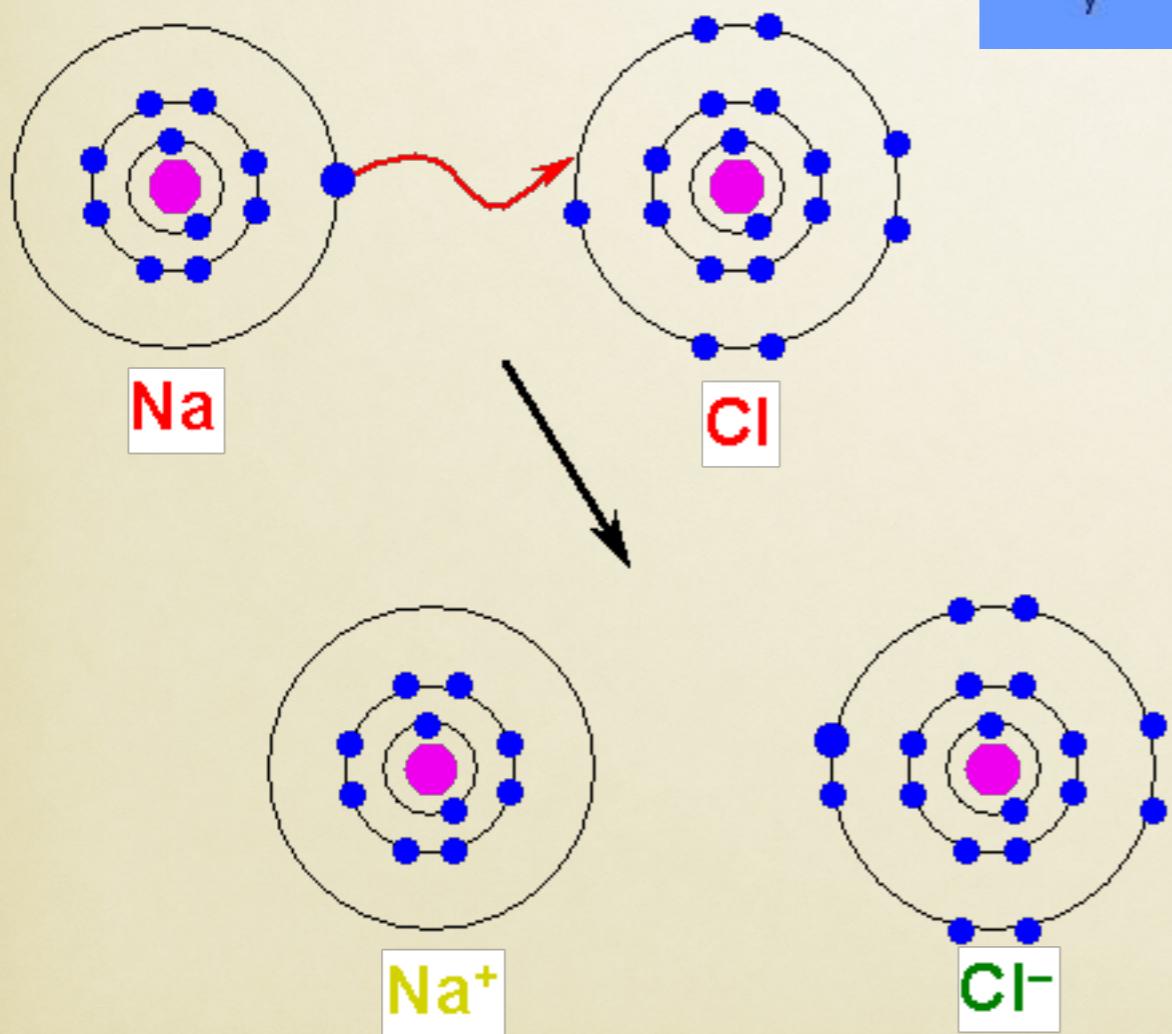
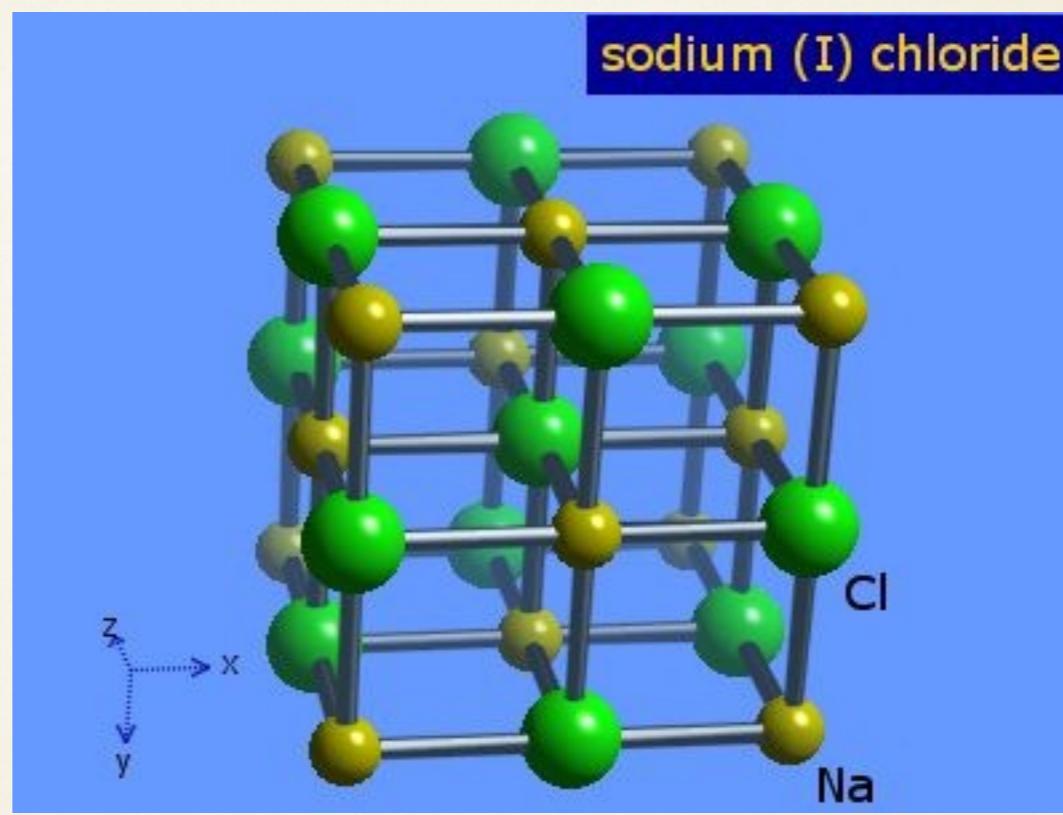


# LIGAÇÕES QUÍMICAS

CAPÍTULO 2: SHACKLEFORD

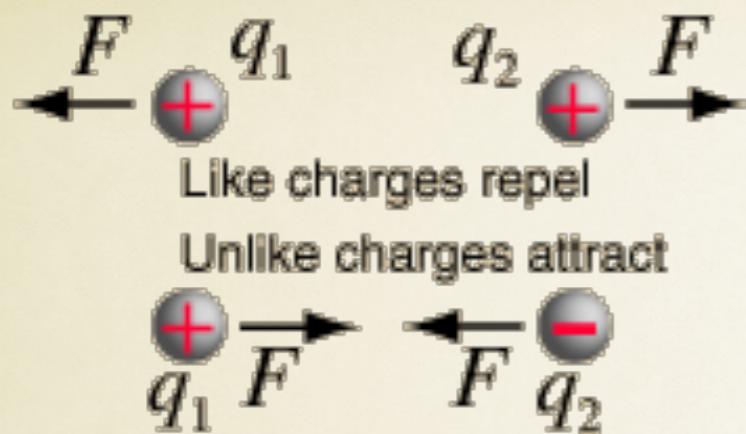
# LIGAÇÃO IÔNICA

- Transferência de elétron, preenchendo a última camada de cada átomo (tornando-os mais estáveis)



