

Introdução à Física do Estado Sólido

Física Moderna II-B

Caetano R. Miranda

AULA 6 – 12/09/2022

Carlos A. Martins Jr.



sampa



crmiranda@usp.br

Cronograma

CRONOGRAMA TENTATIVO - Introdução à Física do Estado Sólido - Física Moderna IIB - 2S 2022					
DATA	aula n°	Segundas (19h - 21h) - Sala 2001 - Ala Central	aula n°	Quartas (21h - 23h) - Sala 2001 - Ala Central	DATA
15-Aug			1	Apresentação - Curso	18-Aug
22-Aug	2	Revisão - Partículas e ondas - Chocolate	3	Átomos e Ions (Elétrons em átomos) - Tabela Periódica	25-Aug
29-Aug	4	Átomos e Ions (Elétrons em átomos) - Simulação	5	Moléculas e sólidos (Elétrons em sólidos) - impressão 3D	01-Sep
05-Sep	Feriado	Independência do Brasil. Não haverá aula.	Feriado	Independência do Brasil. Não haverá aula.	08-Sep
12-Sep	6	Ordem e Simetria	7	Ondas em cristais – Estruturas cristalinas - Corte/Colar - Origem	15-Sep
19-Sep	8	Estruturas - Átomos em cristais - VR1	9	Estruturas - Átomos em cristais - VR2	22-Sep
26-Sep	10	Vibrações térmicas e Fonons	11	Vibrações térmicas e Fonons - Sonificação	29-Sep
03-Oct	12	Elétrons livres	13	Elétrons livres	06-Oct
10-Oct	14	Condutividade elétrica e teoria de bandas	15	Condutividade elétrica e teoria de bandas	13-Oct
17-Oct	16	Semicondutores	17	Semicondutores - VR3	20-Oct
24-Oct	18	Junção PN - Criação Jogos	19	Junção PN	27-Oct
31-Oct	20	Magnetismo	21	Magnetismo	03-Nov
7/11	22	Supercondutividade	23	Supercondutividade	10-Nov
14/11	Feriado	Dia - República. Não haverá aula.	24	Projeto - Escolha do Tema / Oficina - Infográfico	17-Nov
21/11	25	Nanotecnologia	26	Nanotecnologia	24-Nov
28/11	27	Materiais quânticos	27	Materiais quânticos	01-Dec
05-Dec	29	PROJETO	30	PROJETO	08-Dec
12-Dec	31	Vistas - Notas	32		15-Dec

ENTREGA 1

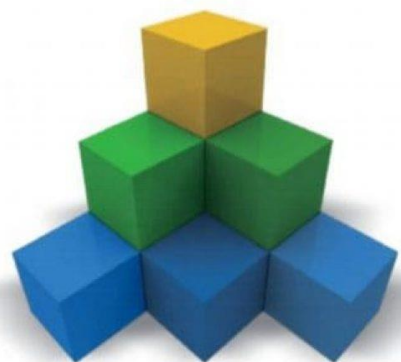
ENTREGA 2

ENTREGA 3

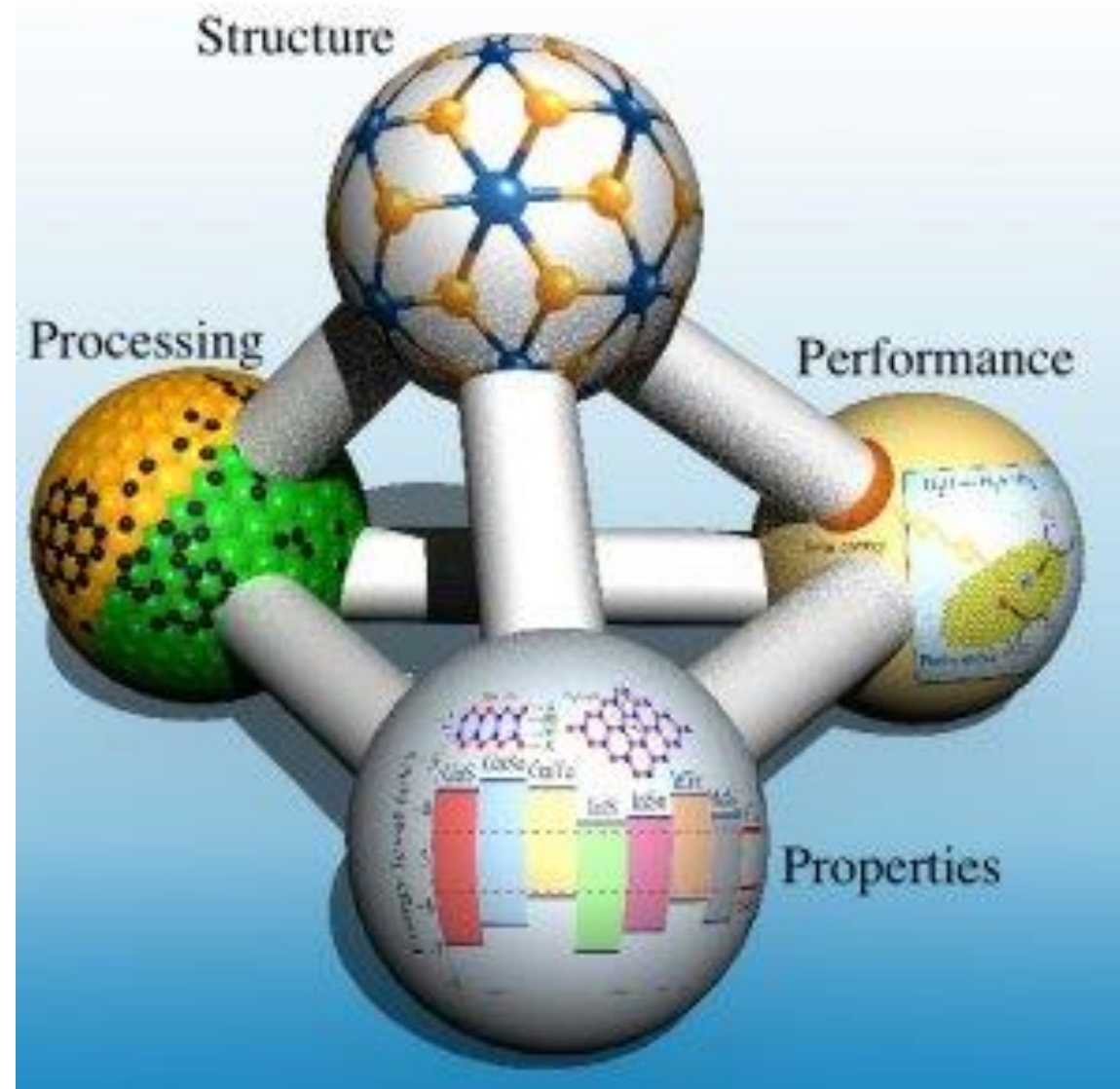
PROJETO

Entrega 1 – 15/09/2022

Mapeando a Física do Estado Sólido no BNCC ...



BASE
NACIONAL
COMUM
CURRICULAR
EDUCAÇÃO É A BASE



Unidade temática: Matéria e Energia / Objetos do conhecimento / Habilidades

Motivação

O que poderíamos ter feito melhor?

8 respostas

Acho que a explicação das ligações não ficou muito clara, mas pode ter sido uma impressão pessoal minha. Não sei indicar como deixar mais claro.

Ficou um pouco confusa a explicação de qual ligação é mais forte? Metálica > covalente > iônica? Iônica > Metálica > covalente?

A parte da explicação do que fazer para primeira entrega poderia ser mais detalhada e com mais exemplos.

De minha parte, acho que preciso de um estudo para lembrar os princípios mais básicos de química (que vi há muito tempo), para aproveitar melhor as discussões.

Nada.

Ter dado uma aprofundada nas ligações, pq não foi visto em introdução à mecânica quântica

Revisão do Átomo de Hidrogênio

Equação de Schrödinger para o átomo de hidrogênio:

$$\frac{-\hbar^2}{8\pi^2m} \nabla^2 \Psi - \frac{e^2}{4\pi\epsilon_0 r} \Psi = E\Psi$$

Revisão do Átomo de Hidrogênio

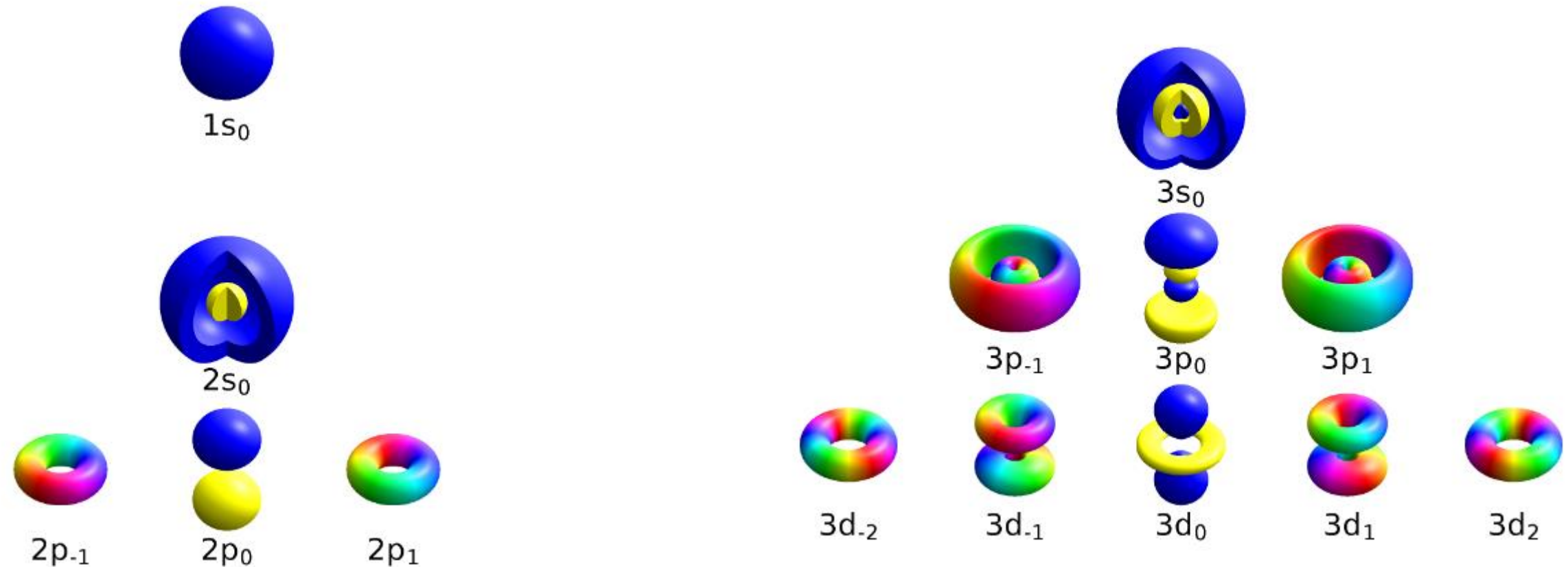
Equação de Schrödinger para o átomo de hidrogênio:

$$\frac{-\hbar^2}{8\pi^2m} \nabla^2 \Psi - \frac{e^2}{4\pi\epsilon_0 r} \Psi = E\Psi$$

**Energia Cinética do
Elétron**

**Potencial
Coulombiano**

Revisão do Átomo de Hidrogênio



Resolvendo a equação, são obtidos três números quânticos (n, l, m). Qual o significado físico de cada um?

Revisão do Átomo de Hidrogênio

$$\Psi(r, \theta, \phi) = R(r) P(\theta) F(\phi)$$

n

ℓ

m_ℓ

Número
quântico
principal

Número
quântico
orbital

Número quântico
magnético

$$E = -\frac{m_e Z^2 e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2}$$

De átomos para moléculas

Como saímos de orbitais atômicos para orbitais moleculares?

Como resolvemos a equação de Schroedinger para moléculas?

De átomos para moléculas

Como resolvemos a equação de Schroedinger para moléculas?

1. Não é possível obter a solução da equação para mais de um elétron -> Problema de muitos corpos
2. Um bom começo são os orbitais atômicos -> Combinação Linear de Orbitais Atômicos (LCAO)

LCAO - Exemplo Molécula de H₂

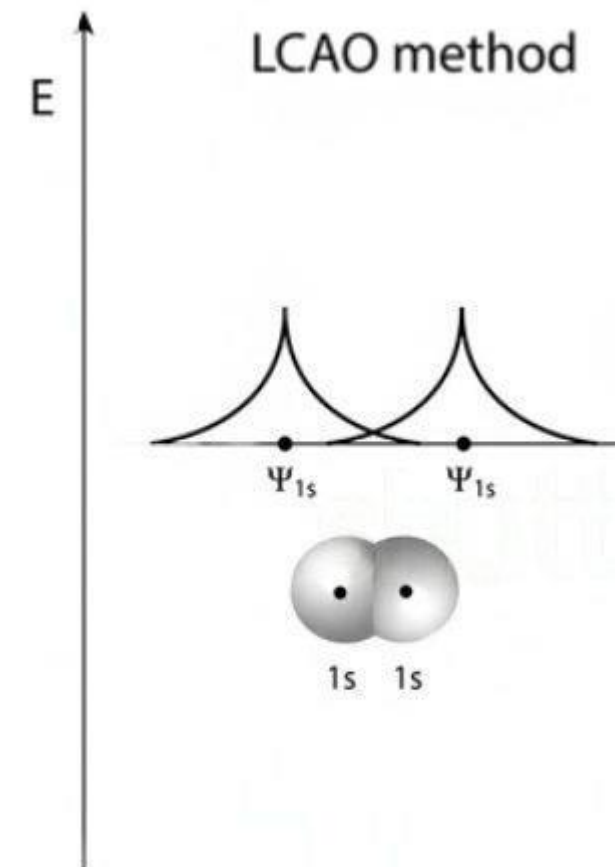
$E_a = E_b = e$ (Energia de átomo isolado)

X : Interação do elétron do átomo 1 com o elétron do átomo 2

$$\begin{pmatrix} e & X \\ X & e \end{pmatrix}$$

Autovalor: Energias do sistema

Autovetor: Função de onda do sistema

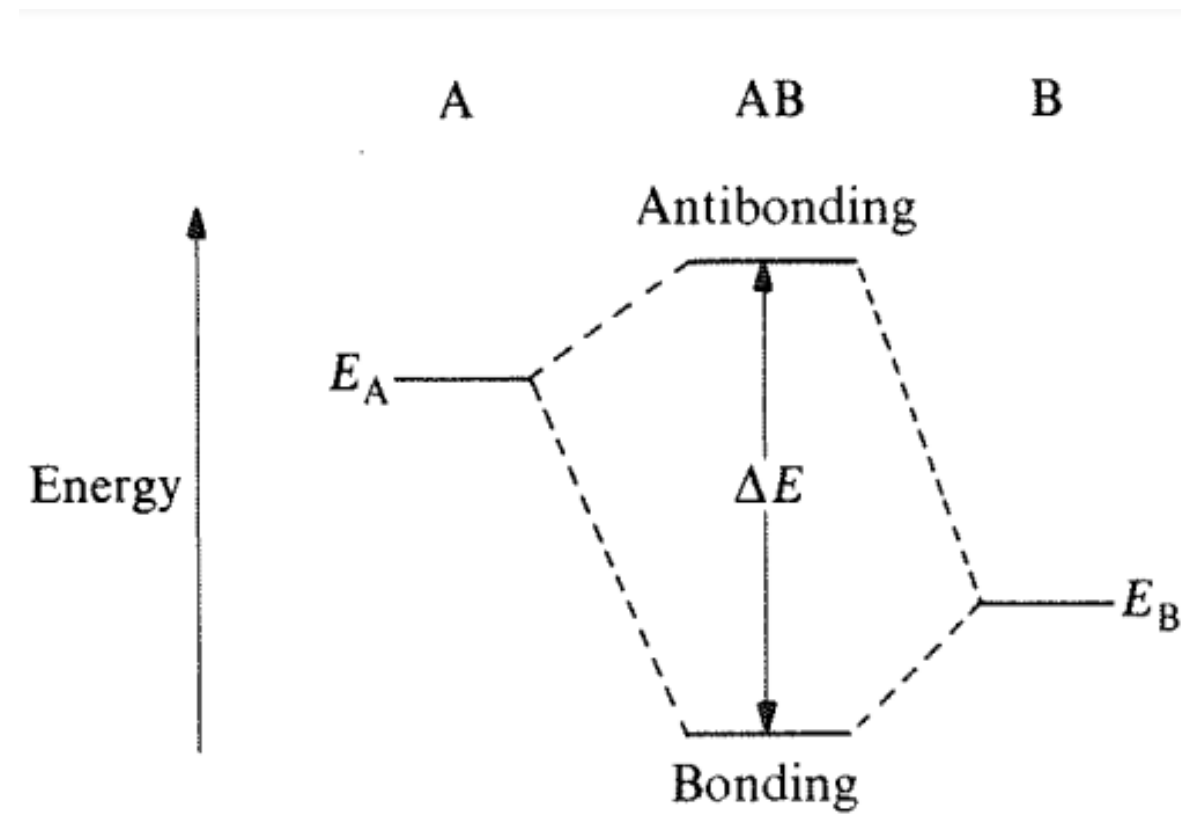


LCAO - Energia Molécula de H₂

Energias:

1^o autovalor: $e-X$

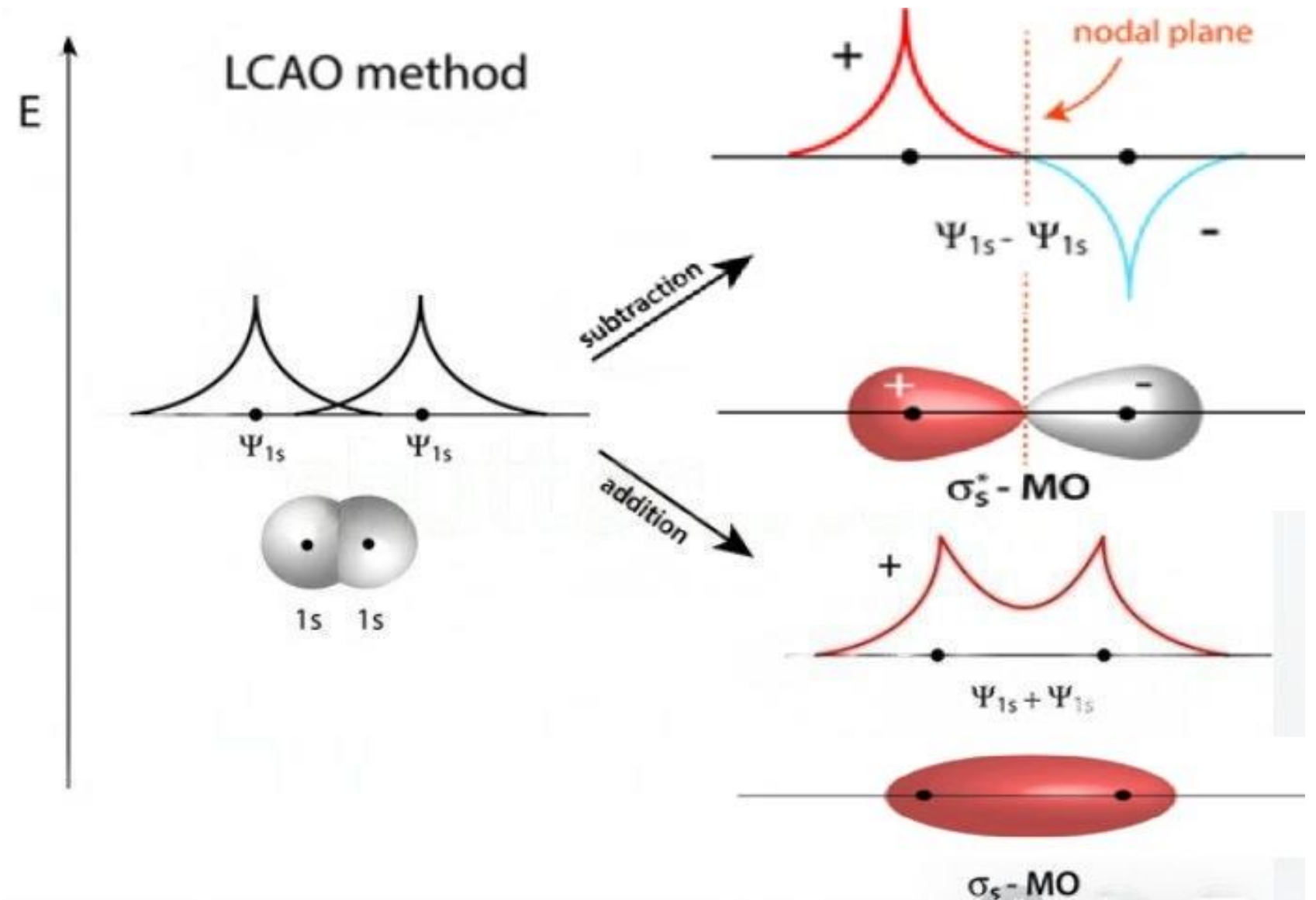
2^o autovalor: $e+X$



LCAO - Função de onda do H_2

Autovetores:

$(1,1)$ e $(1,-1)$



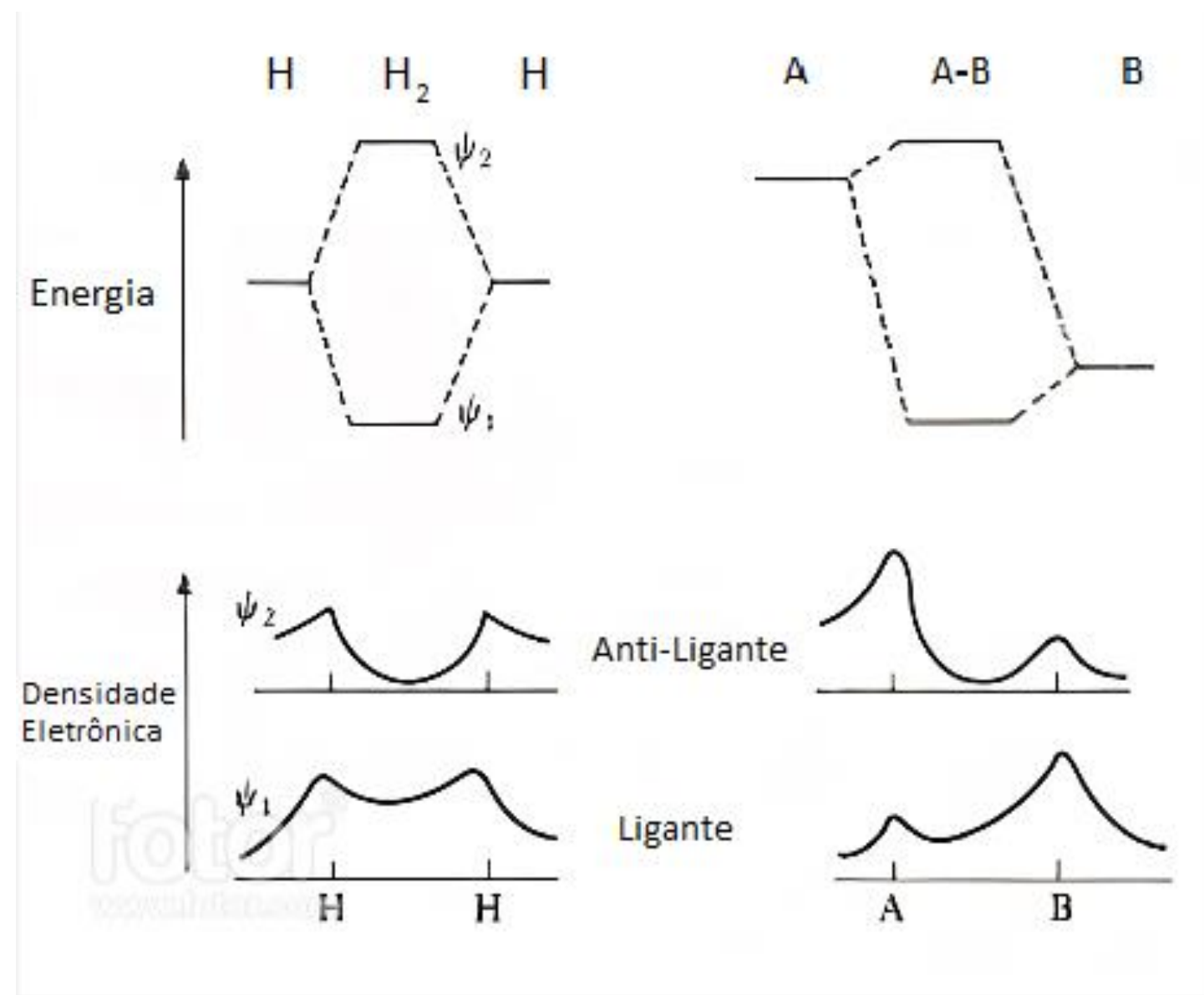
LCAO - Ligação Iônica e Covalente

Ligação Covalente:

Átomos têm a mesma energia ($E_a = E_b = e$)

Ligação Iônica:

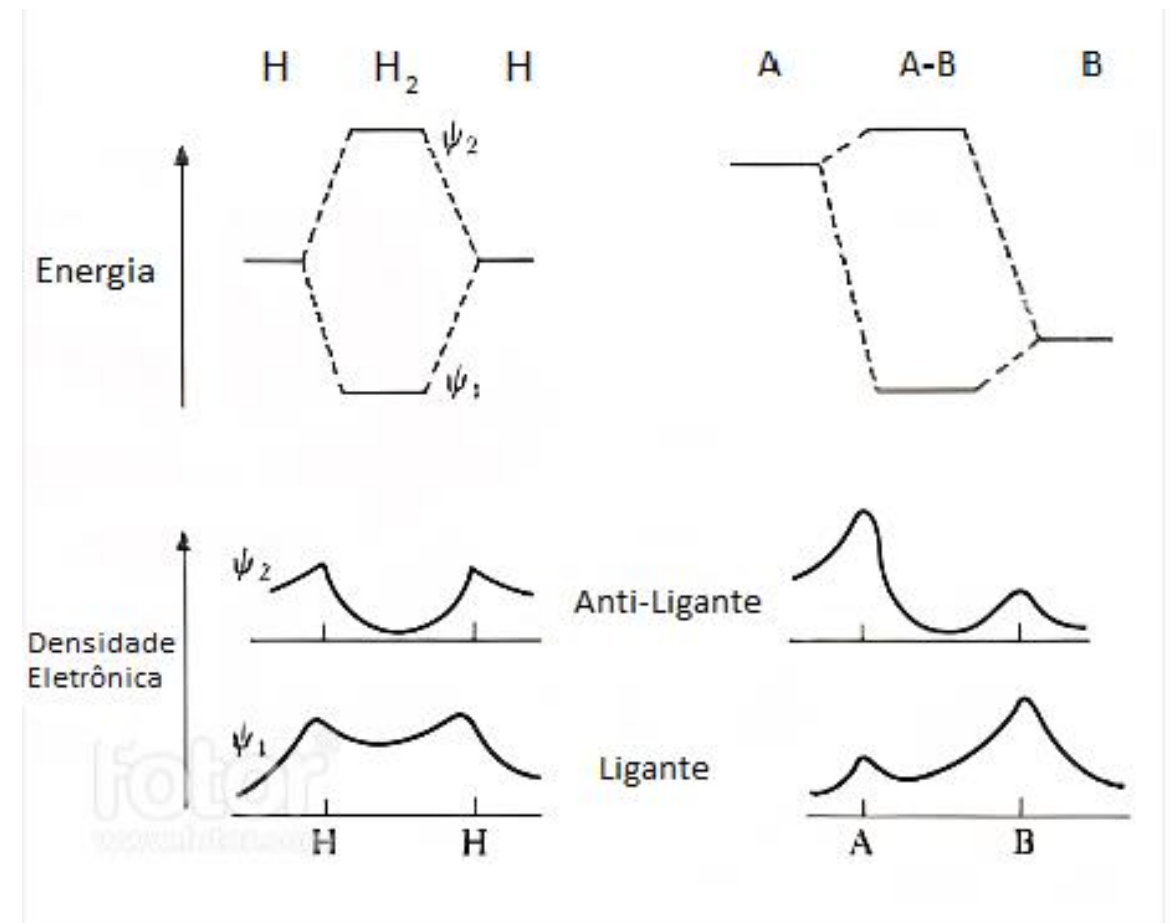
Átomos têm energias diferentes ($E_a > E_b$)



LCAO - Ligação Iônica e Covalente

Ligação Iônica:

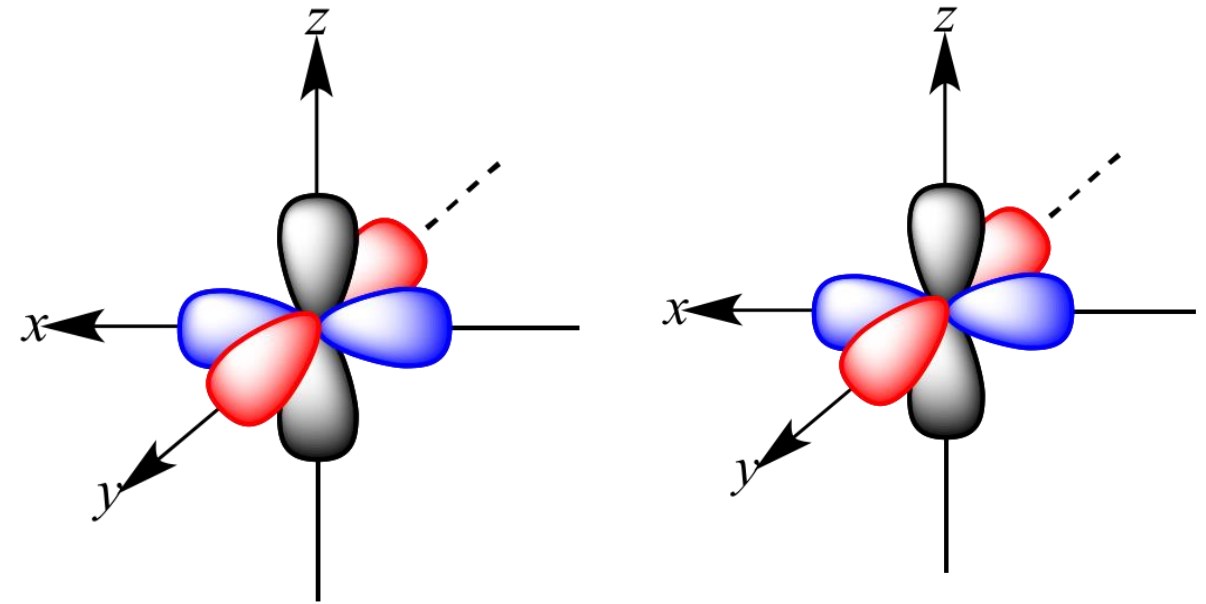
- ⌘ Maior densidade eletrônica no átomo mais eletronegativo
- ⌘ Ainda apresenta um caráter covalente (compartilhamento de elétrons)



LCAO - Orbitais p

Orbitais p_x : ligação σ

Orbitais p_y e p_z : ligação π



LCAO - Orbitais p

Orbitais p_x : ligação σ (s)

Orbitais p_y e p_z : ligação π (p)

$$\begin{array}{cccccc} p_{x1} & p_{y1} & p_{z1} & p_{x2} & p_{y2} & p_{z2} \\ \left(\begin{array}{cccccc} e & 0 & 0 & s & 0 & 0 \\ 0 & e & 0 & 0 & -p & 0 \\ 0 & 0 & e & 0 & 0 & -p \\ s & 0 & 0 & e & 0 & 0 \\ 0 & -p & 0 & 0 & e & 0 \\ 0 & 0 & -p & 0 & 0 & e \end{array} \right) & \begin{array}{l} p_{x1} \\ p_{y1} \\ p_{z1} \\ p_{x2} \\ p_{y2} \\ p_{z2} \end{array} \end{array}$$

LCAO - Autovalores de Orbitais p

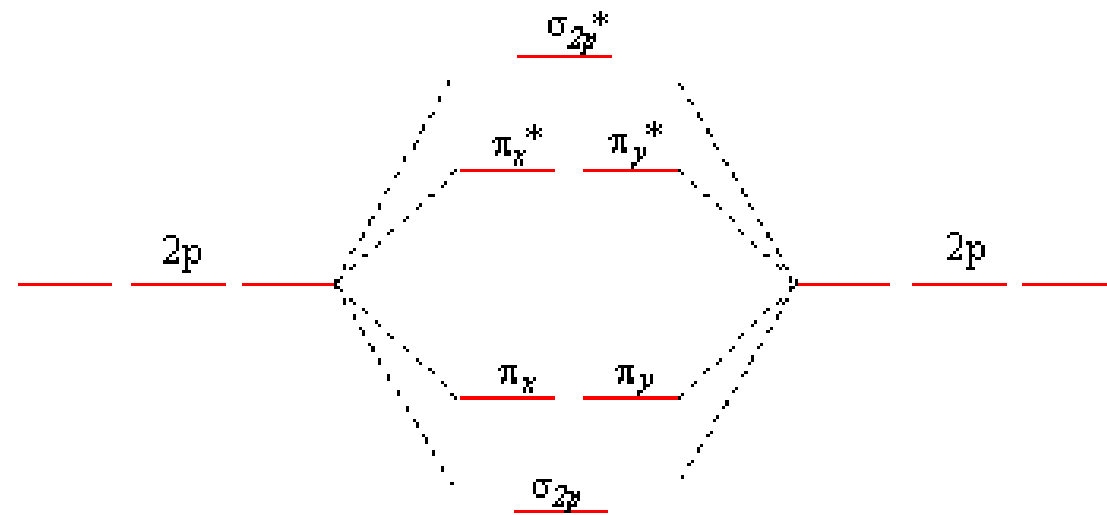
Autovalores:

e-s

e+s

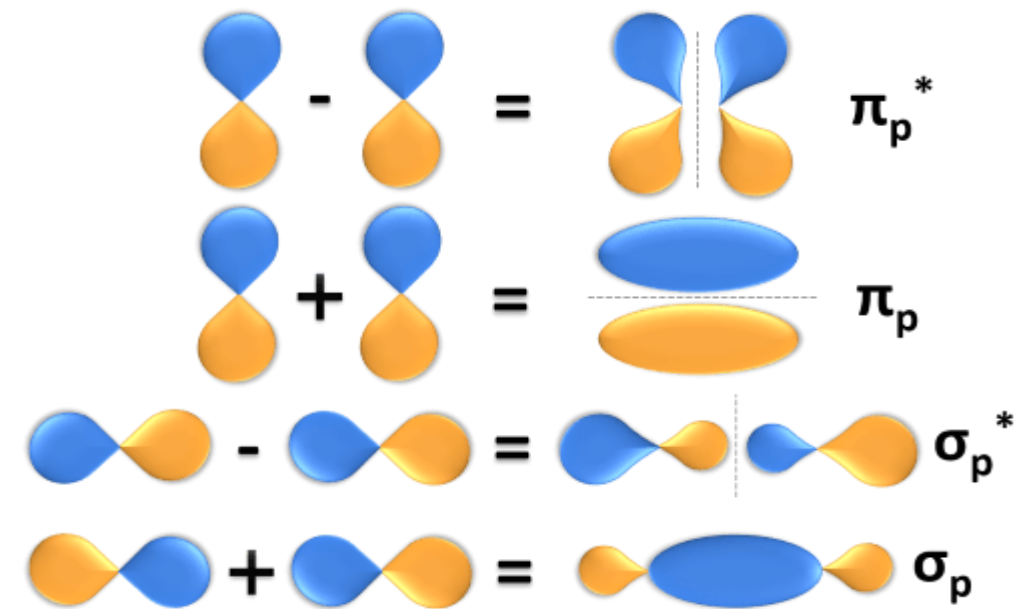
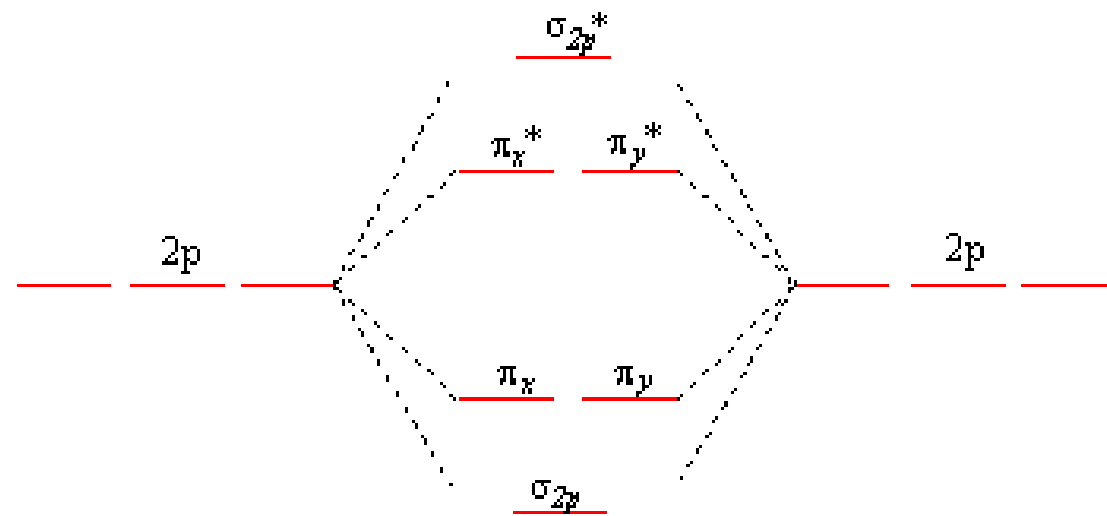
e-p (2)

e+p (2)