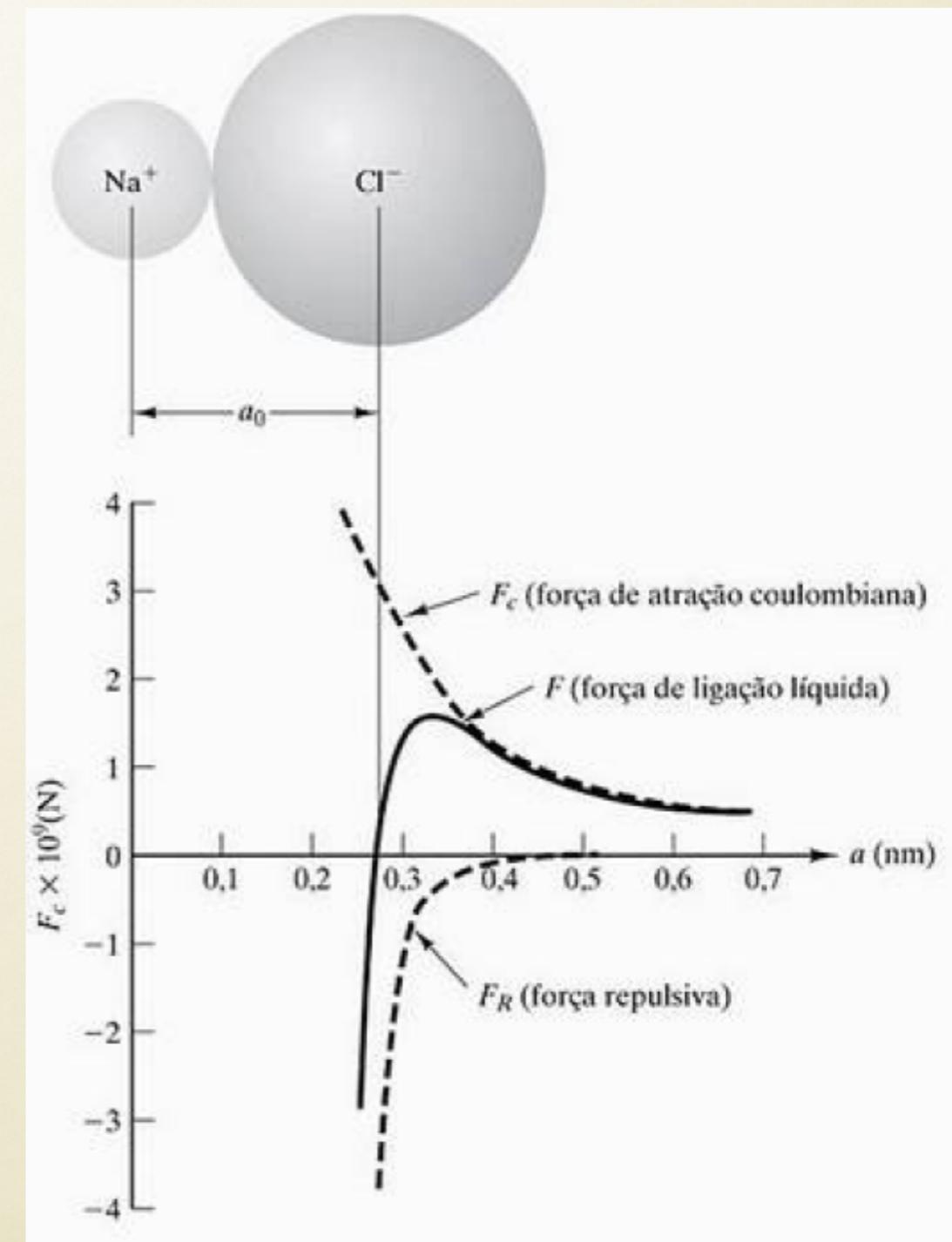
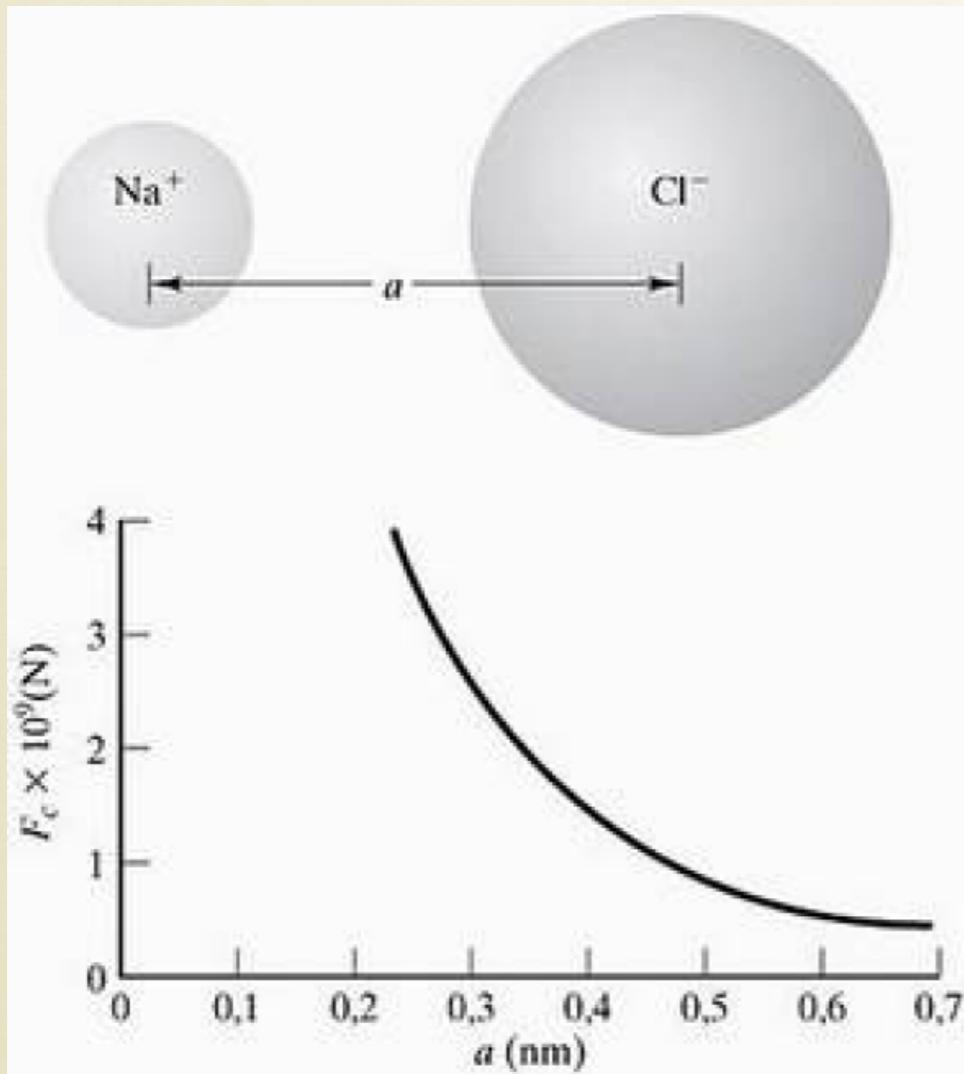
# LIGAÇÃO IÔNICA

- Depois da transferência de elétrons, as cargas se atraem e se repelem de acordo com a força elétrica, Lei de Coulomb.
- Núcleos se repelem, nuvens eletrônicas também
- Mas o núcleo atrai a nuvem eletrônica. Assim há forças atrativas e repulsivas
- Força repulsiva:  $F_r = \lambda e^{-a/\rho}$
- Força atrativa domina para grande distância e repulsiva domina para curtas distâncias



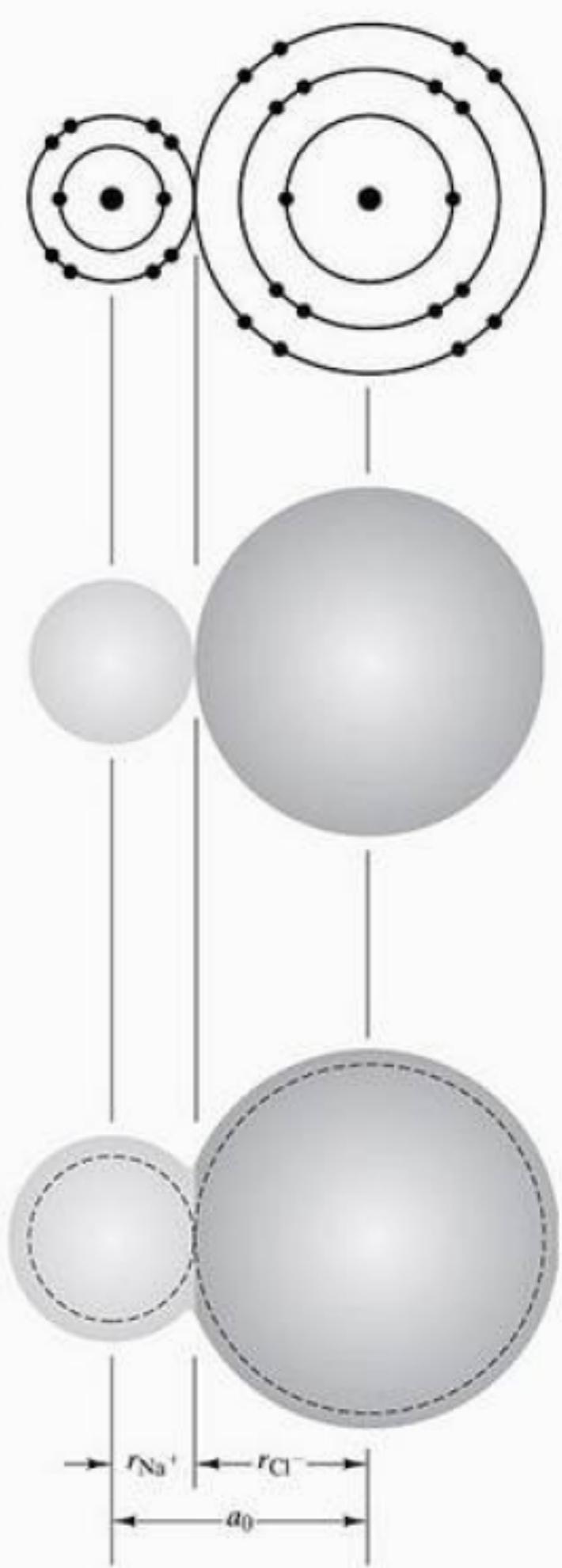
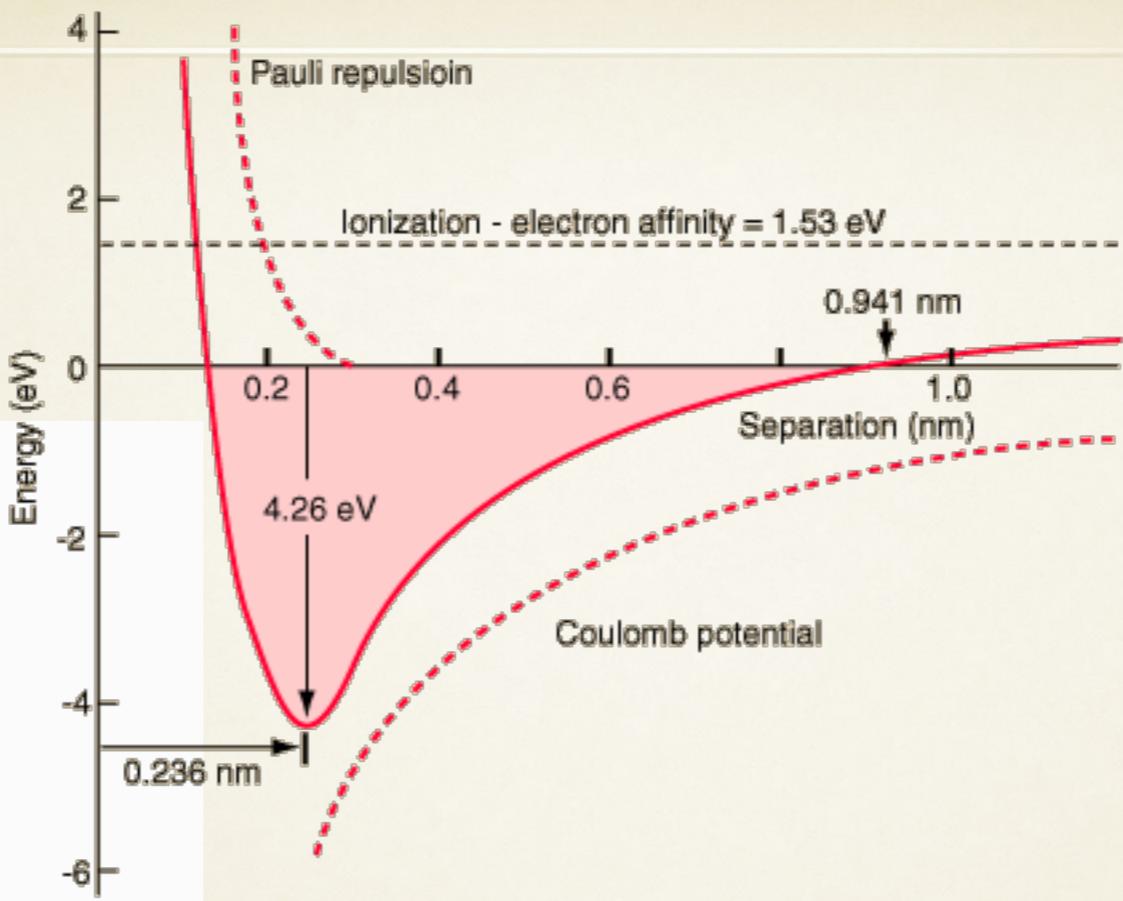
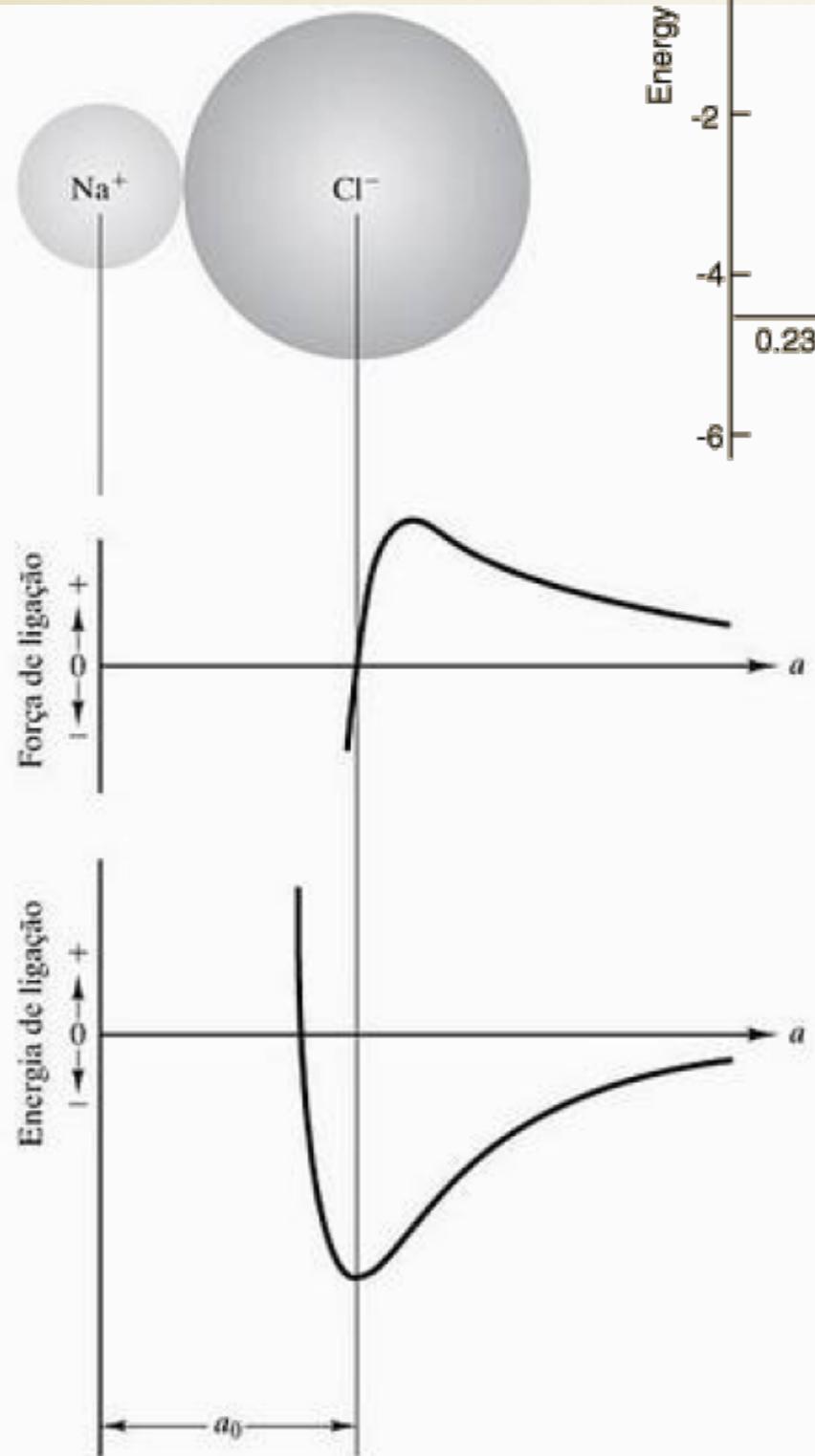
$$F = \frac{kq_1q_2}{r^2} = \frac{q_1q_2}{4\pi\epsilon_0 r^2}$$