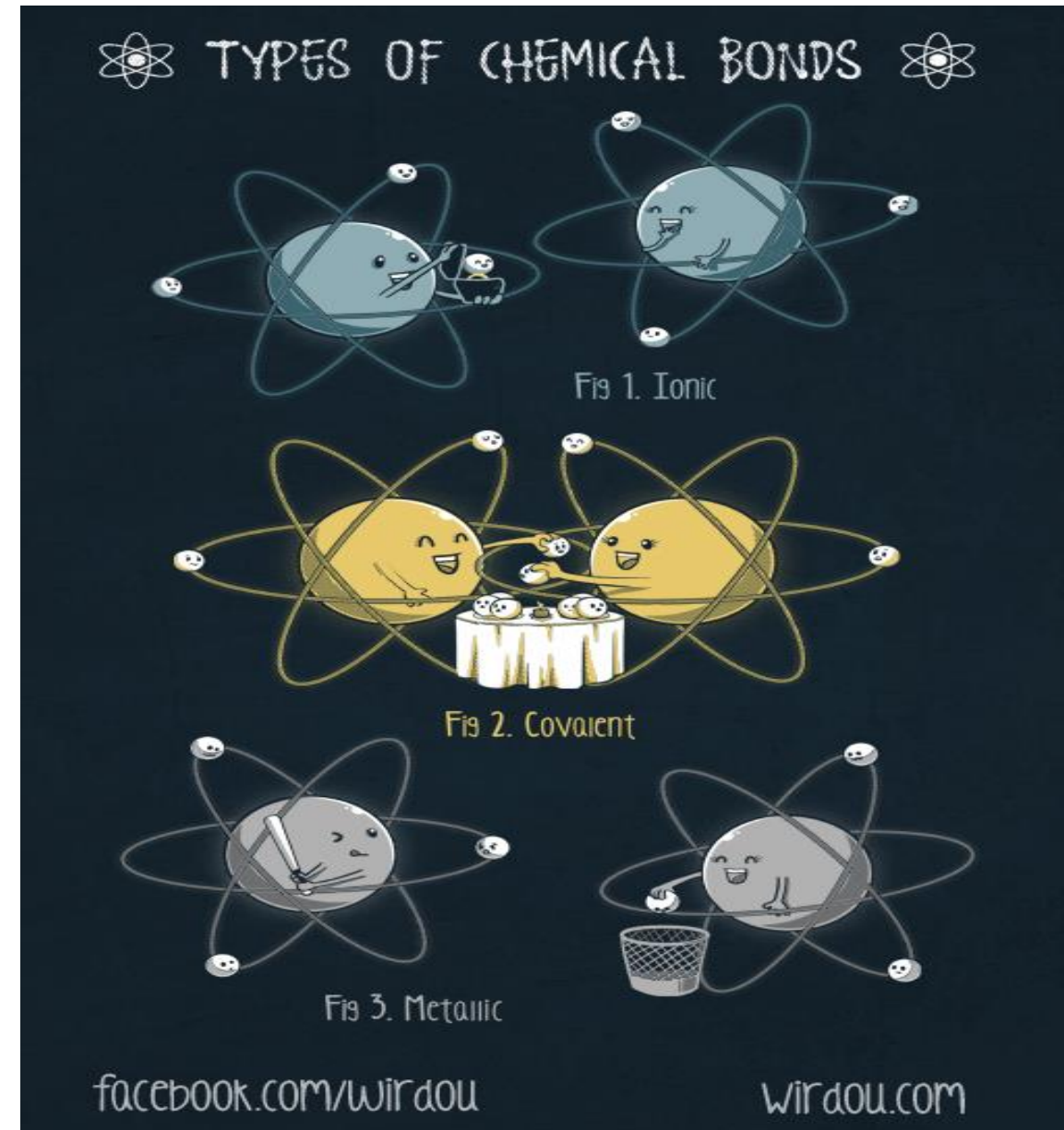
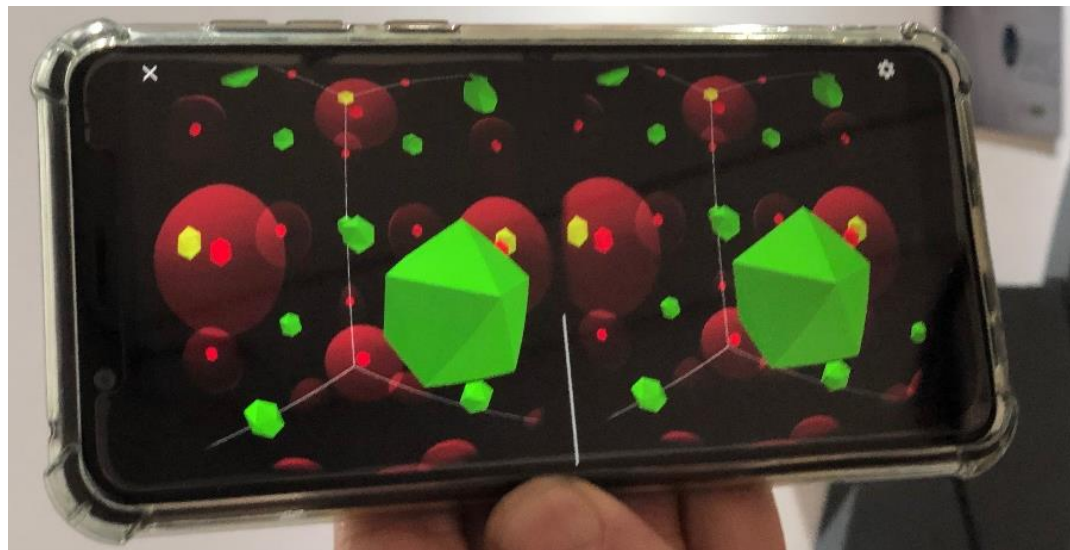
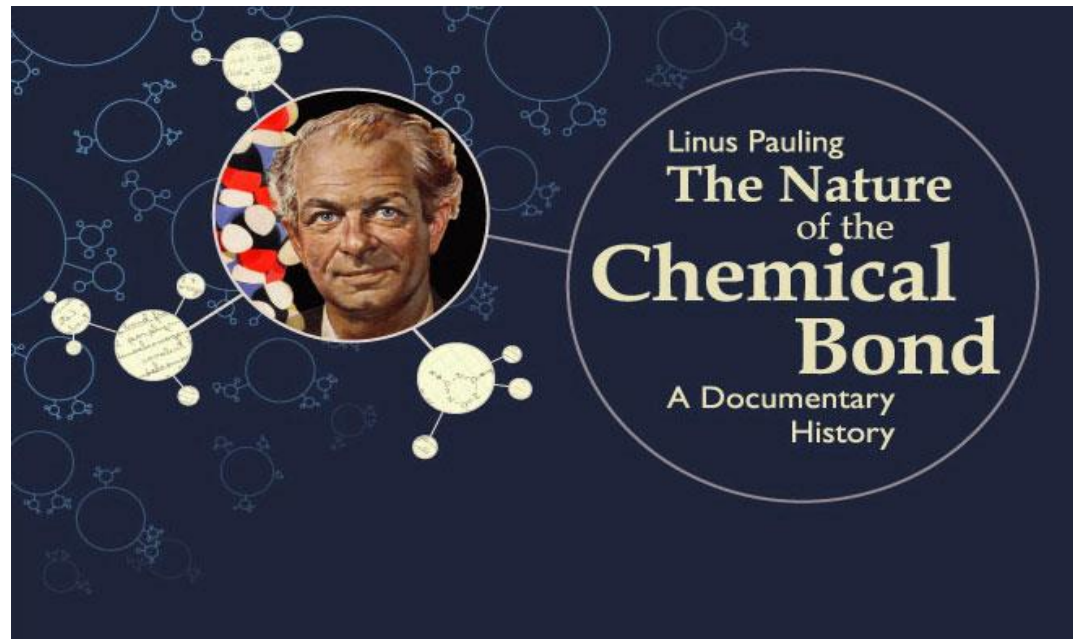


$$\begin{pmatrix} e & 0 & 0 & s & 0 & 0 \\ 0 & e & 0 & 0 & -p & 0 \\ 0 & 0 & e & 0 & 0 & -p \\ s & 0 & 0 & e & 0 & 0 \\ 0 & -p & 0 & 0 & e & 0 \\ 0 & 0 & -p & 0 & 0 & e \end{pmatrix}$$

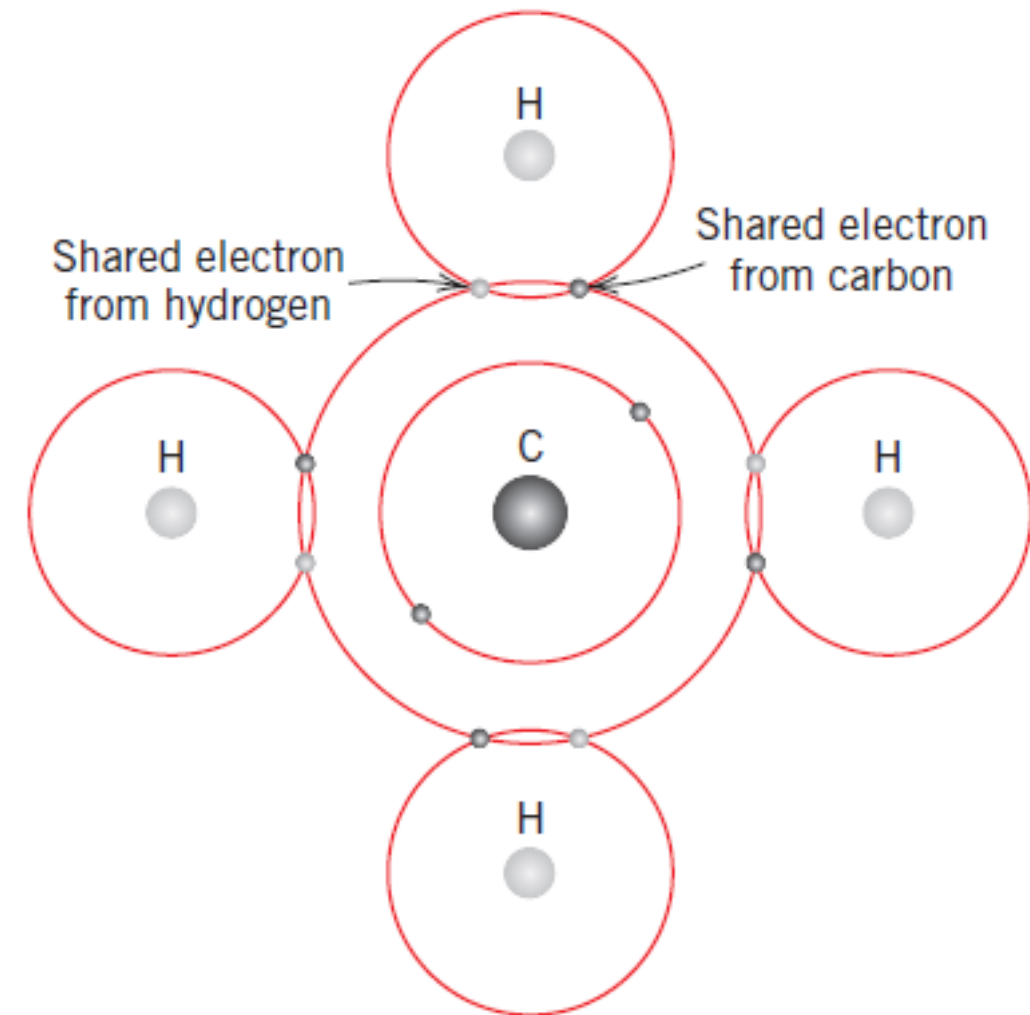
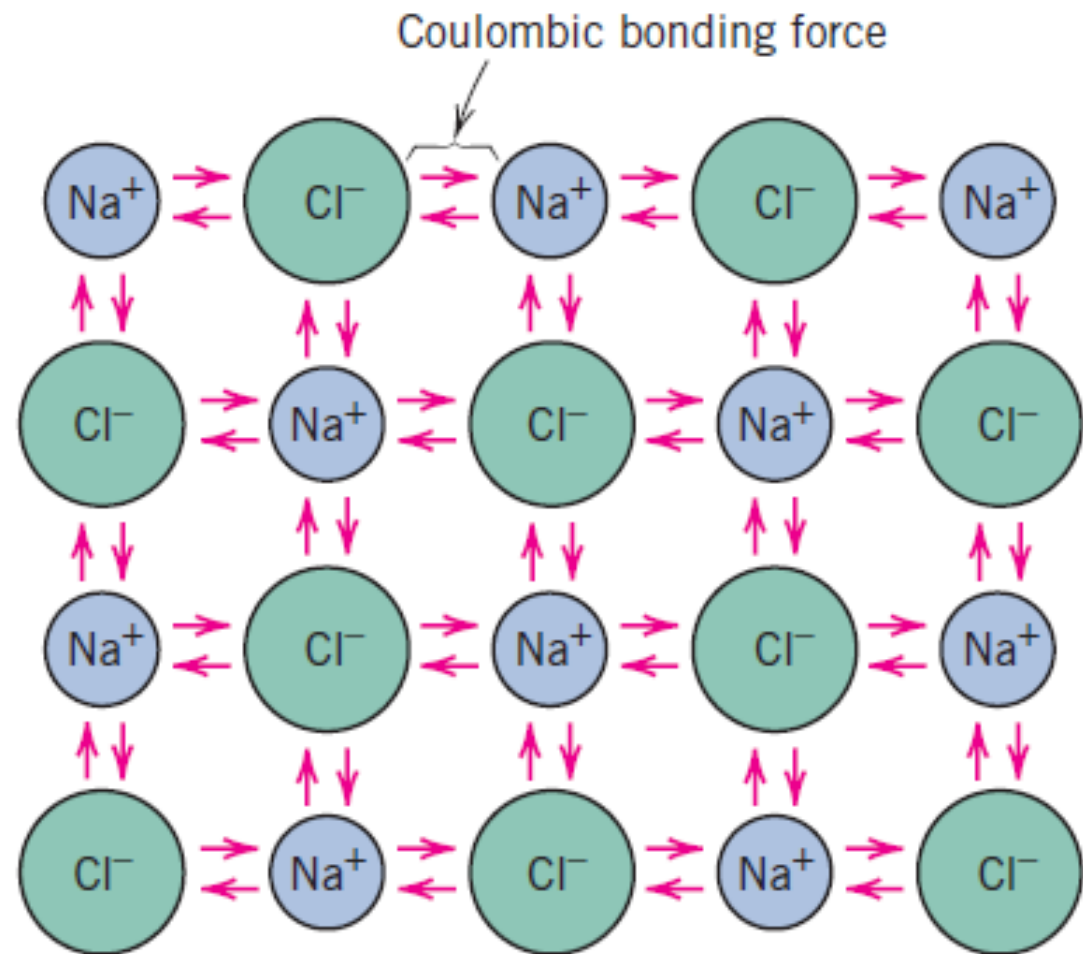
LCAO - Ligação sigma e pi



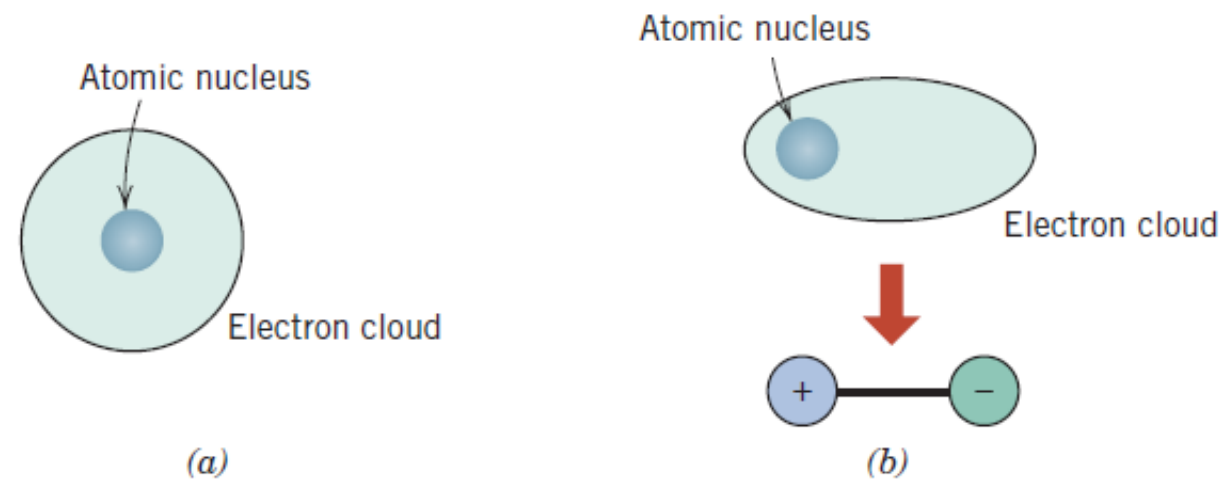
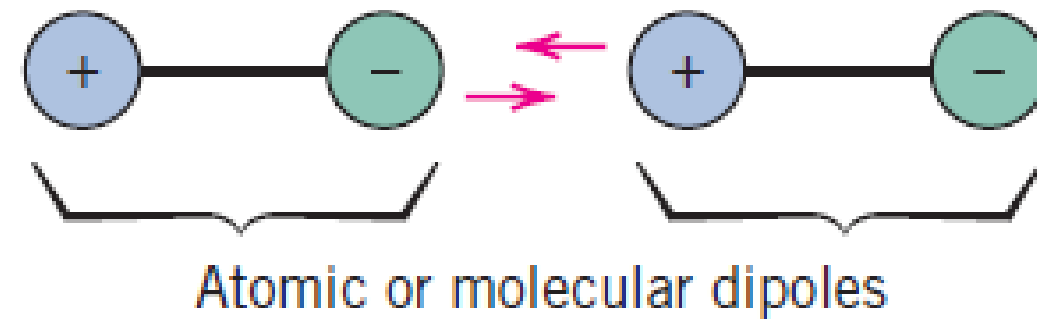
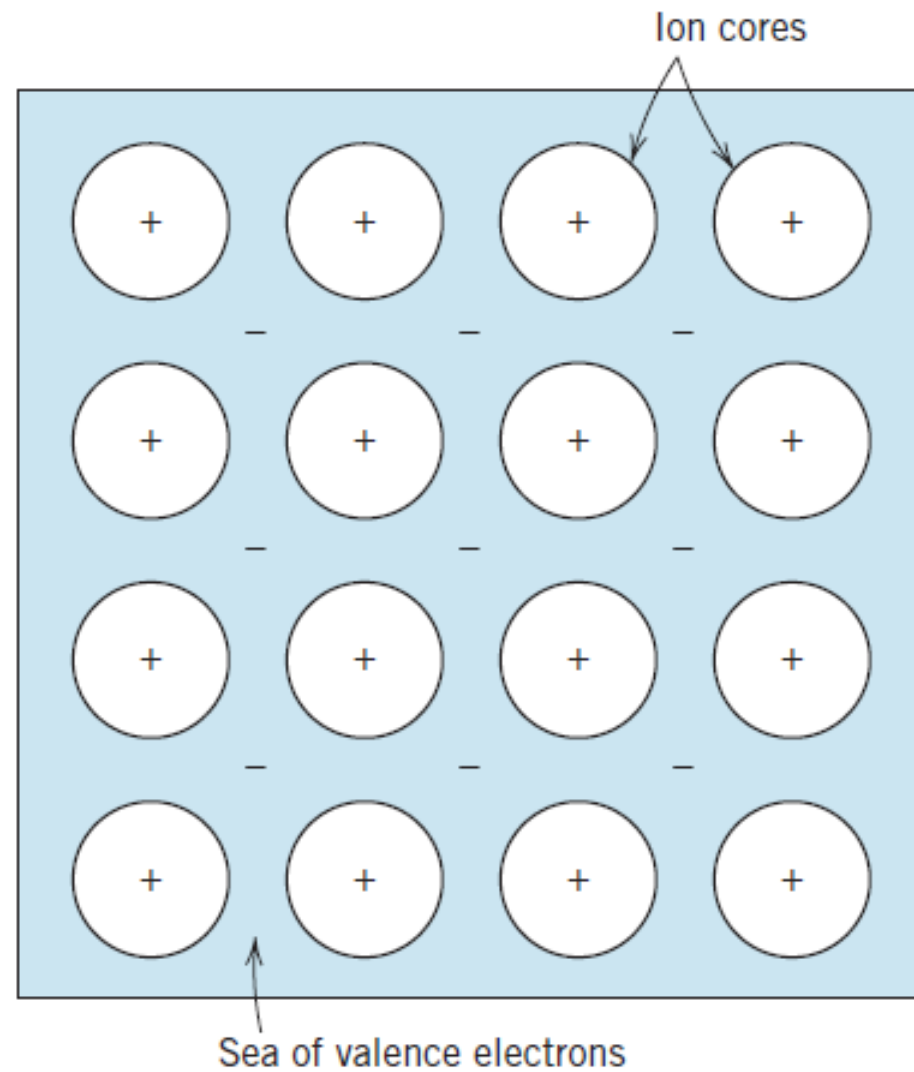
A natureza da ligação química



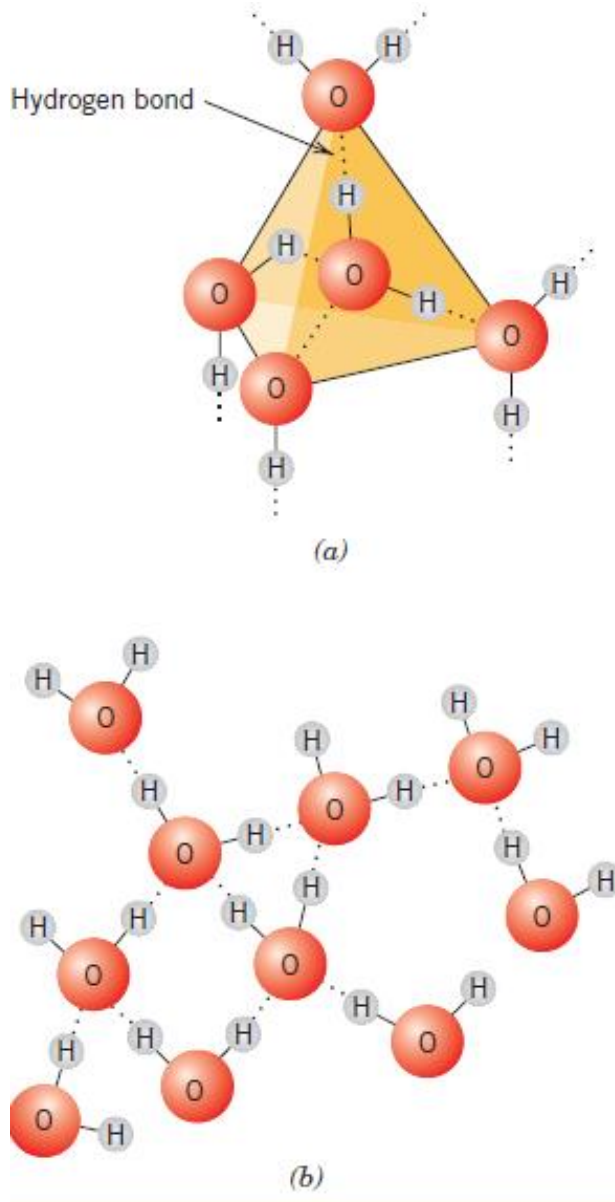
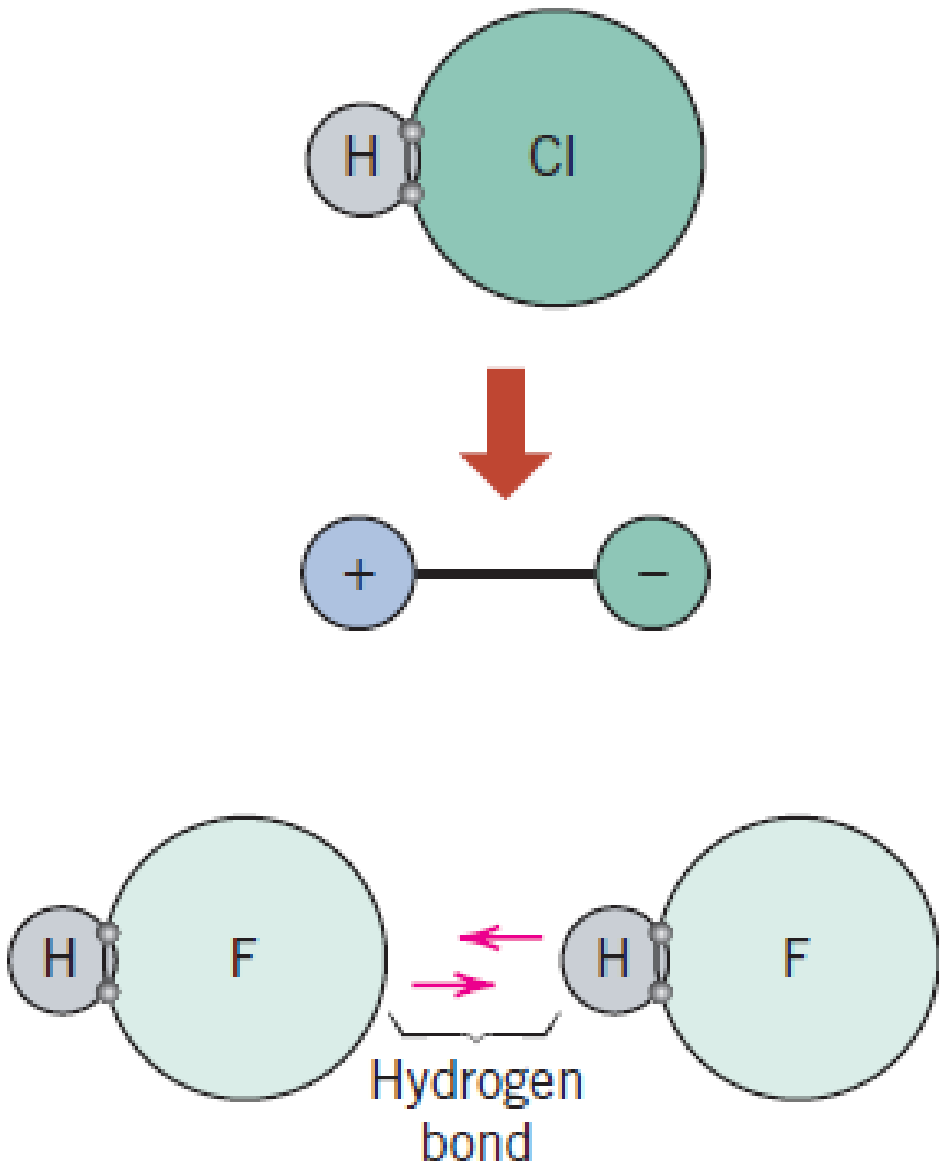
Tipos de ligação



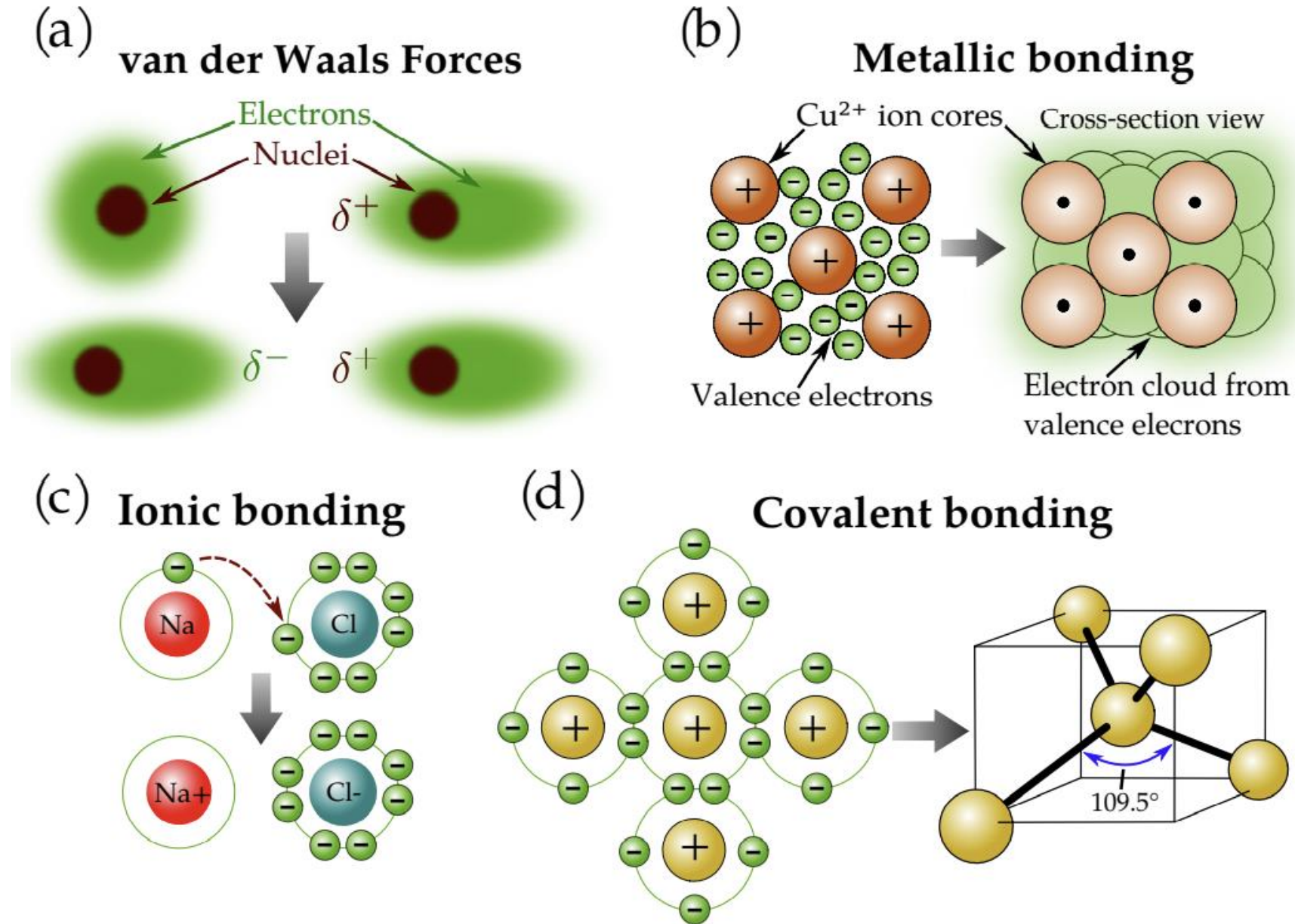
Tipos de ligação



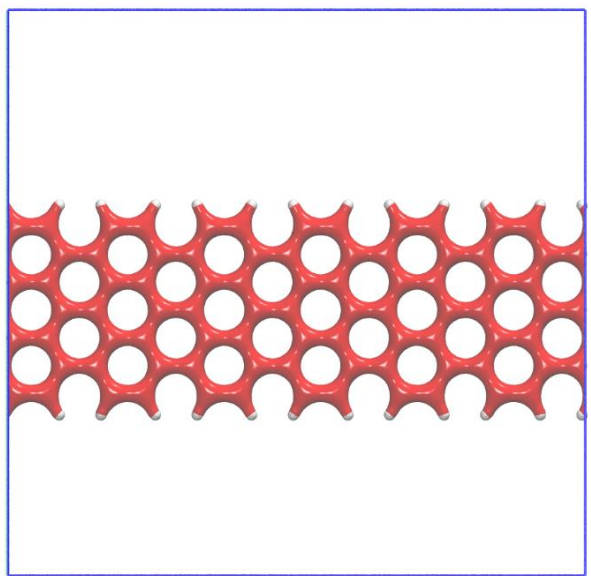
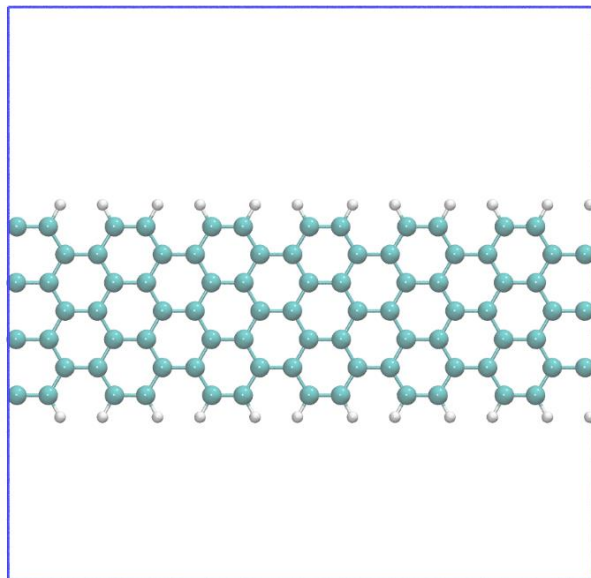
Tipos de ligação



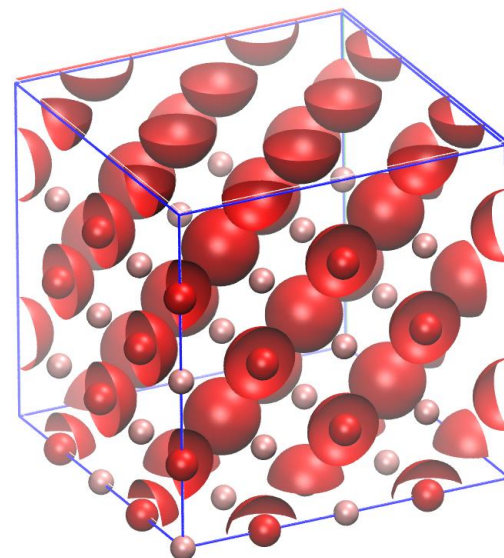
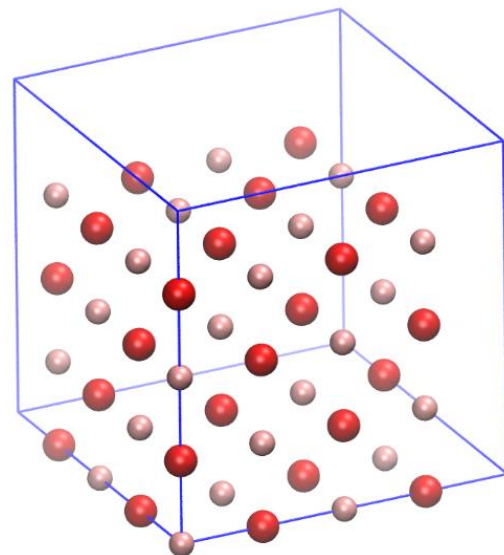
Direcional ou não direcional



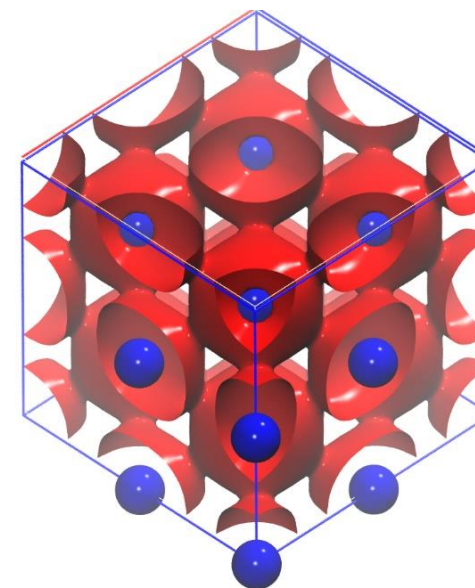
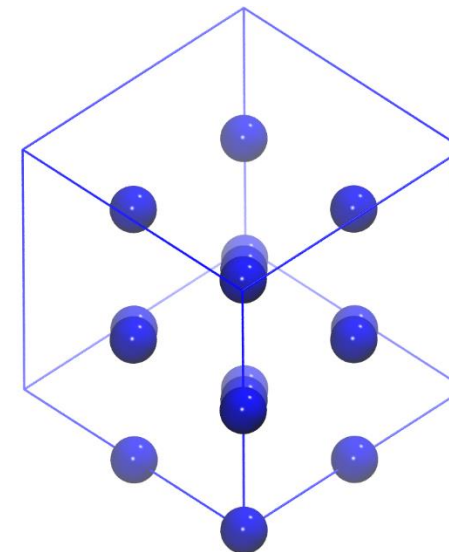
Experimentando as ligações químicas ...



Grafeno - ligação covalente



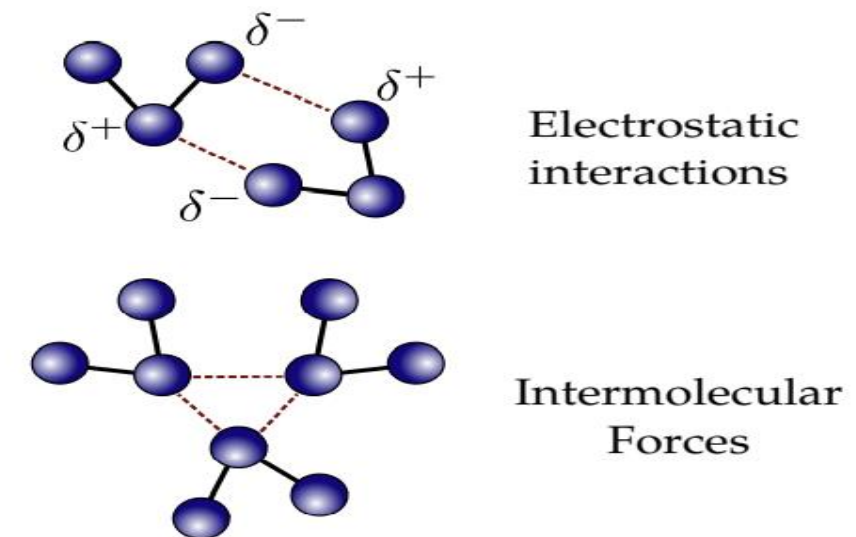
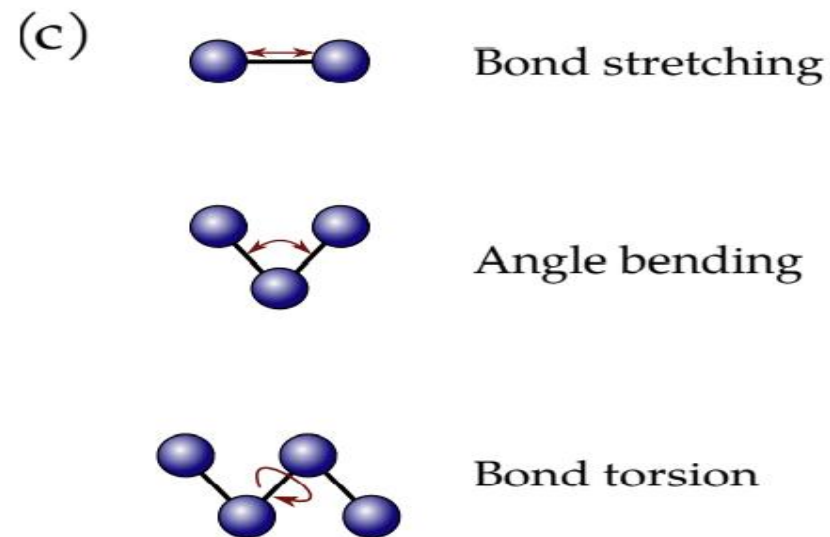
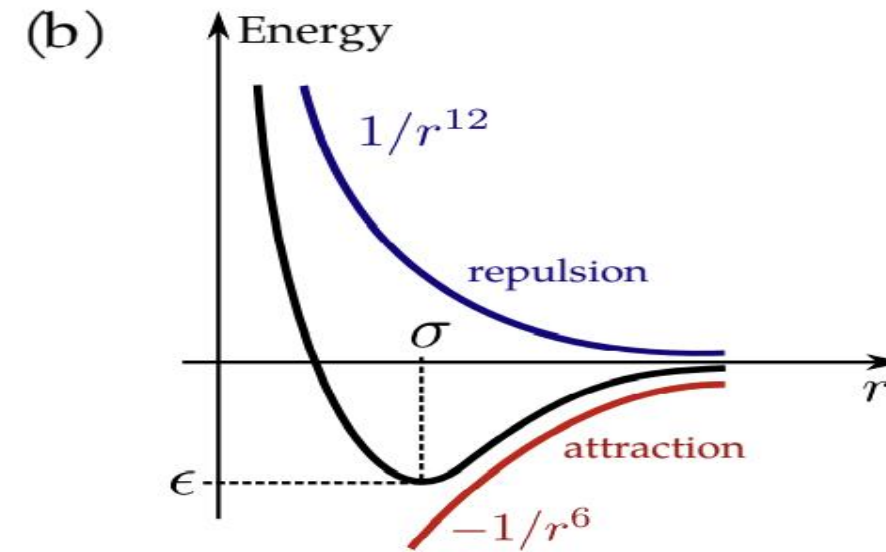
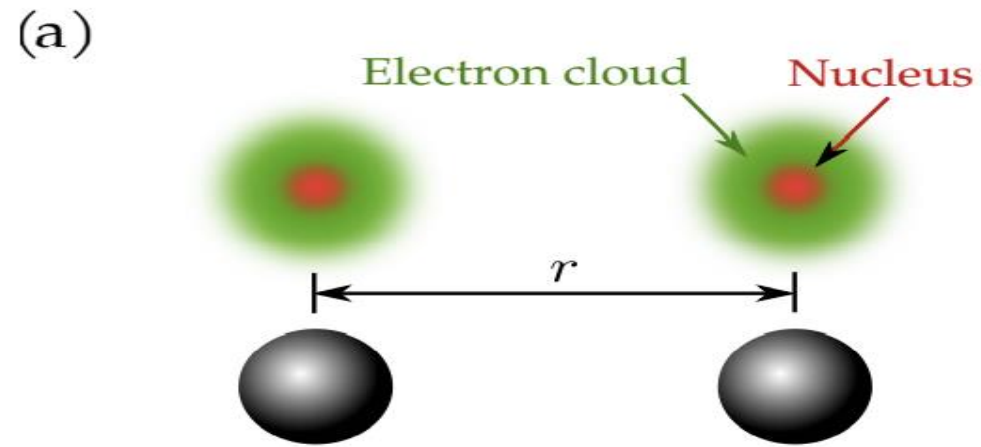
MgO – ligação iônica