Coulomb's Law



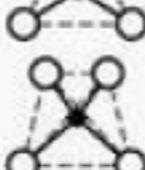
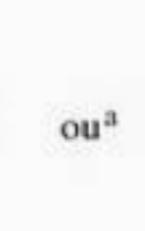
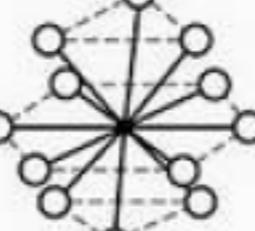
# LIGAÇÃO IÔNICA

- Distância de equilíbrio:  $r = a_0$ , quando  $F_r = F_a$
- Em termos de energia  $E$ , em  $r = a_0$  a energia é mínima.  $F = dE/da$ , logo  $E(r=a_0) = E_0$  é a energia mínima.
- Para mover os íons de suas posições de equilíbrio, energia deve ser cedida ao sistema.



# LIGAÇÃO IÔNICA

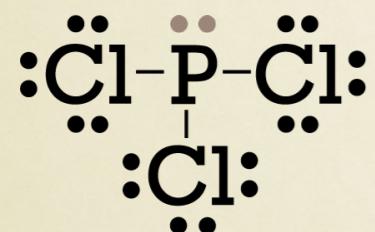
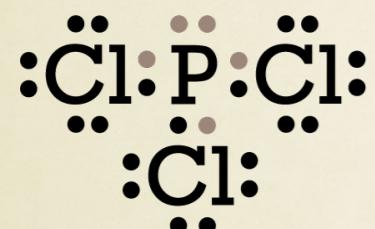
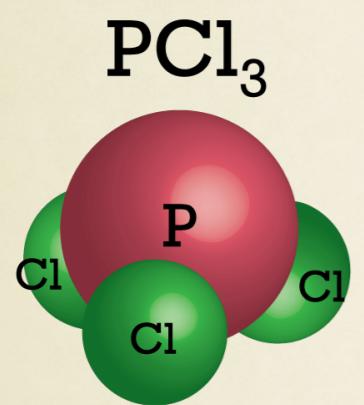
- $N_c$  = Número de coordenação = número de primeiros vizinhos
- Depende do tamanho relativo dos raios dos íons
- Já foi observado  $N_c$  até 12, sendo que 5, 7, 9, 10 e 11 nunca foram observados.

Número de coordenação	Razão dos raios, $r/R$	Geometria de coordenação	Packing Geometry		
			Minimum Radius Ratio <b>Rc / Ra</b>	Coordination Number <b>C. N.</b>	
2	$0 < \frac{r}{R} < 0,155$		< 0.155	2	Linear
3	$0,155 \leq \frac{r}{R} < 0,225$		0.155	3	Corners of an equilateral triangle (triangular coordination)
4	$0,225 \leq \frac{r}{R} < 0,414$		0.225	4	Corners of a tetrahedron (tetrahedral coordination)
6	$0,414 \leq \frac{r}{R} < 0,732$		0.414	6	Corners of an octahedron (octahedral coordination)
8	$0,732 \leq \frac{r}{R} < 1$		0.732	8	Corners of a cube (cubic coordination)
12	1	 ou <sup>a</sup> 	1.0	12	Corners of a cuboctahedron (close packing)

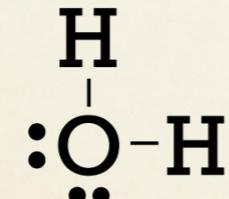
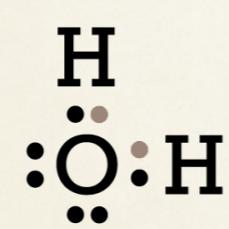
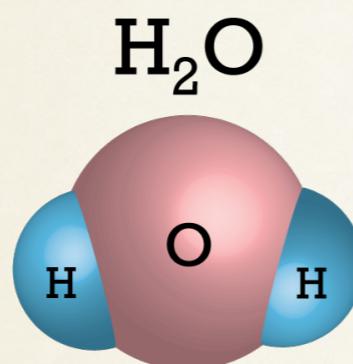
# LIGAÇÃO COVALENTE

- Direção característica,
- Compartilhamento de elétrons de valência
- Número de coordenação menor que no caso irônico
- Quando o C faz 4 ligações, o ângulo entre elas é de 109.5 graus.

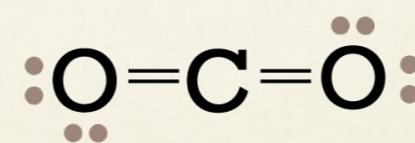
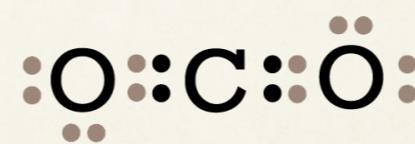
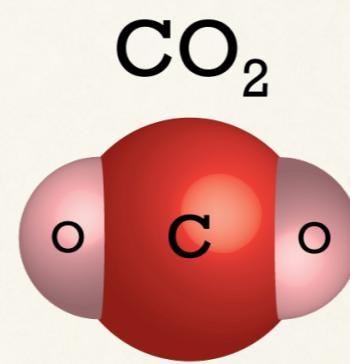
Phosphorus Trichloride