Nb - ligação metálica



Modelos interatômicos



Modelos interatômicos

$$nA/r_0^{n+1} = mB/r_0^{m+1}.$$

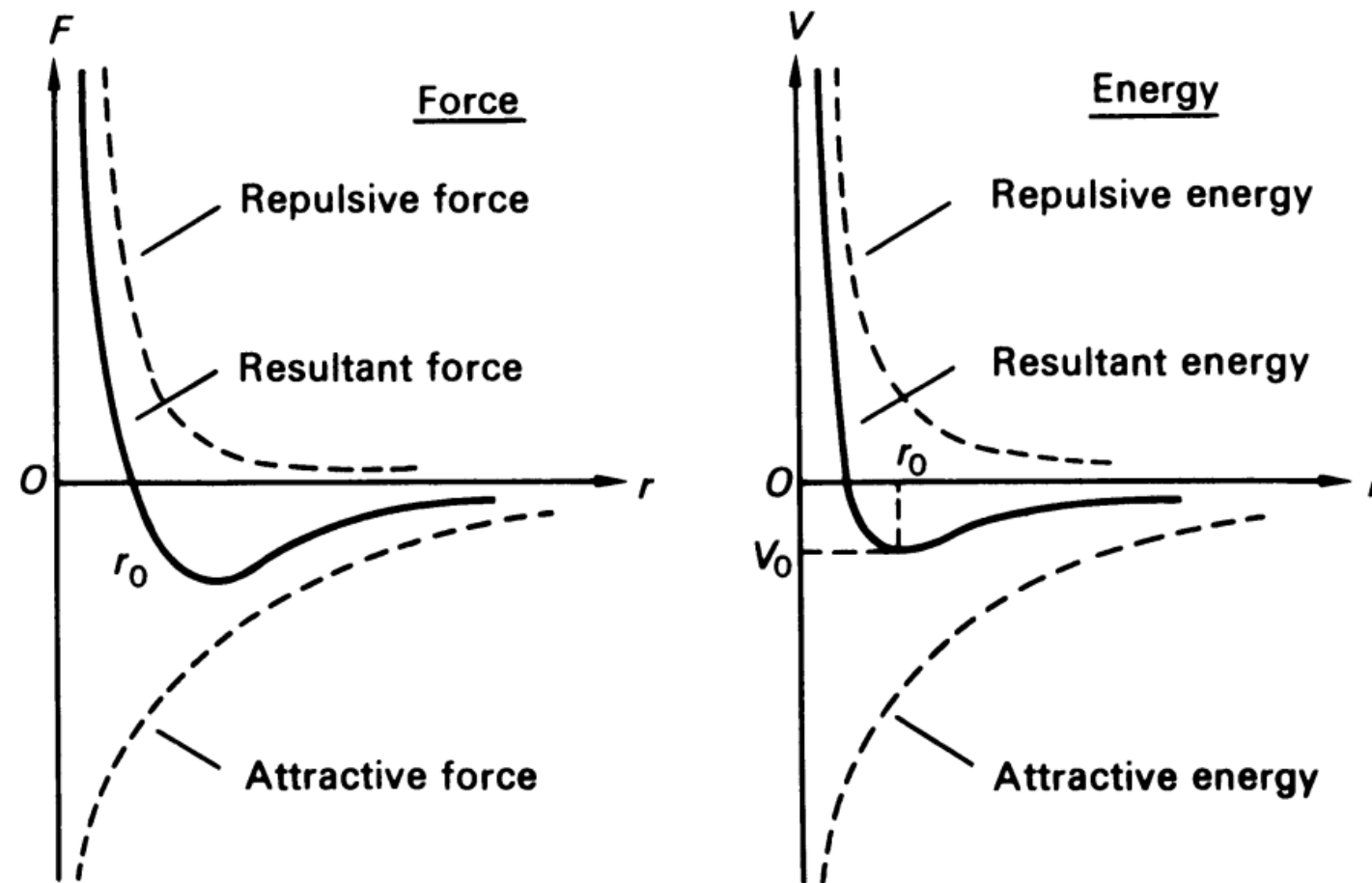
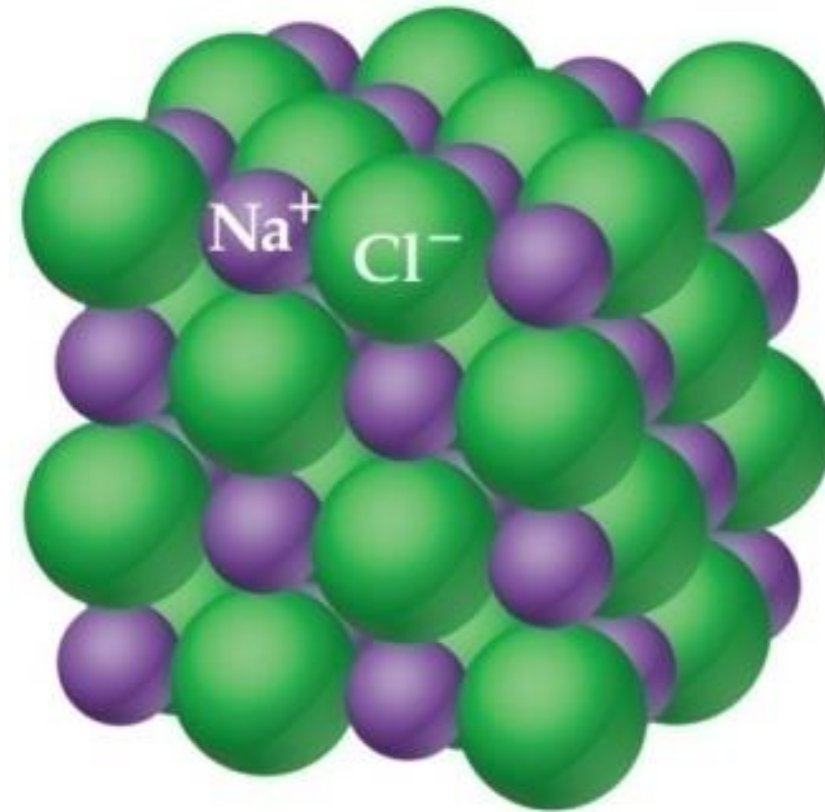
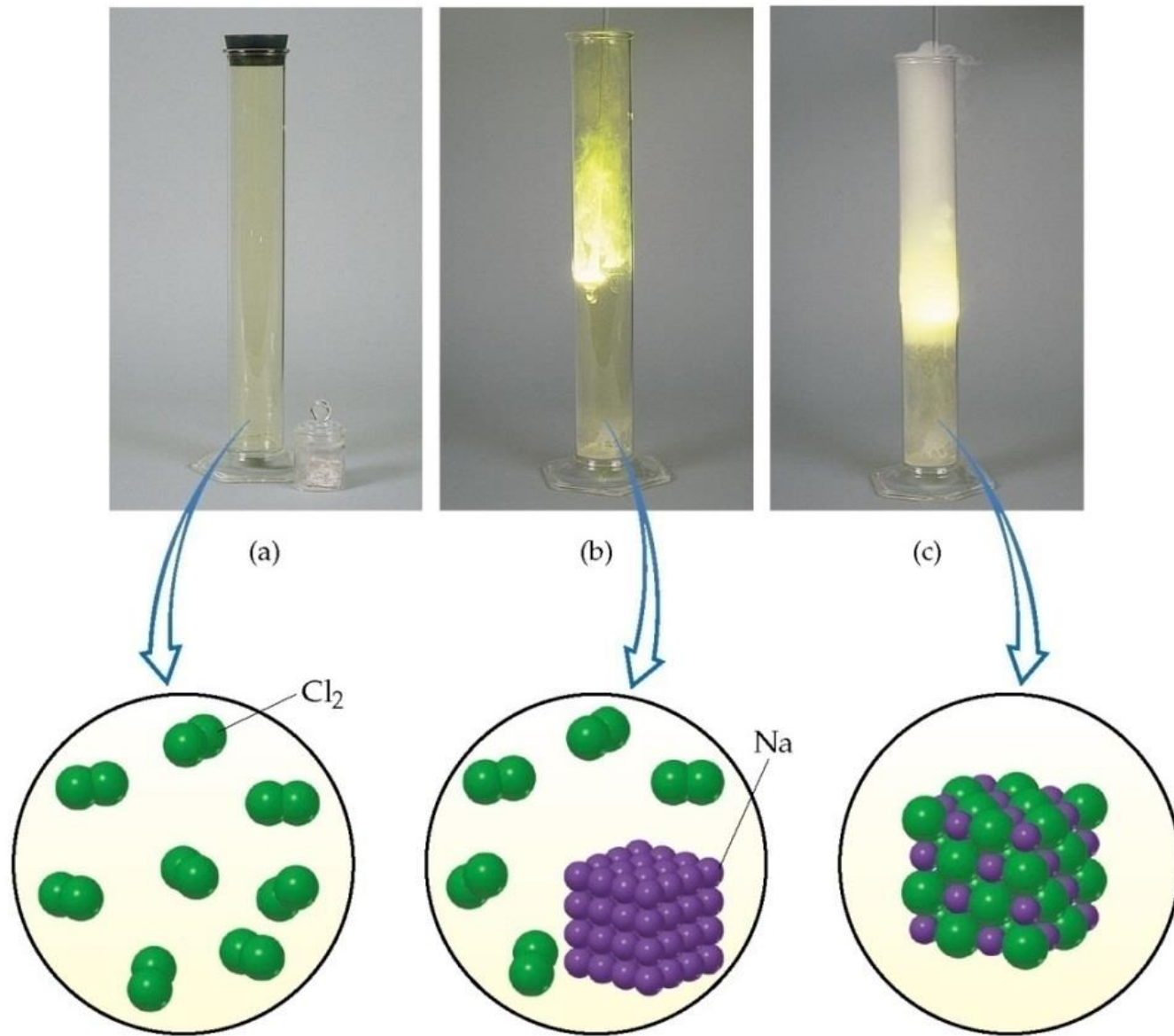


Fig. 2.1 Force and potential energy as a function of distance between two atoms.

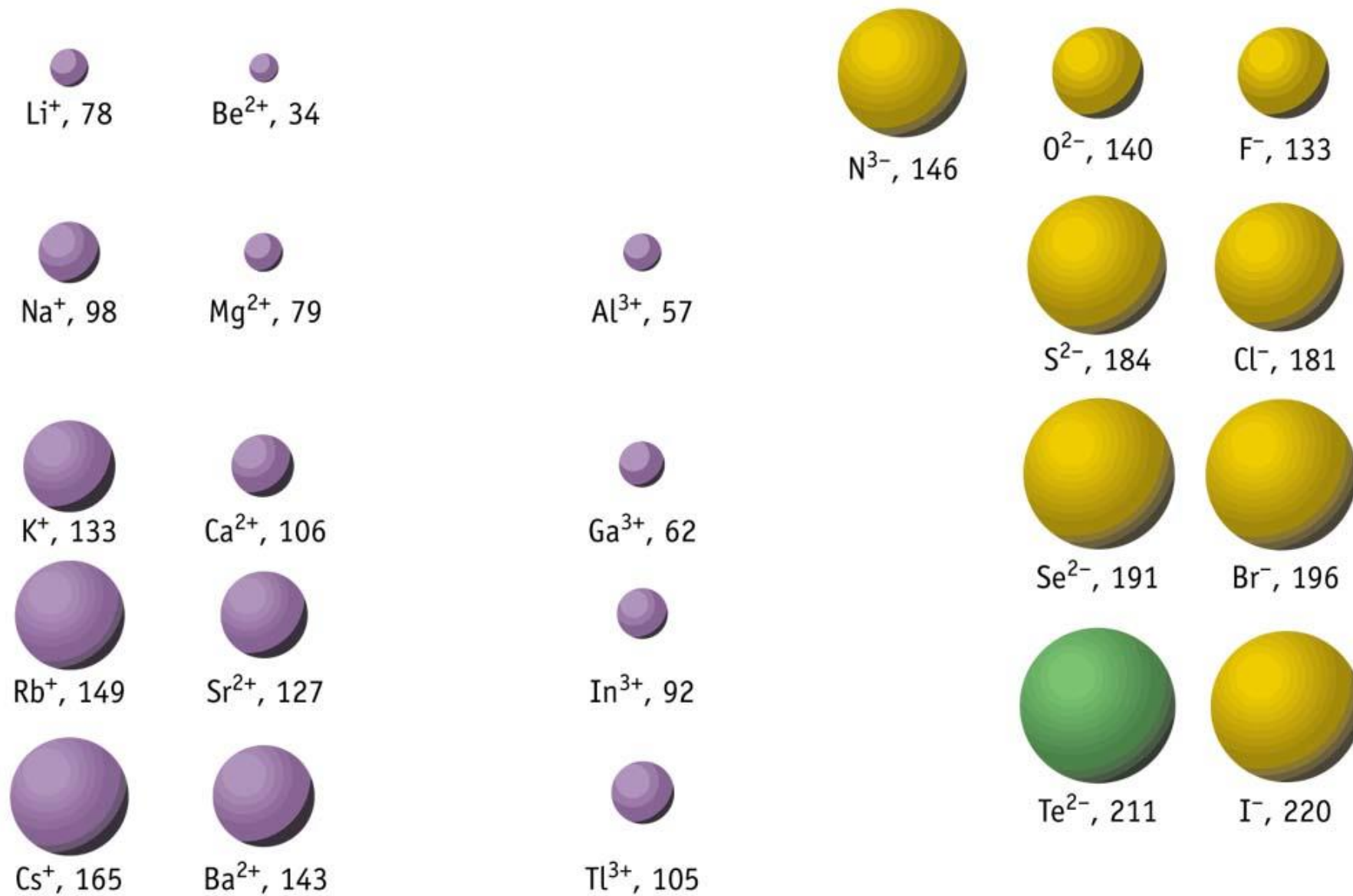
Classification of solids

<i>Property</i>	<i>Ionic</i>	<i>Covalent</i>	<i>Metallic</i>	<i>Molecular</i>
(i) Typical examples	NaCl, LiF, CaCl ₂	Diamond, Si, Ge, SiC	Na, Fe, Cu	Ar, Ne, I (C ₆ H ₁₂ O ₆) ₂ sugar
(ii) Bonding energy (J mole ⁻¹)	6-10 × 10 ⁴	2-10 × 10 ⁴	1-4 × 10 ⁴	10 ³
(iii) Melting point (K)	700-3300	500-3700	230-4150	< 600
(iv) Electrical resistivity (Ωm)	10 ¹² -10 ²⁰	10-10 ²⁰	10 ⁻³ -10 ⁻⁶	10 ¹² -10 ²⁰
(v) Thermal conductivity (Wm ⁻¹ K ⁻¹)	2-20	4-600	40-400	0.04-4
(vi) Hardness	hard but cleavable	hard	malleable	

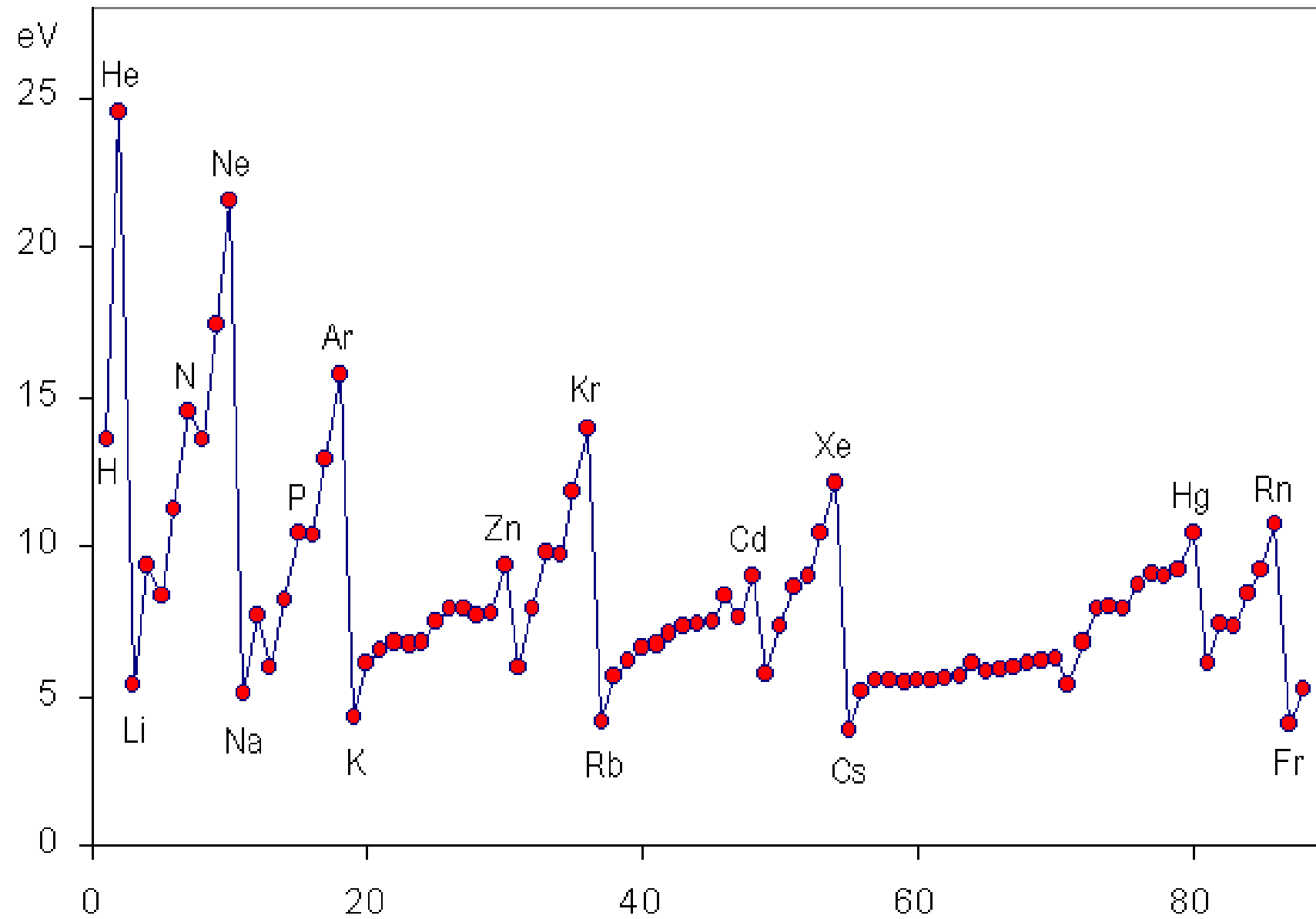
Experimento ...




Raios iônicos

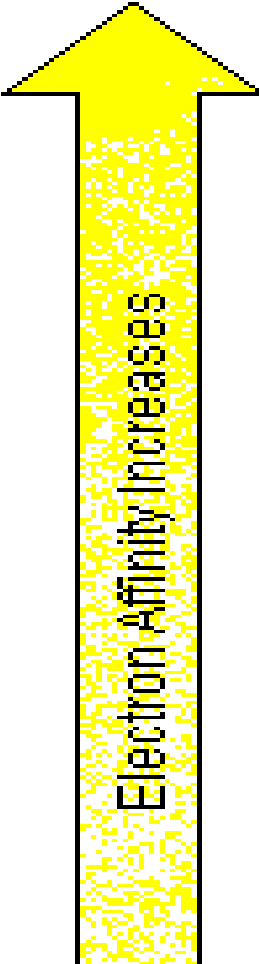


Energia de ionização



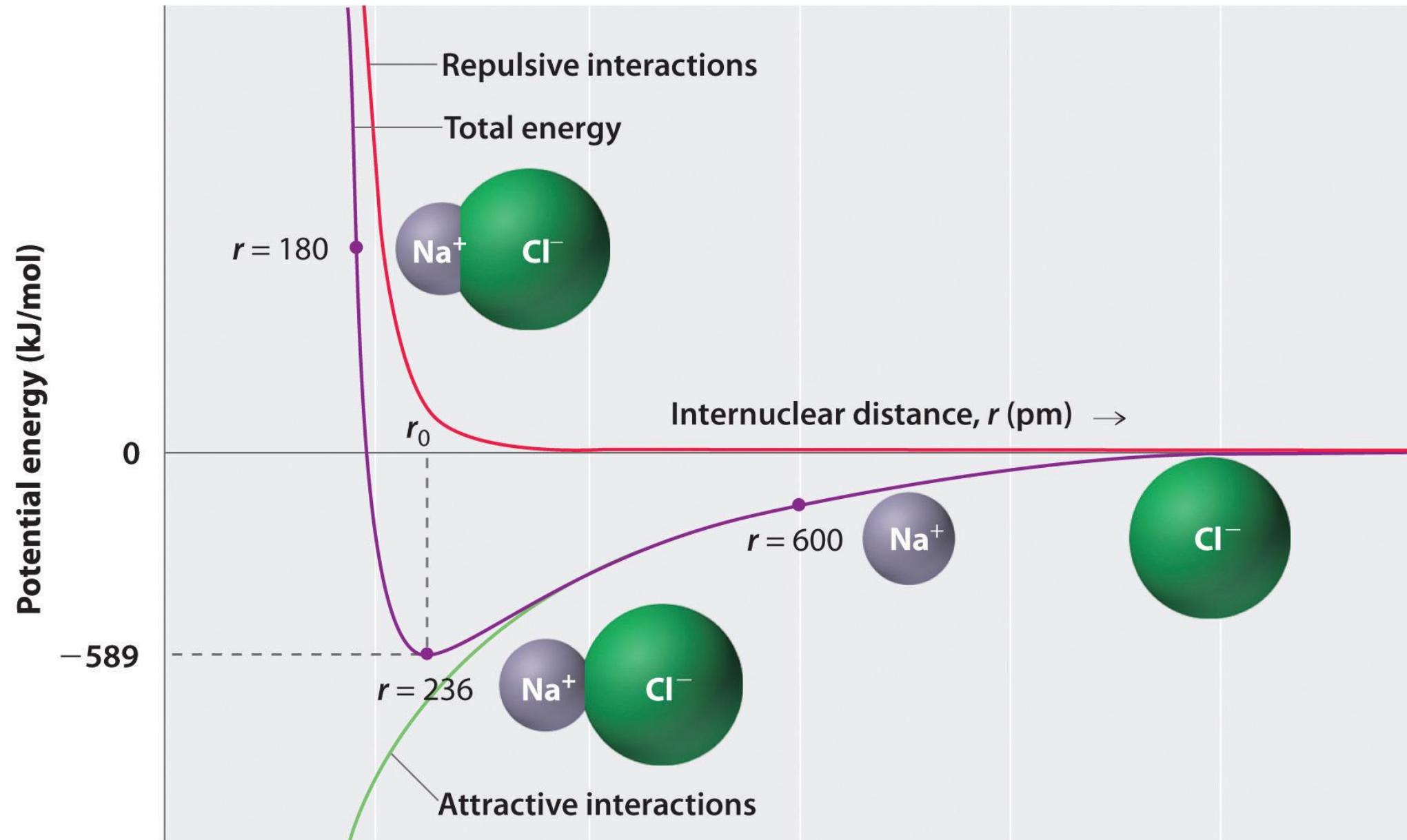
Afinidade eletrônica

Electron Affinity Increases 

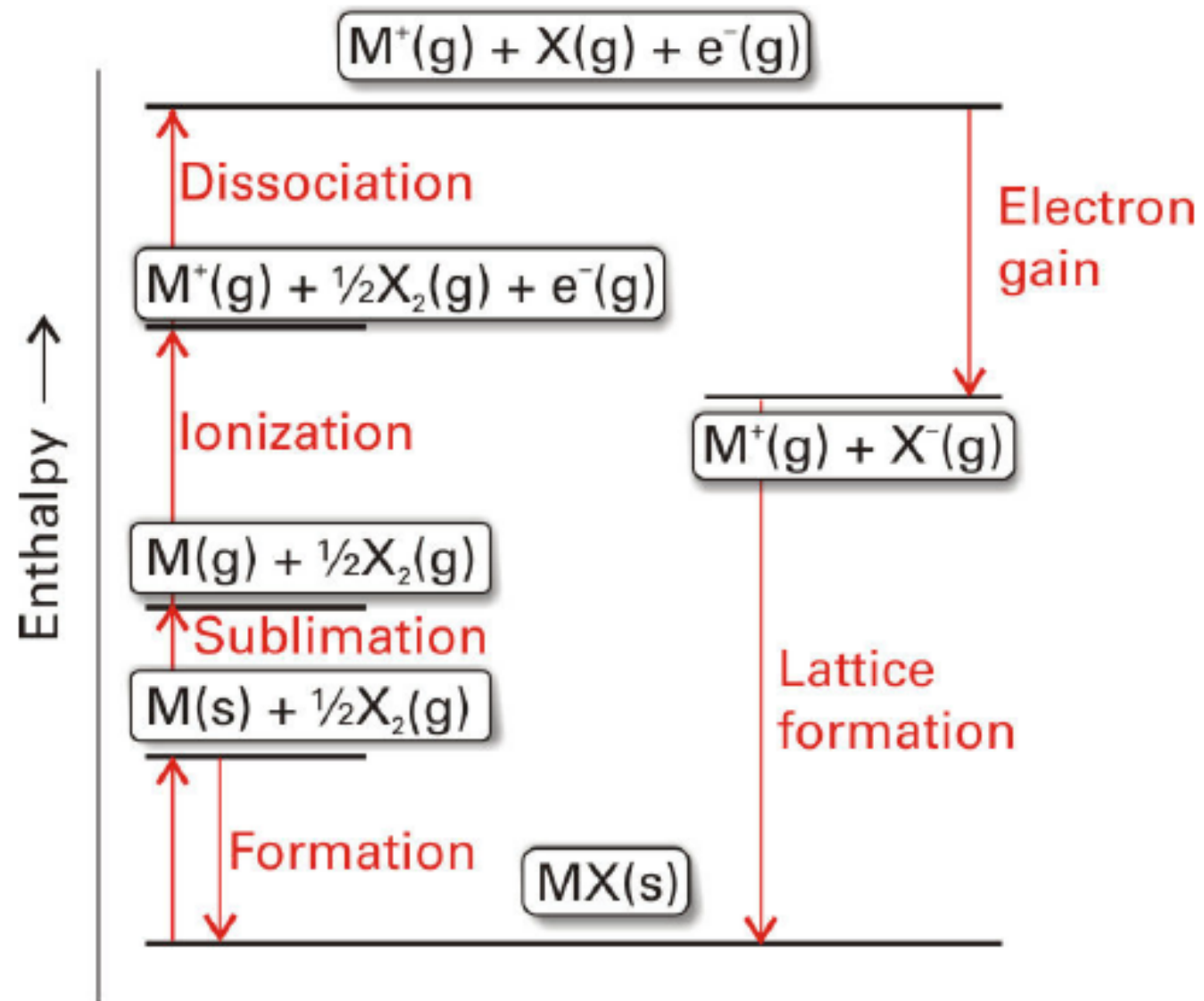
 Electron Affinity Increases

IA	IIA	III A	IV A	V A	VI A	VII A	VIII A
H 73.5	Be *	B 27	C 123.4	N -7	O 142.5	H 73.5	He *
Li 60.4	Mg *	Al 45	Si 135.0	P 72.4	S 202.5	F 331.4	Ne *
Na 53.2	Ca *	Ga 30	Ge 120	As 78	Se 197.0	Cl 352.4	Ar *
K 48.9	Sr *	In 29	Sn 122	Sb 102	Te 192.1	B 327.9	Kr *
Rb 47.4	Ba *	Tl 30	Pb 110	Bi 110	Po 190	I 298.4	Xe *
Cs 46.0	Ra *					At 270	Rn *
Fr 44.5							

Experimento imaginário ...

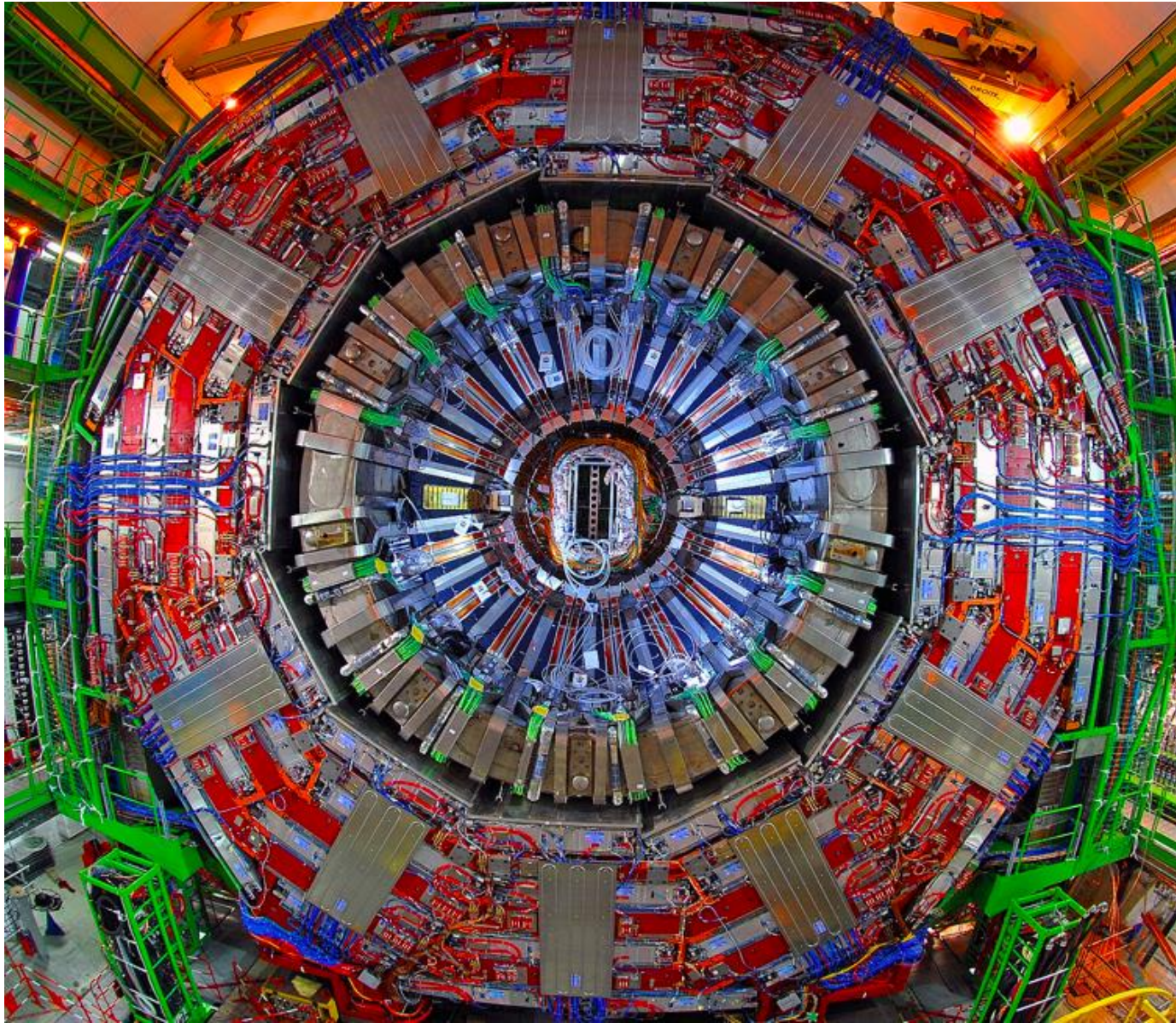


Ciclo de Born-Harber



UNIVERSOS SOB DIFERENTES PERSPECTIVAS

Simetria em ciência & arte



Simetrias

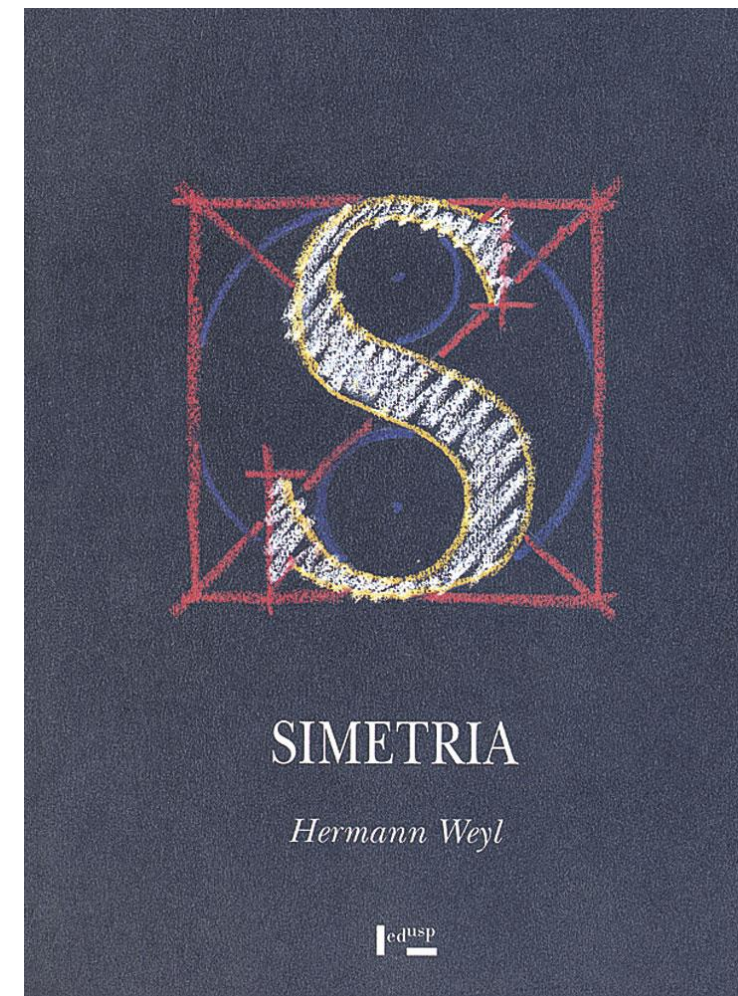
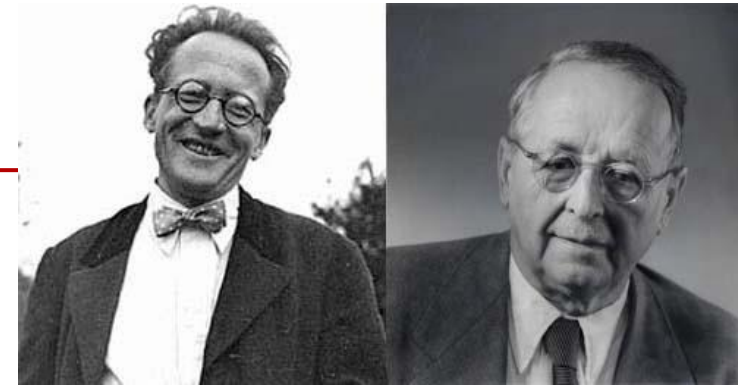
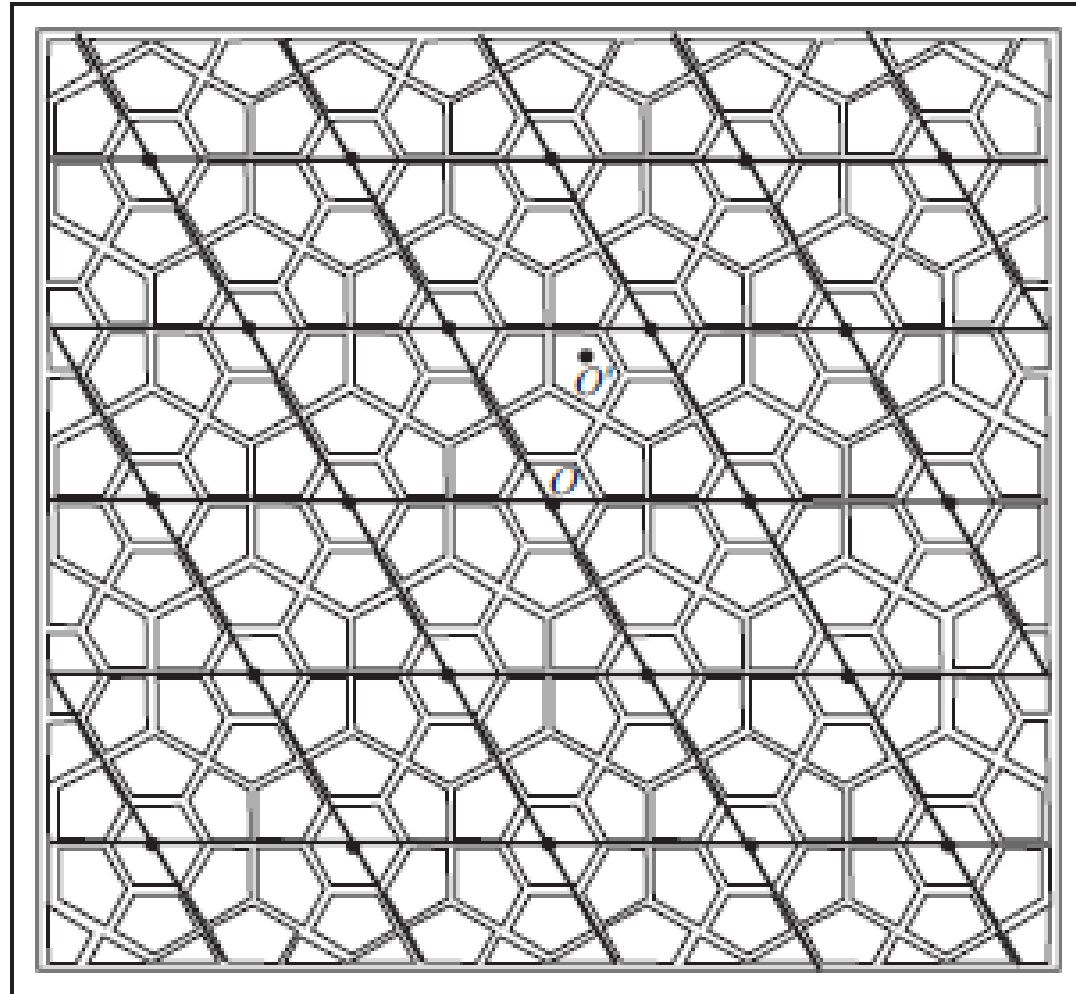
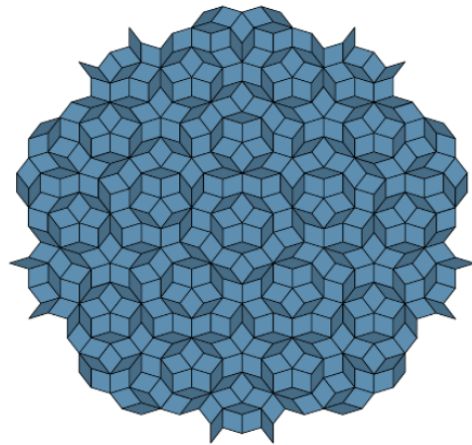


Figure 1.3.1 A 2D periodical figure and its lattice.

Ordem e desordem

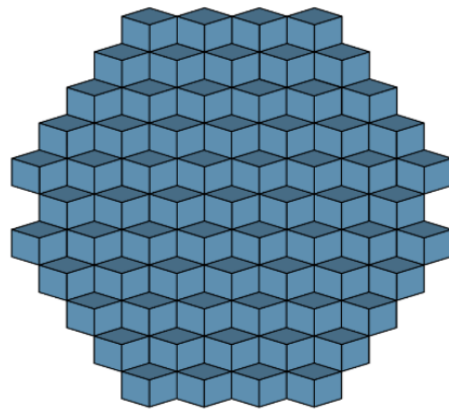


a) Dense + Regular



Quasicrystals

b) Dense + Regular + Periodic

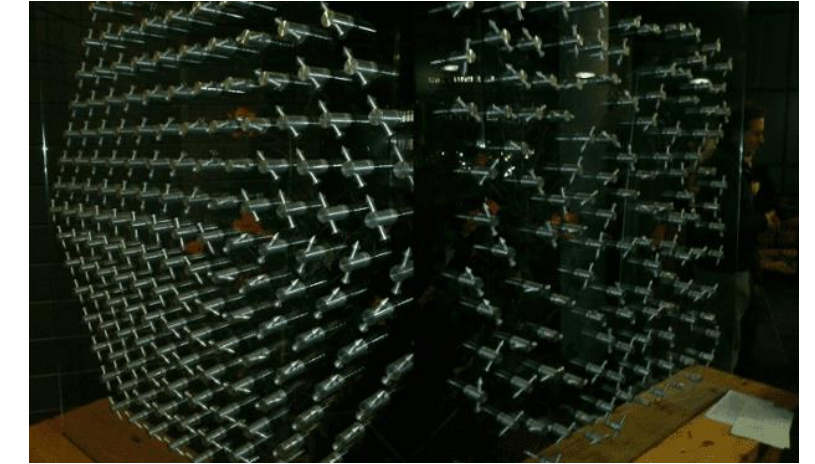
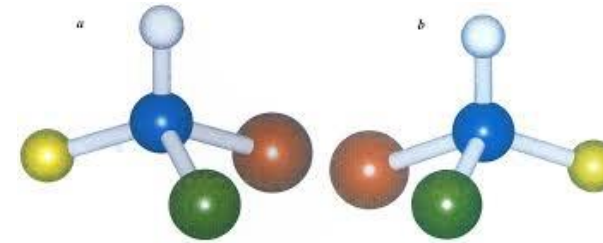


Ordinary crystals

c) Dense



Glasses

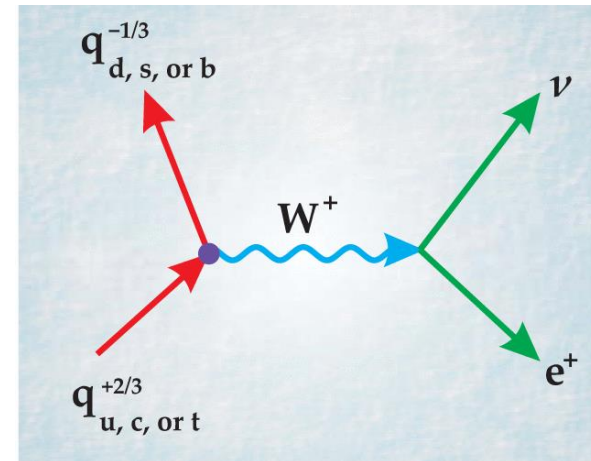
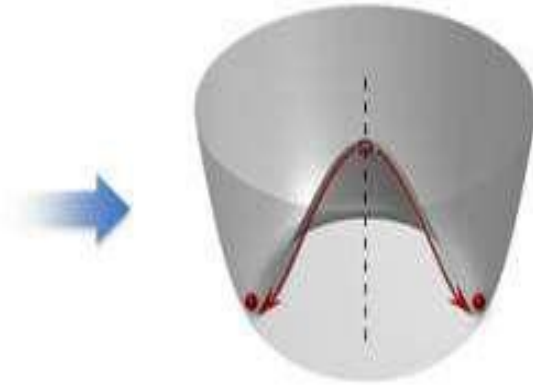


Quebra espontânea de simetria em um ferromagneto.