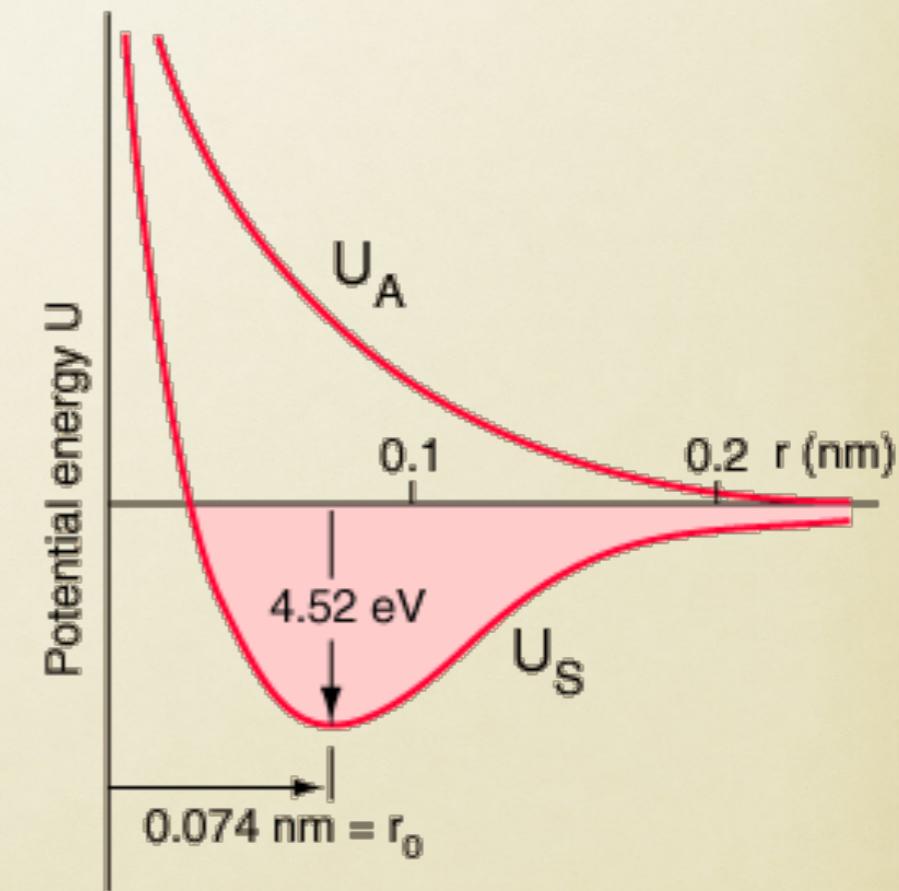
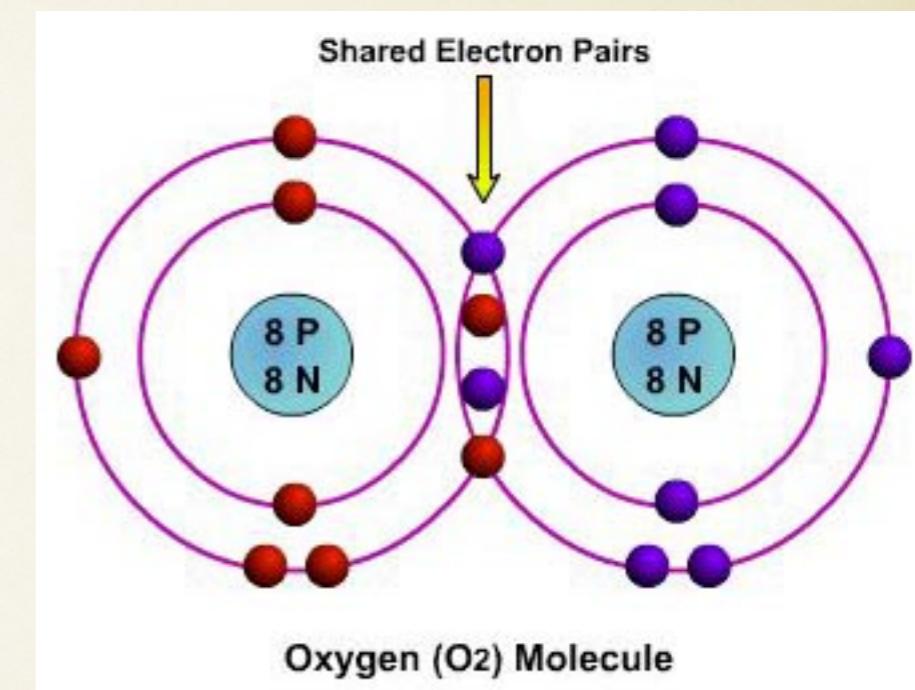
Water

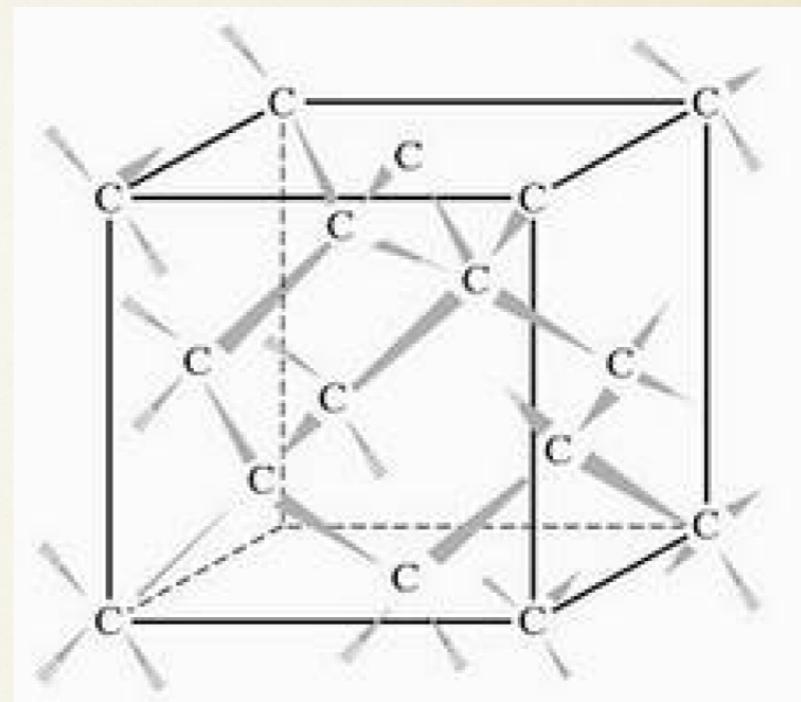
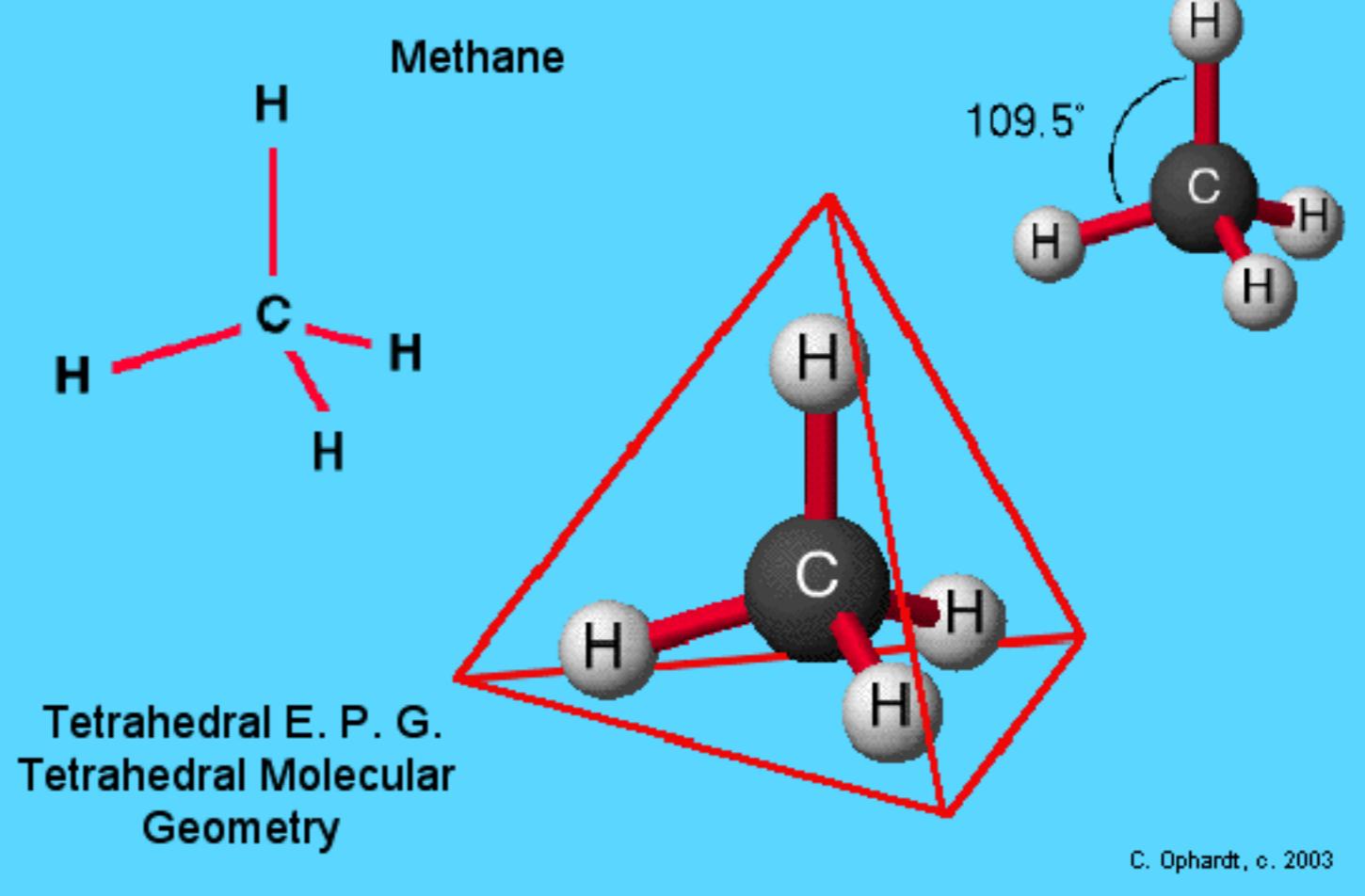
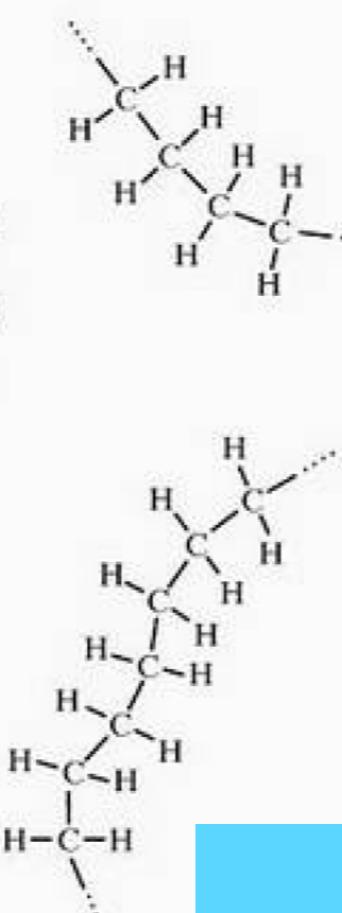
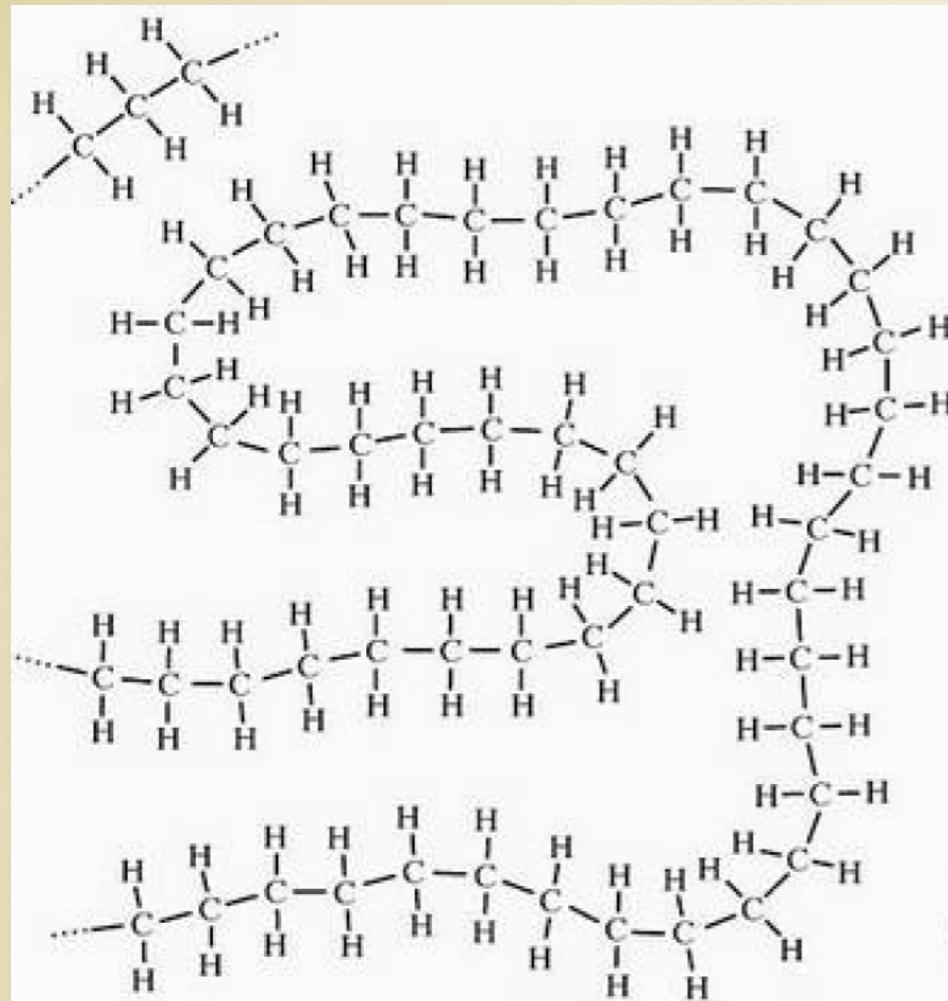