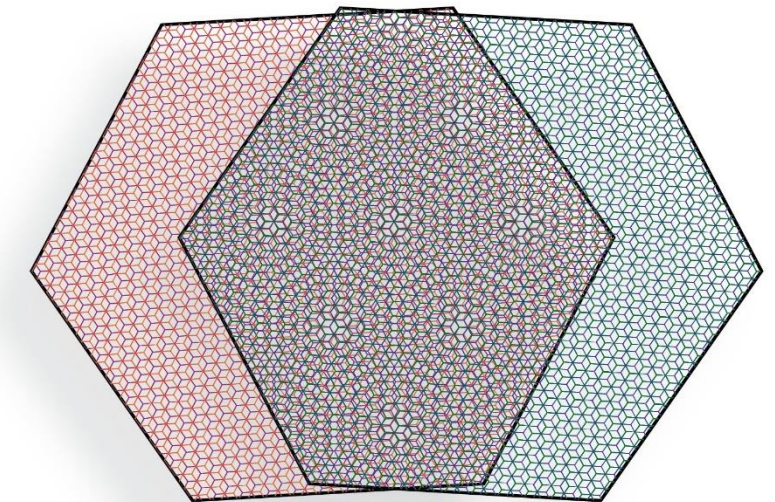
Unbroken Symmetry



Broken Symmetry



Quebra de simetria em física de partículas



Quebra espontânea de simetria em grafeno de dupla camada torcida

Simetria ?

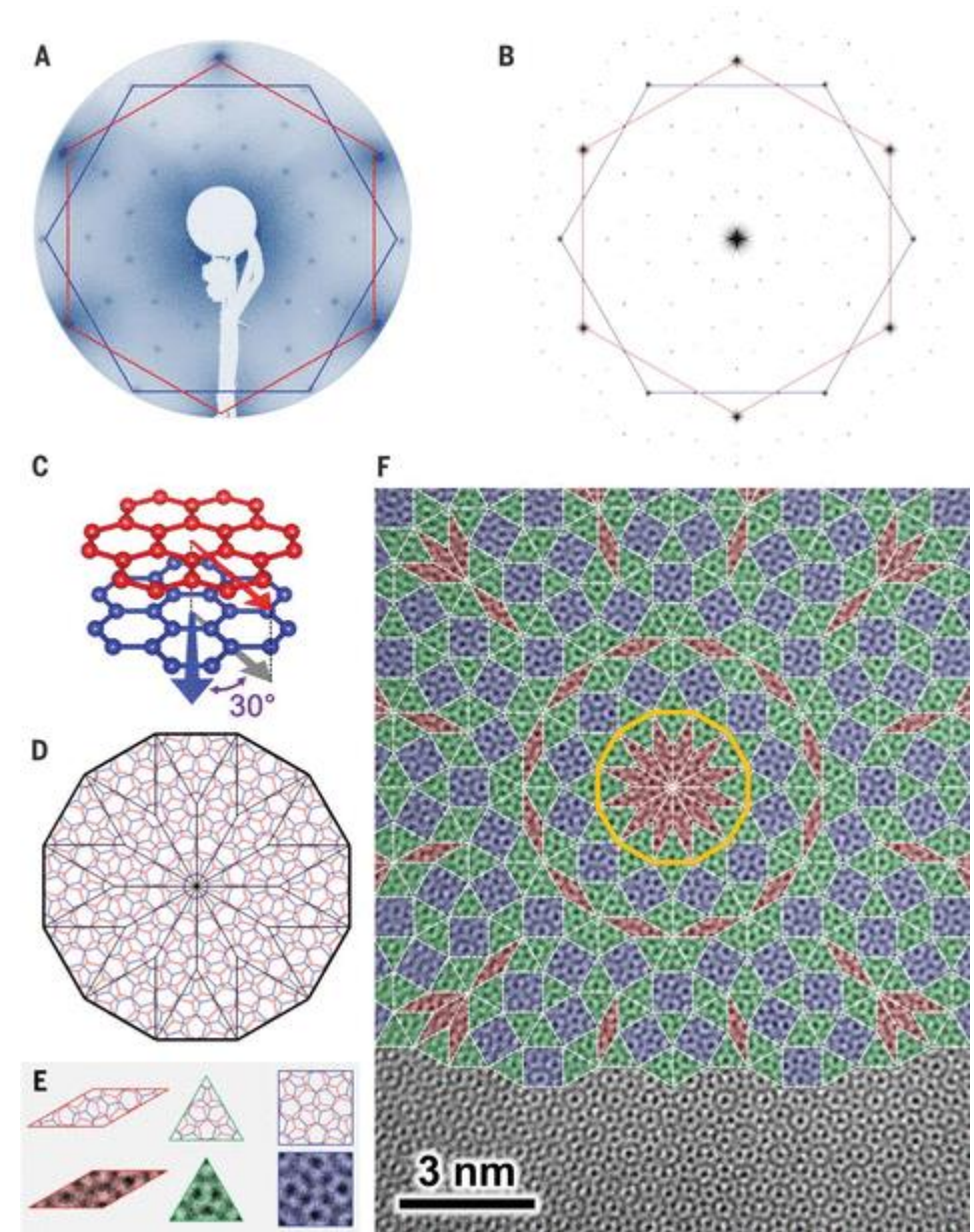
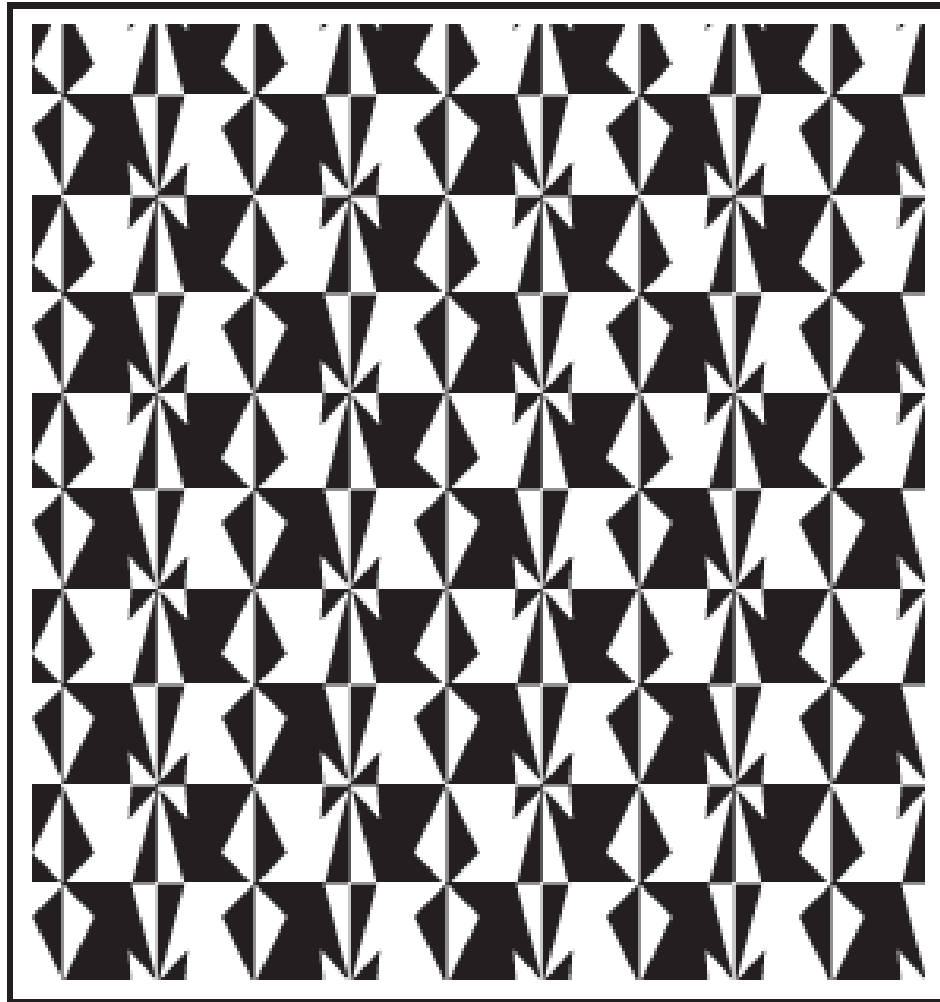


Figure 1.5.1 A figure of black-white symmetry.

Ornamentos e Simetrias

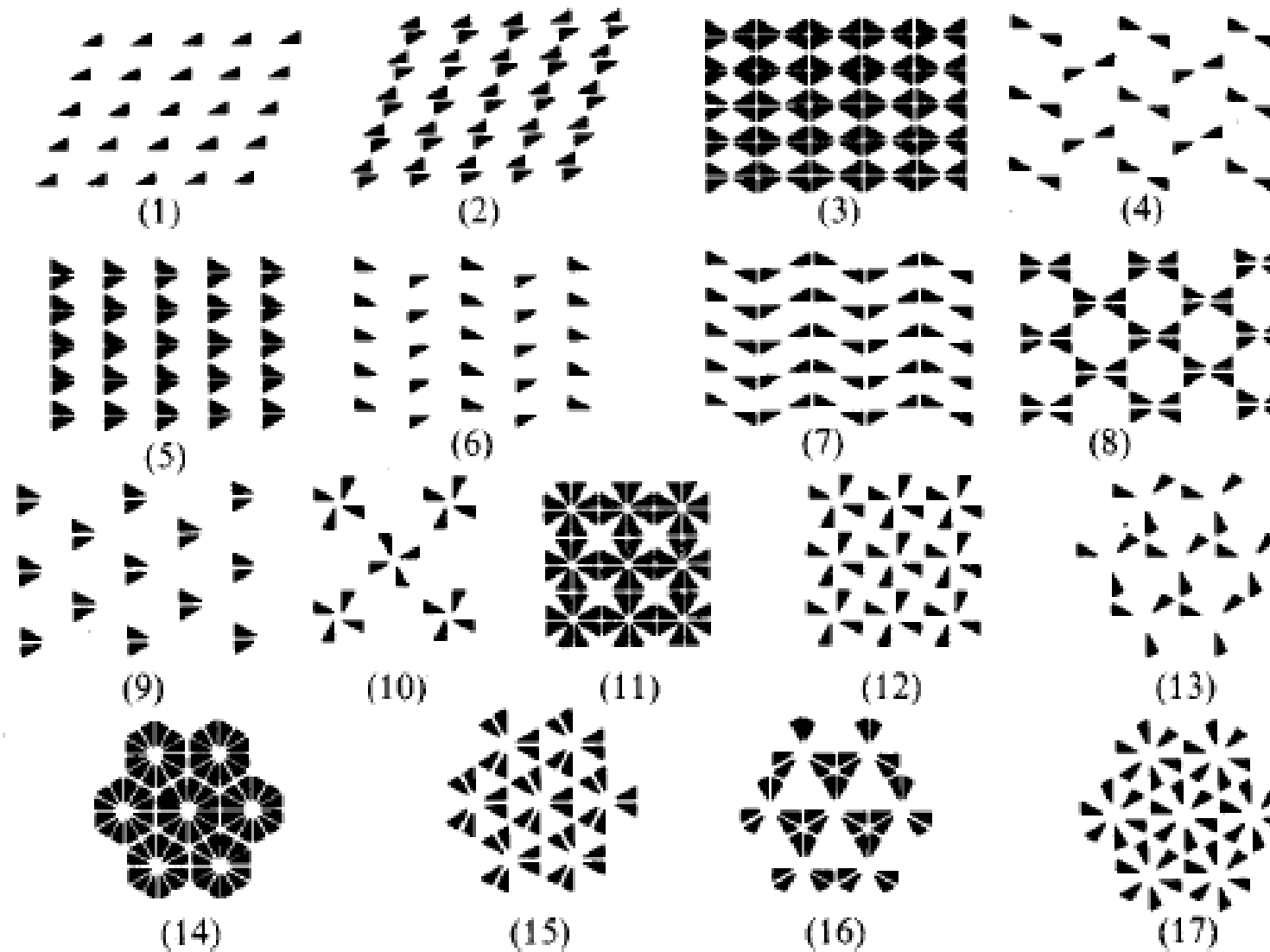
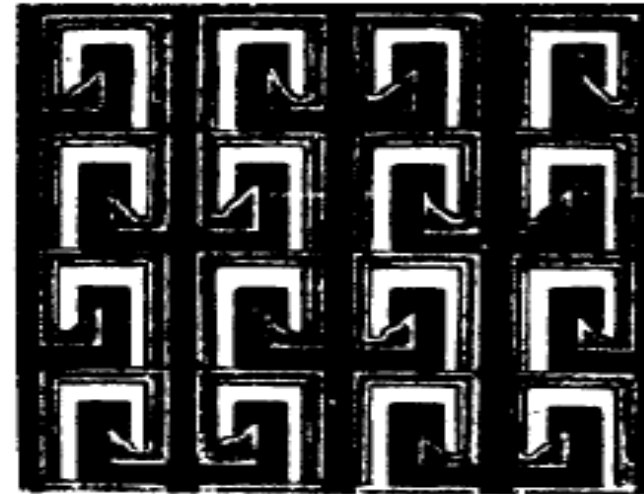


Fig. 19. Ornament groups of the plane

Ornamentos e Simetrias



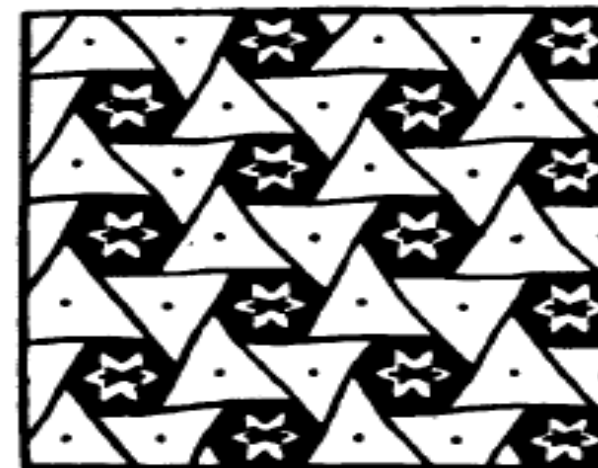
(8) India



(9) China



(12) Egypt



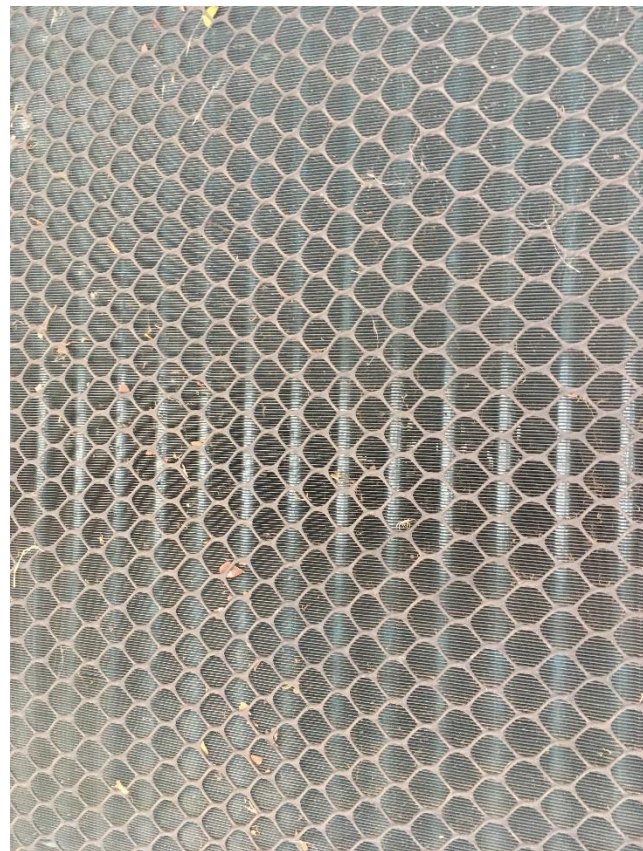
(17) Persia

Fig. 20. Ornaments from various cultures

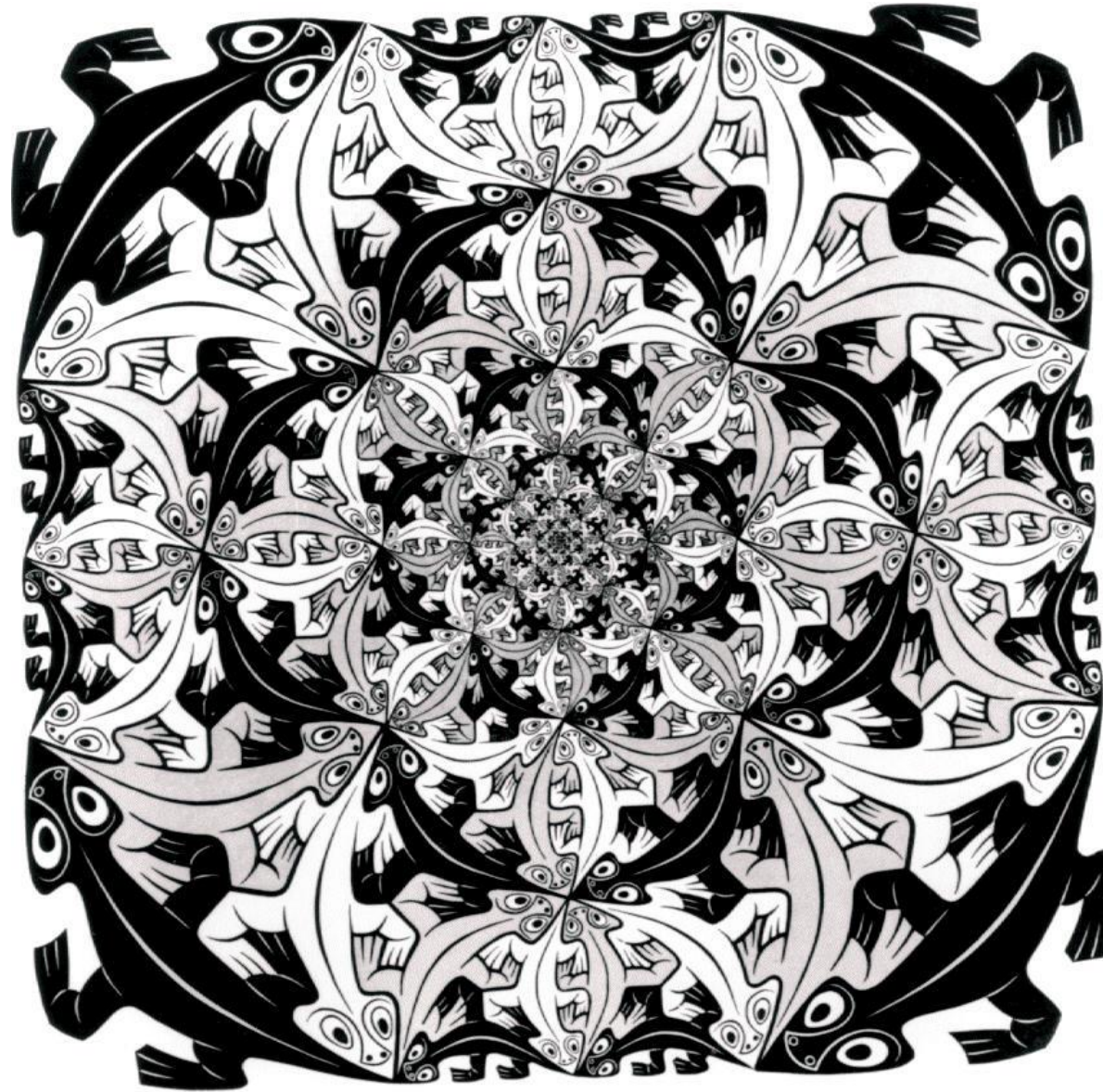
Exemplos no cotidiano (ponto de ônibus do circular)