Carbon Dioxide



Shared Electron Pairs



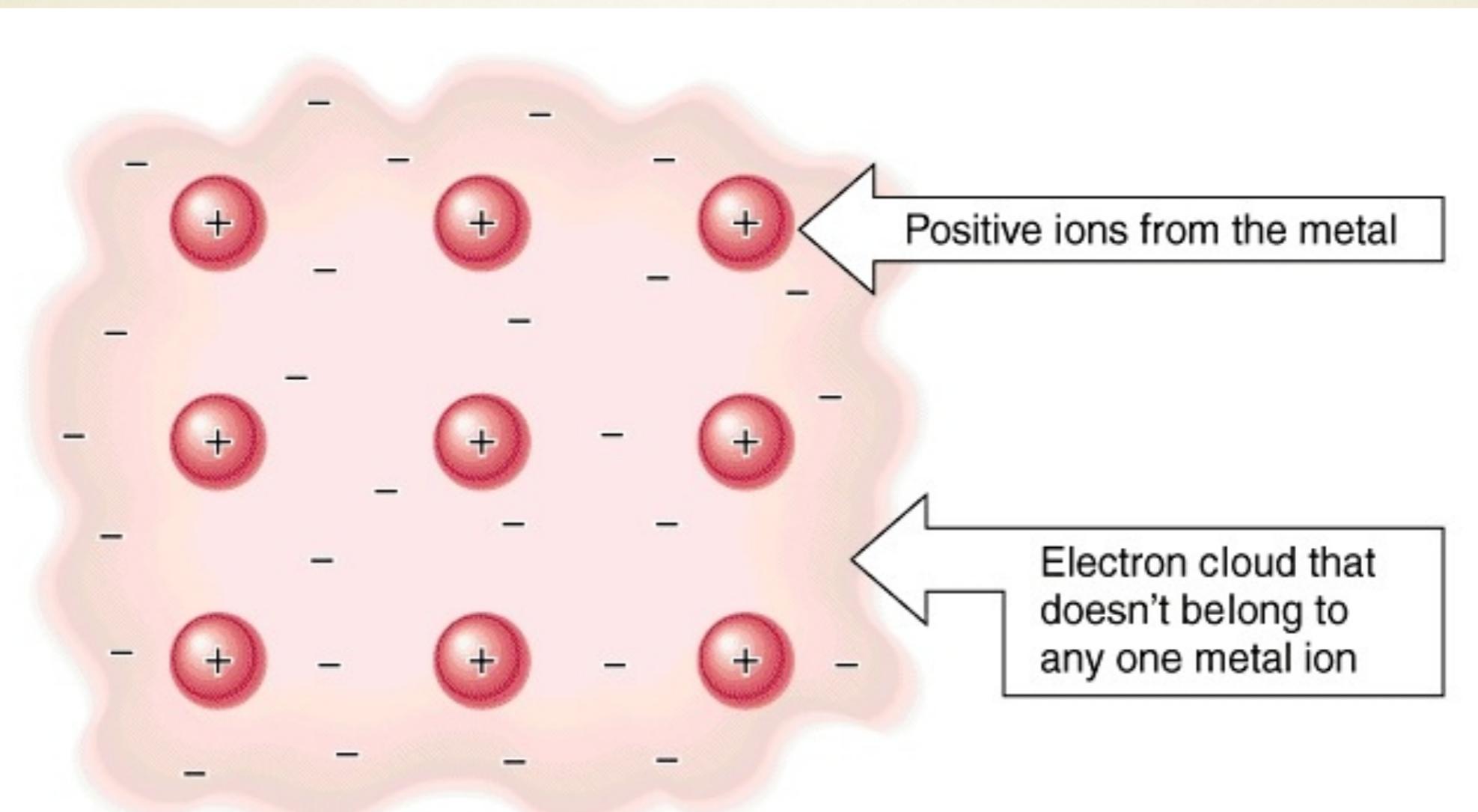


**Tabela 2.2** Energias e comprimentos de ligação para ligações covalentes representativas

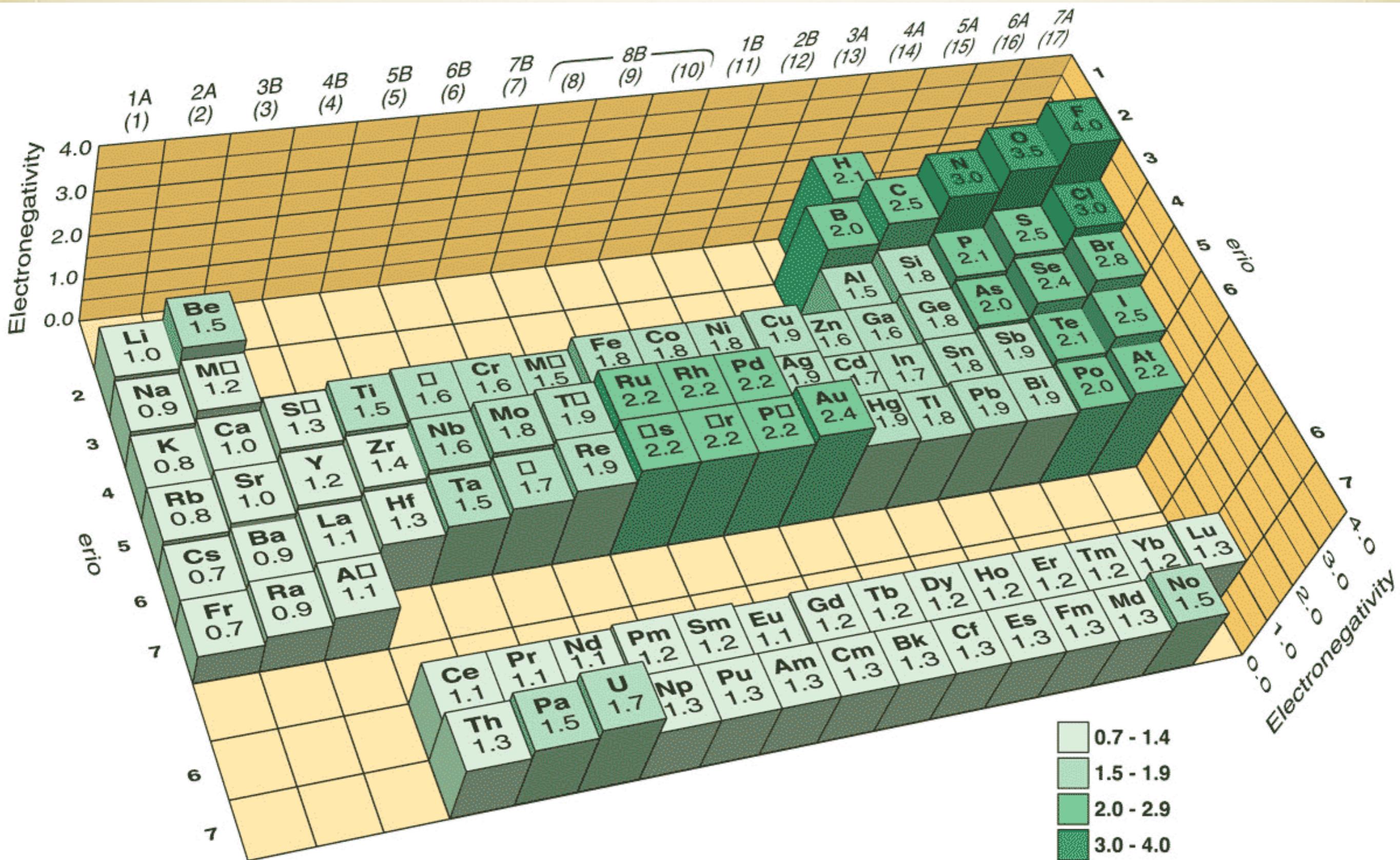
Ligação	Energia de ligação <sup>a</sup>		Comprimento da ligação, nm
	kcal/mol	kJ/mol	
C—C	88 <sup>b</sup>	370	0,154
C=C	162	680	0,130
C≡C	213	890	0,120
C—H	104	435	0,110
C—N	73	305	0,150
C—O	86	360	0,140
C=O	128	535	0,120
C—F	108	450	0,140
C—Cl	81	340	0,180
O—H	119	500	0,100
O=O	52	220	0,150
O—Si	90	375	0,160
N—H	103	430	0,100
N—O	60	250	0,120
F—F	38	160	0,140
H—H	104	435	0,074

# LIGAÇÃO METÁLICA

- Sem direção característica
- Elétrons de valênciadelocalizados: gás de elétrons
- Responsável pela alta condutividade elétrica
- Mesmos conceitos de energia mínima e distância de equilíbrio entre os átomos
- Alto número de coordenação



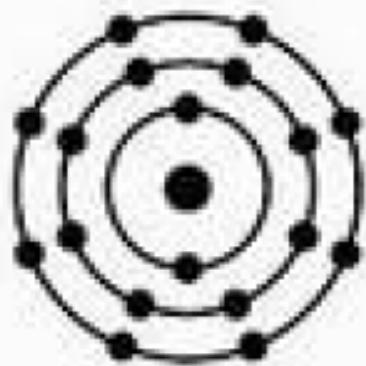
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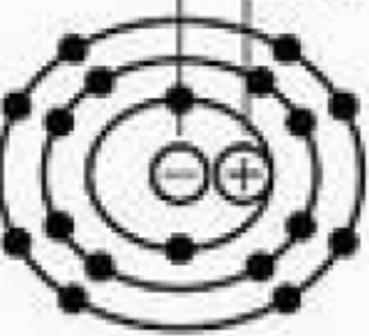
# LIGAÇÃO DE VAN DER WAALS

- Ligação secundária: mais fraca
- Atração eletrostática, mas sem troca de elétrons
- Criada pela distribuição assimétrica de cargas negativa e positiva: formação de dipolo elétrico nas moléculas
- Dipolos: temporários ou permanente
- Permanente: pontes de hidrogênio (mais fortes)

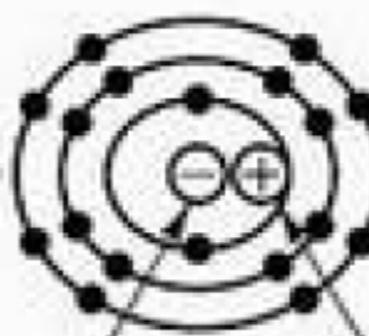
Átomo de Ar isolado



Magnitude do momento  
do dipolo

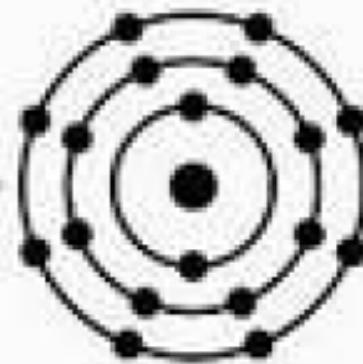


Ligação  
secundária

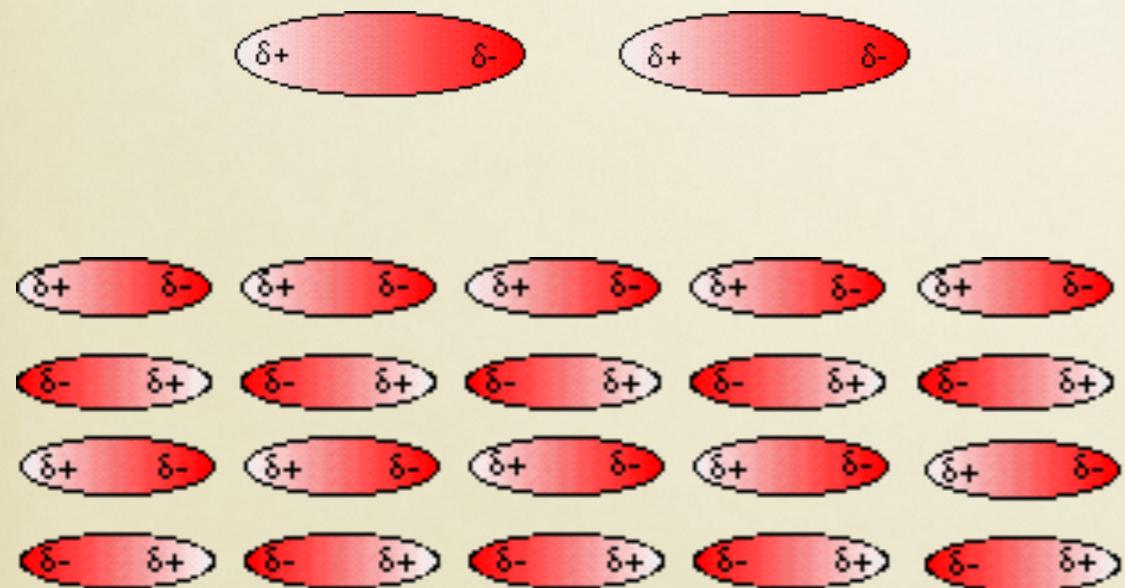
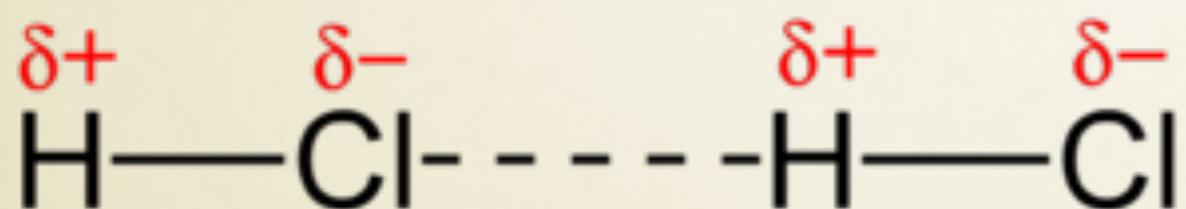


Centro da carga  
negativa (elétron)

Átomo de Ar isolado

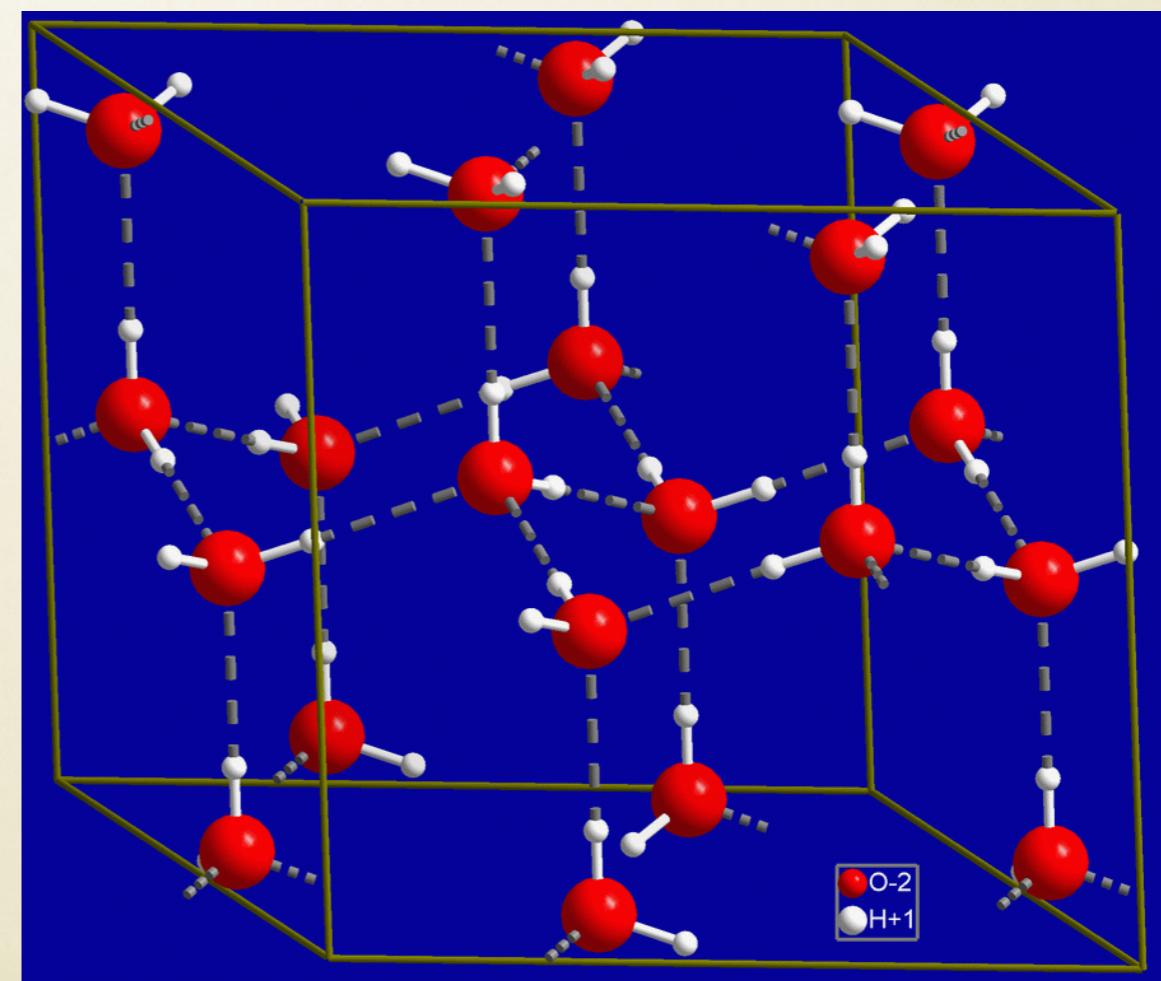
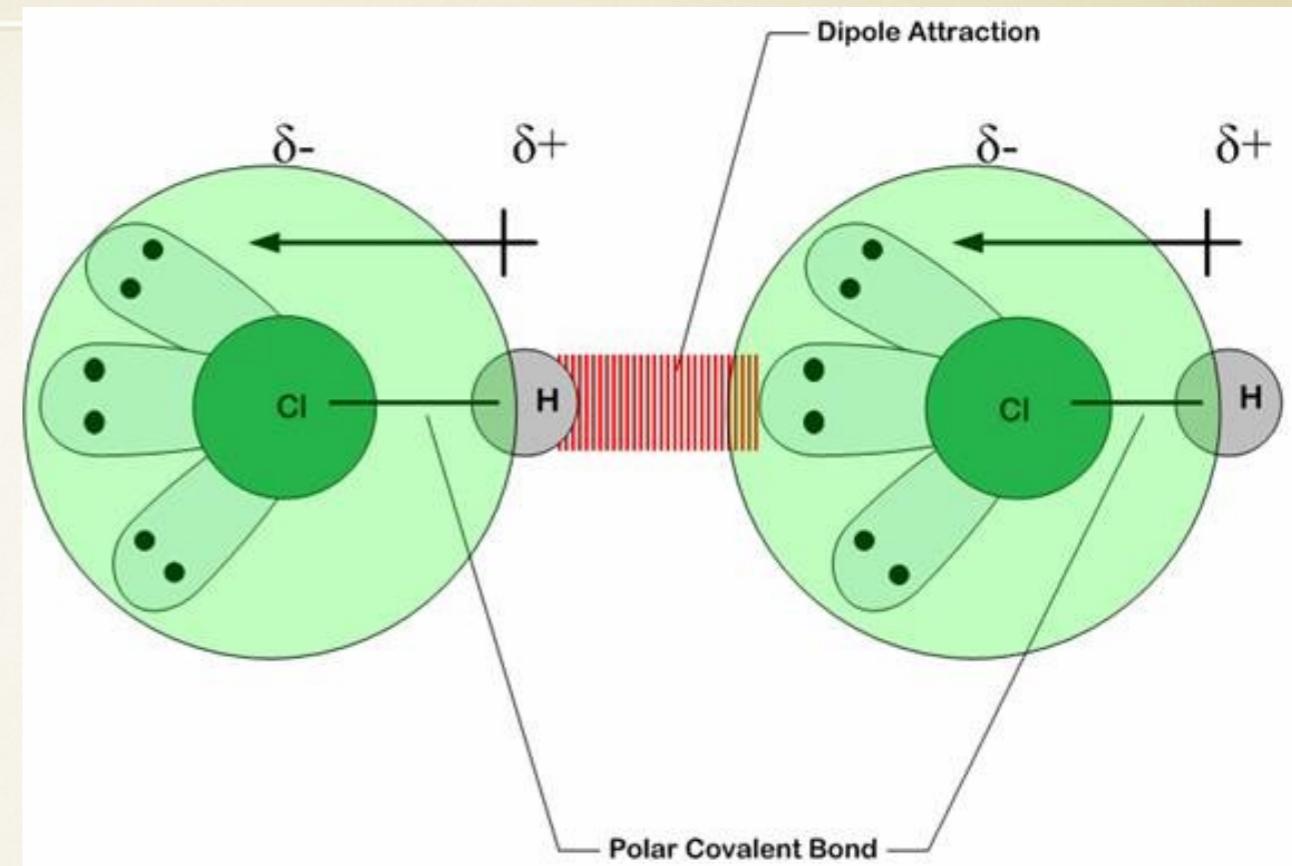
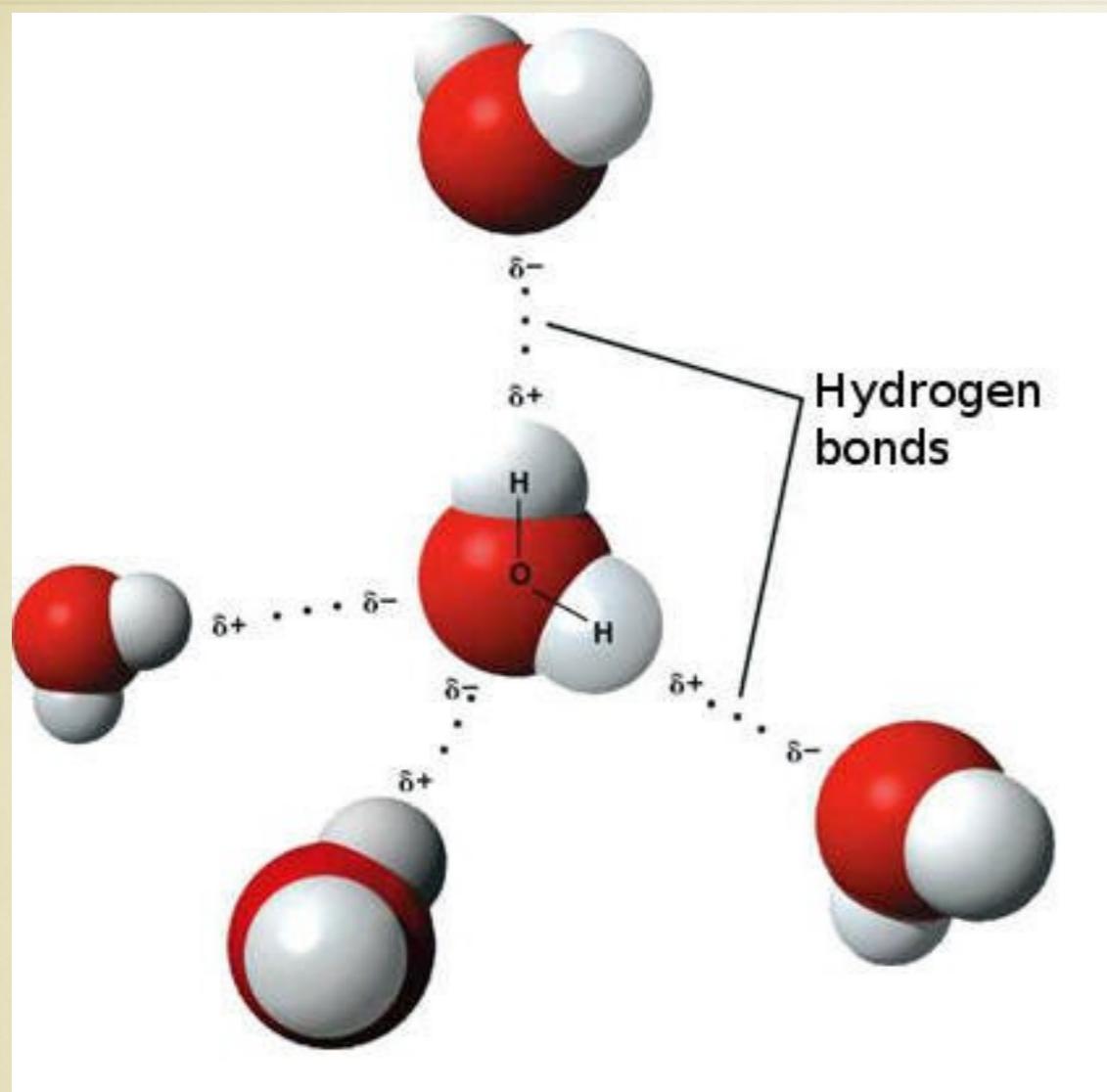


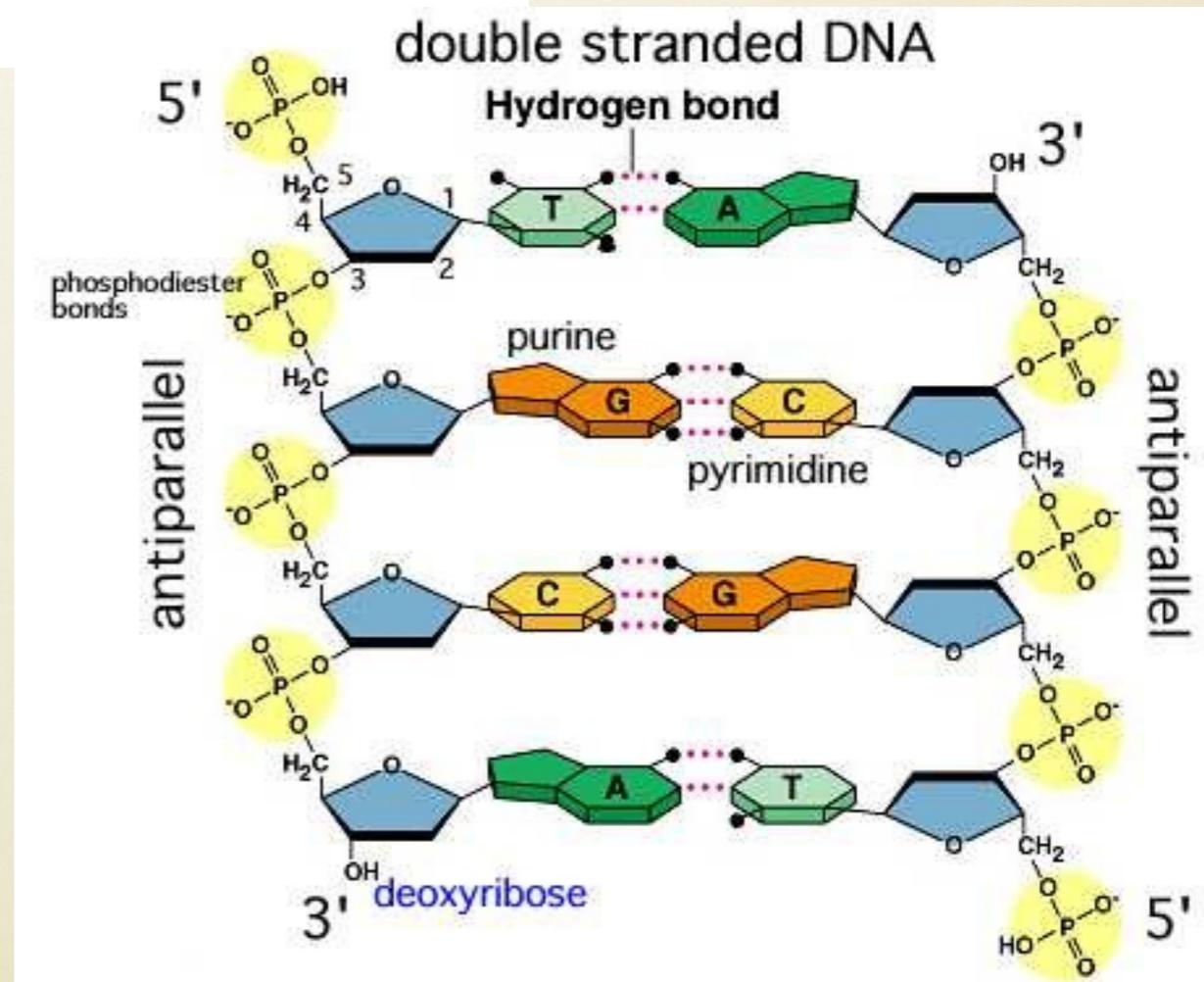
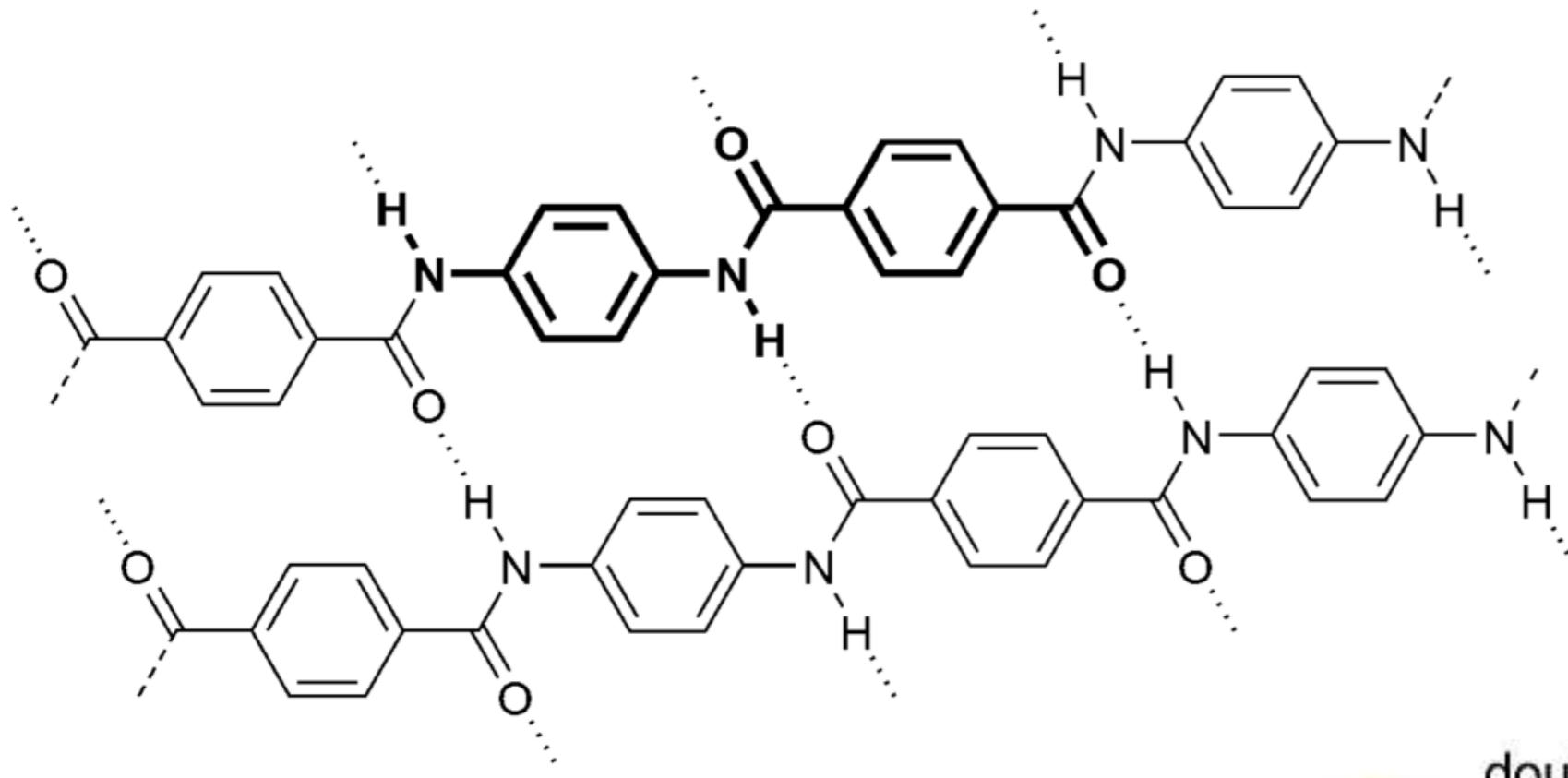
Centro da carga  
positiva (núcleo)

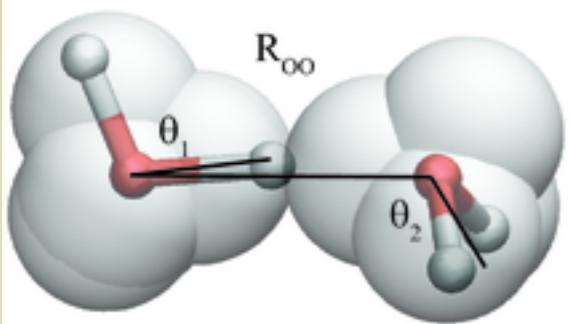


# LIGAÇÃO DE VAN DER WAALS

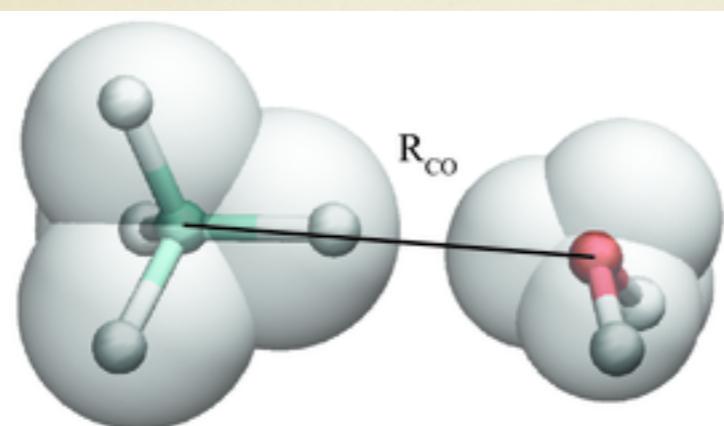
- Dipolos permanentes: pontes de hidrogênio
- Interação mais forte
- Alta coesão entre moléculas
- Água, por exemplo, cada molécula faz 4 ligações com outras 4 moléculas.
- Isso explica a expansão anômala da água antes de congelar
- Outro exemplo: polietileno



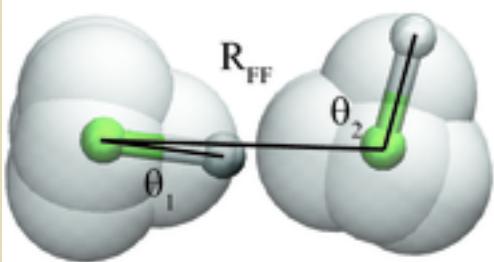




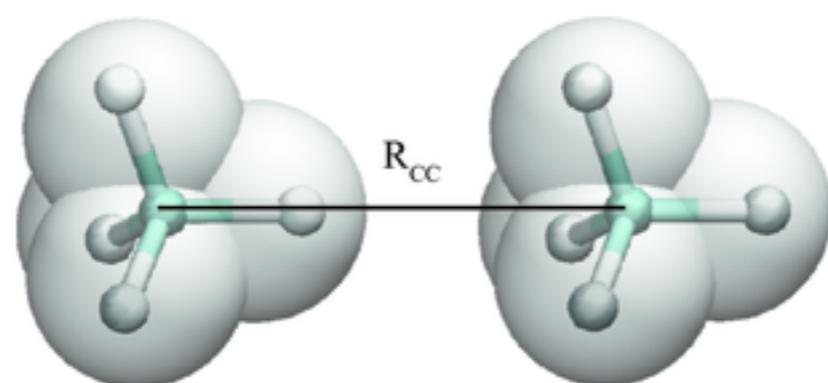
$(\text{H}_2\text{O})_2$      $E = -35.5$  (-5.44 kcal/mol)  
 $R_{\text{OO}} = 2.29$  (2.92 Å),  
 $\theta_1 = 4.6^\circ$  ( $6^\circ$ ),  $\theta_2 = 112.4^\circ$  ( $123^\circ$ )



$\text{CH}_4 \cdot \text{OH}_2$      $E = -3.9$  (-0.9 kcal/mol)  
 $R_{\text{OC}} = 3.18$  (3.51 Å)

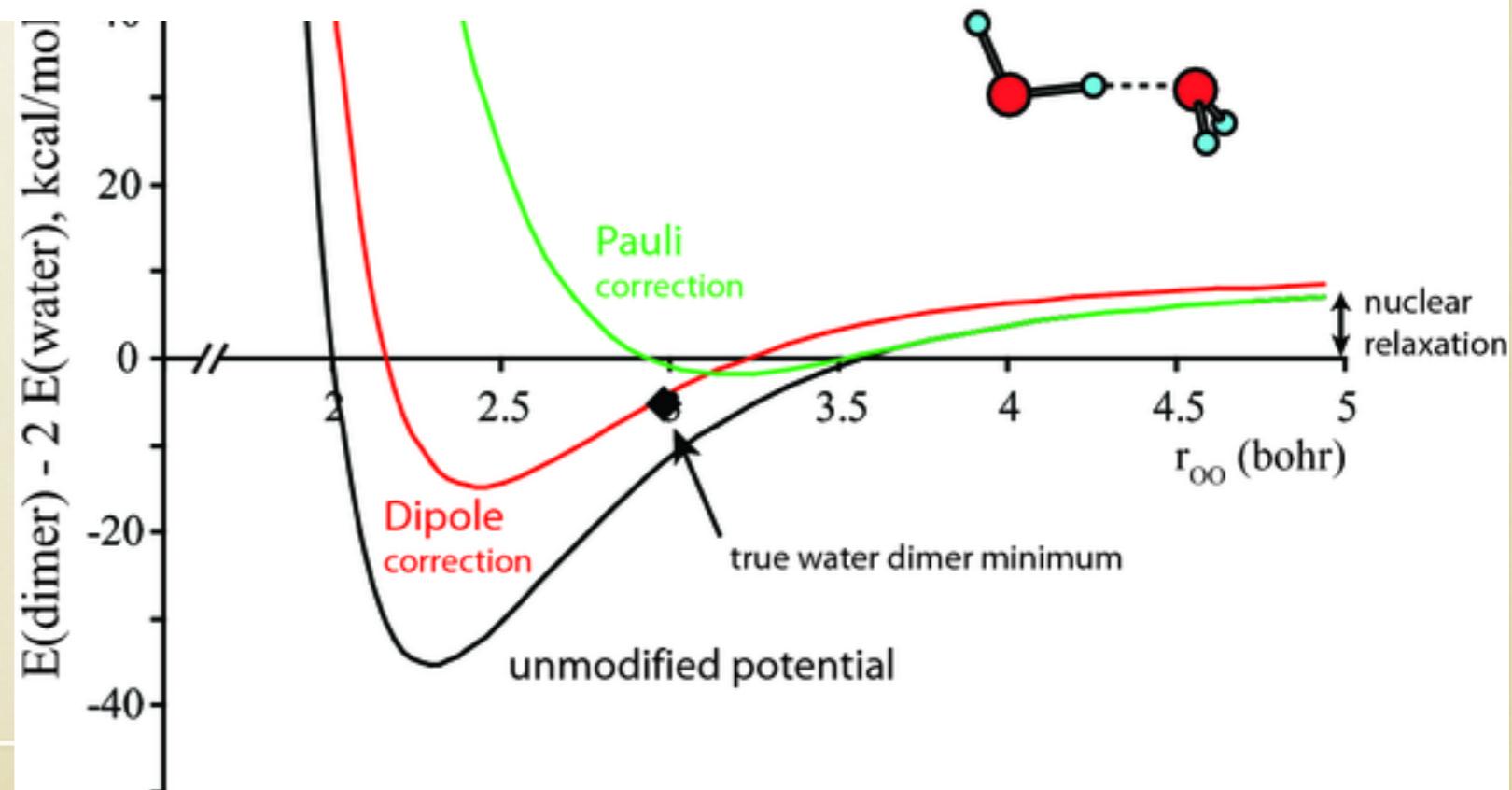


$(\text{HF})_2$      $E = -53.7$  (-4.56 kcal/mol)  
 $R_{\text{FF}} = 2.13$  (2.73 Å),  
 $\theta_1 = 5.8^\circ$  ( $7^\circ$ ),  $\theta_2 = 103.5^\circ$  ( $112^\circ$ )



$(\text{CH}_4)_2$      $E = -0.5$  (-0.3 kcal/mol)  
 $R_{\text{CC}} = 3.91$  (4.13 Å)

### Water dimer potential



# CLASSIFICAÇÃO

- Metais: ligação metálica
- Vidros e Cerâmicas: ligações iônicas e covalentes
- Polímeros: ligações covalentes e secundárias
- Semicondutores: ligações covalentes e jônicas