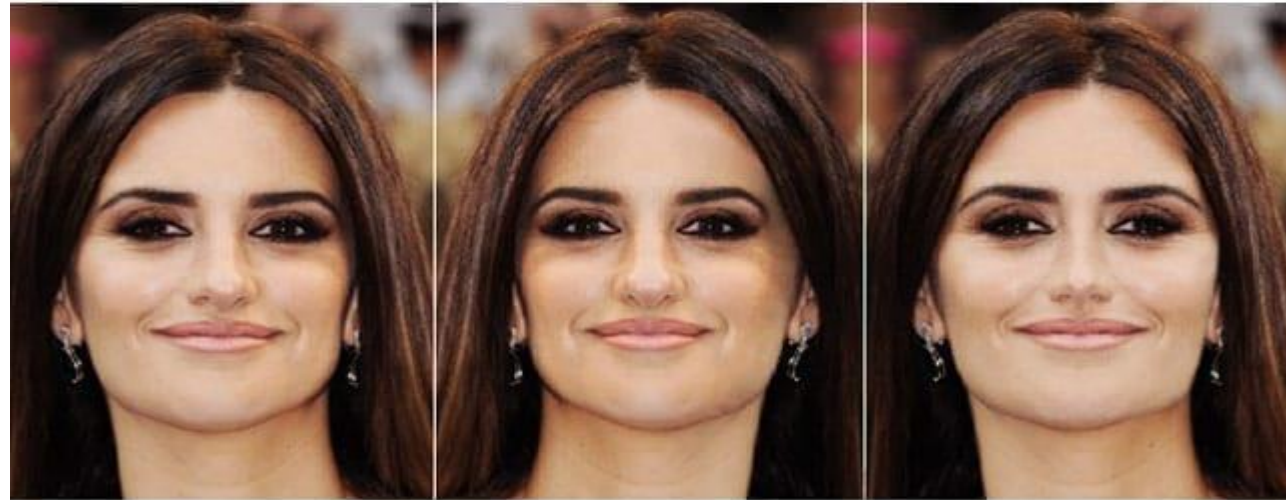
Exemplos no IFUSP



Simetrias



Simetrias



Original

Left Symmetry

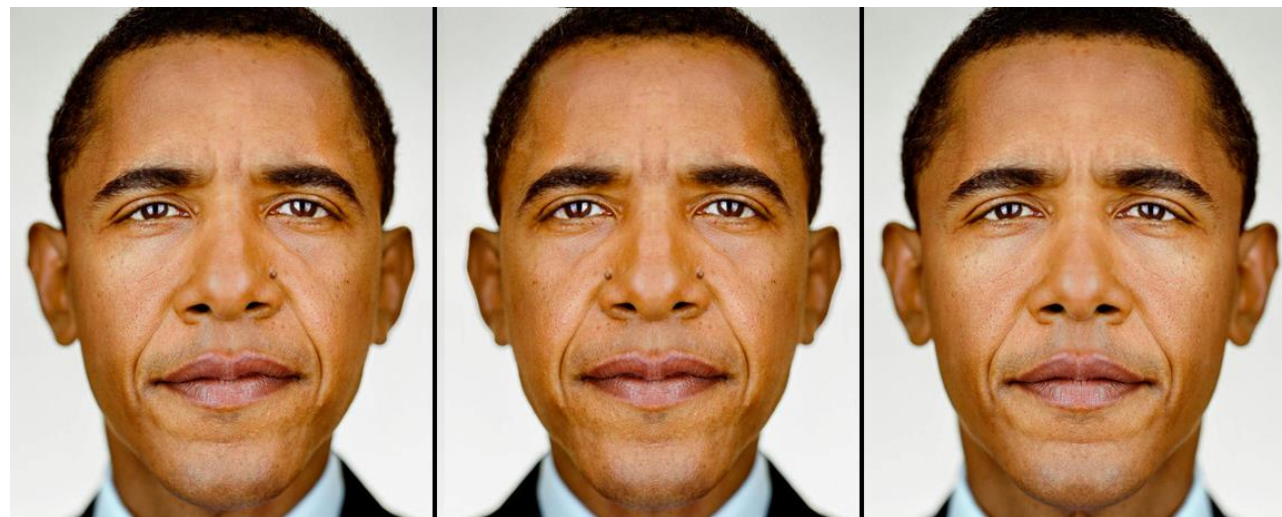
Right Symmetry



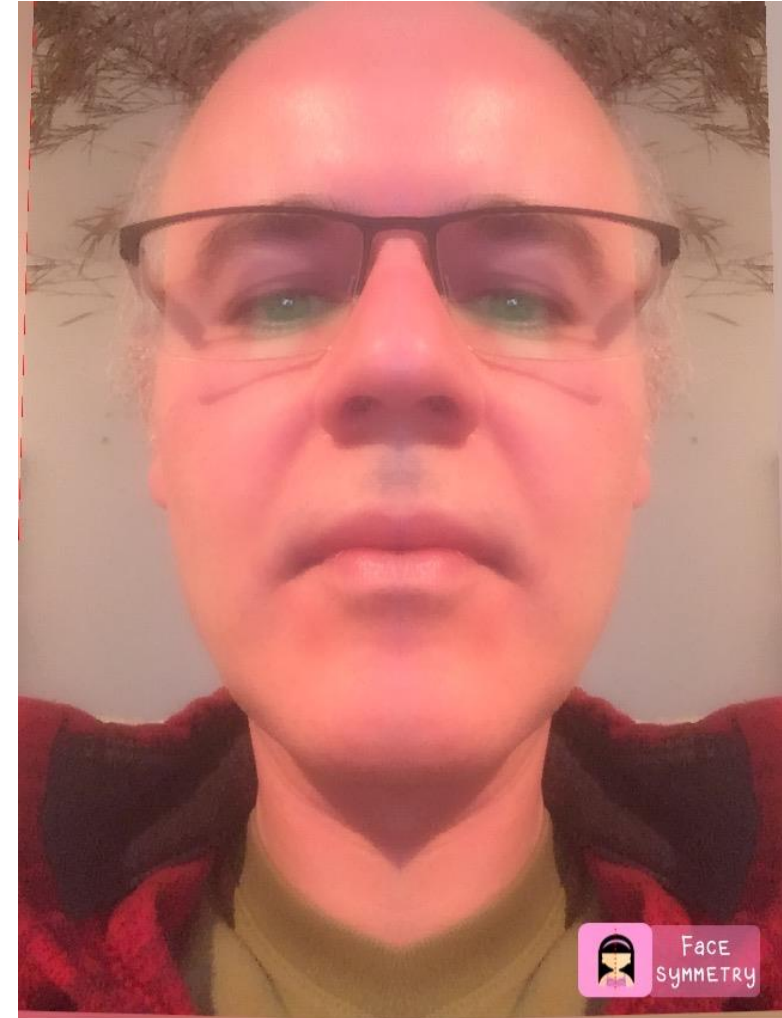
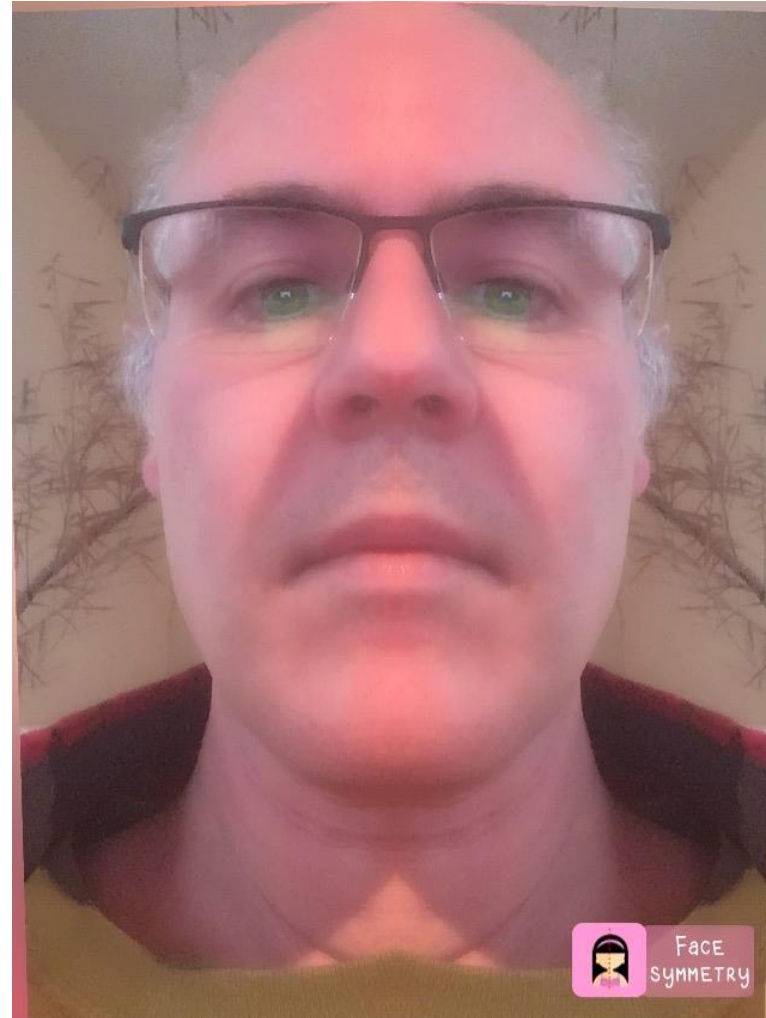
Original

Left Symmetry

Right Symmetry



Simetrias



Simetria

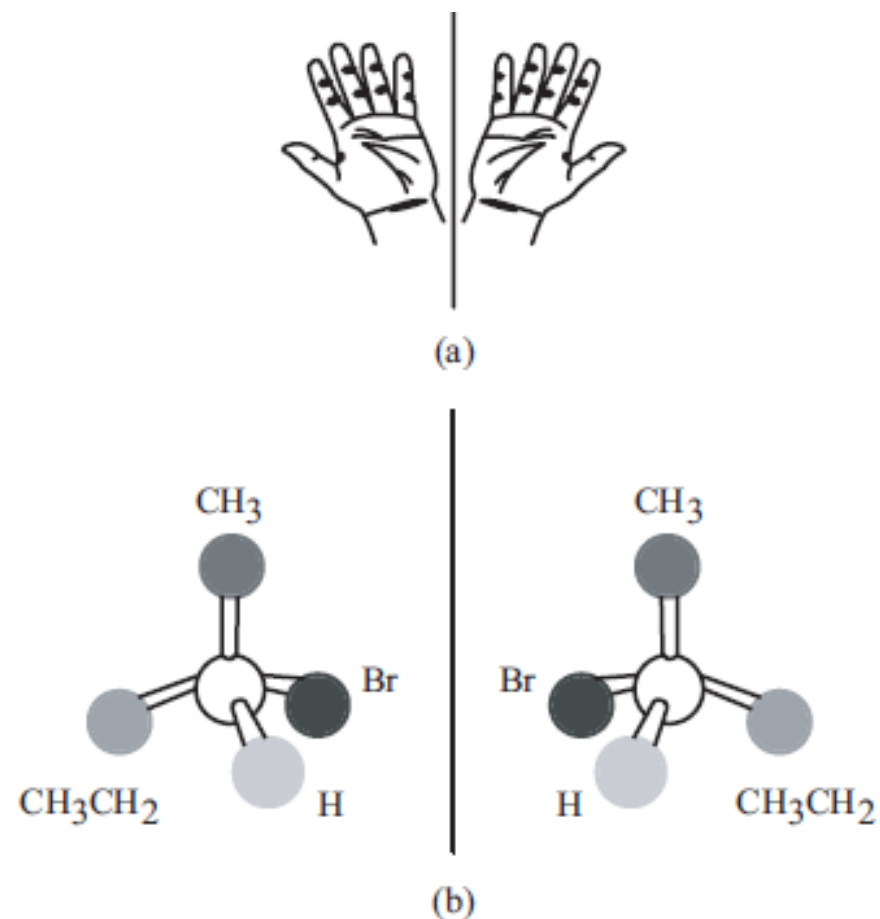


Figure 1.1.2 The schematic diagram of handedness. (a) The left hand and the right hand; (b) the mirror reflection of a chiral molecule.

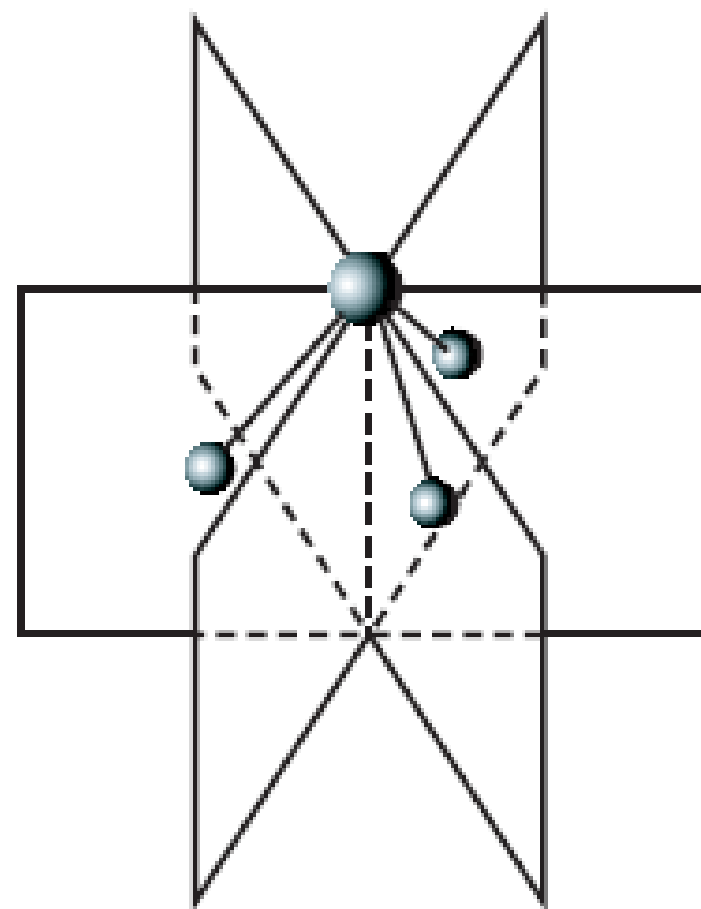
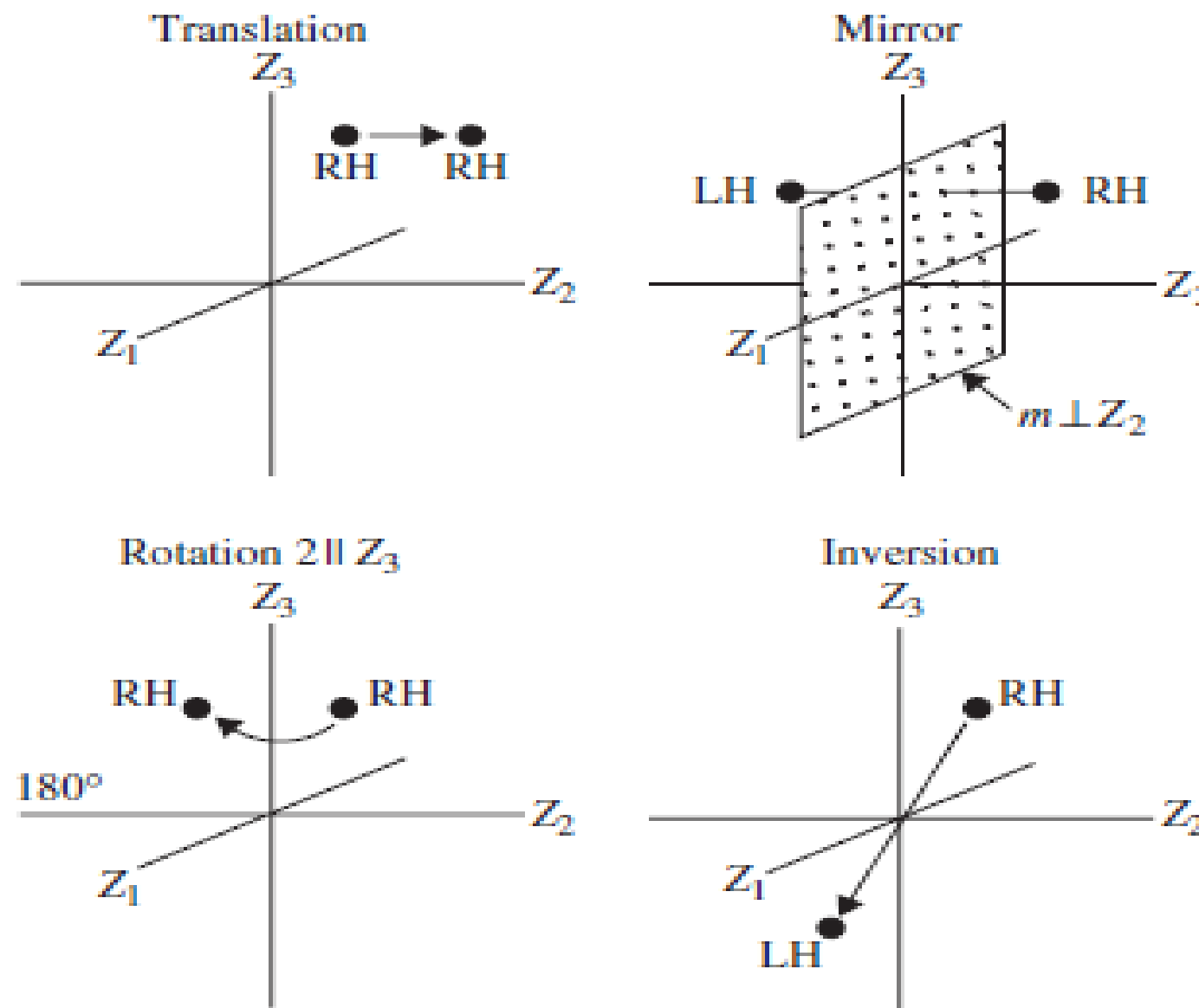


Figure 1.1.7 A NH₃ molecule with its rotation axis and mirror planes.

Simetria



Simetria planar (reflexão e translação)

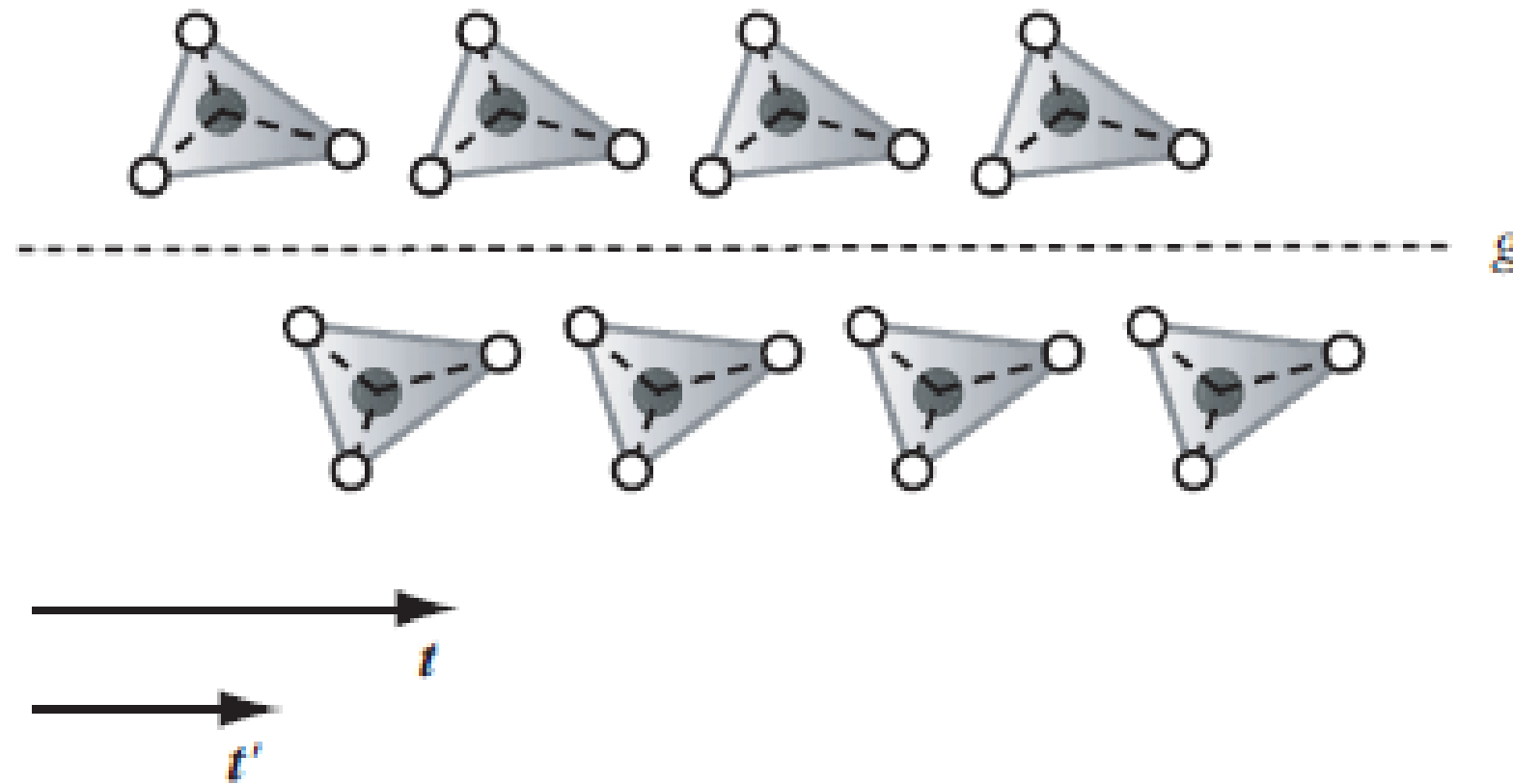


Figure 1.3.4 The schematic diagram of a glide reflecting plane.

Screw (“parafuso”: rotação + translação)

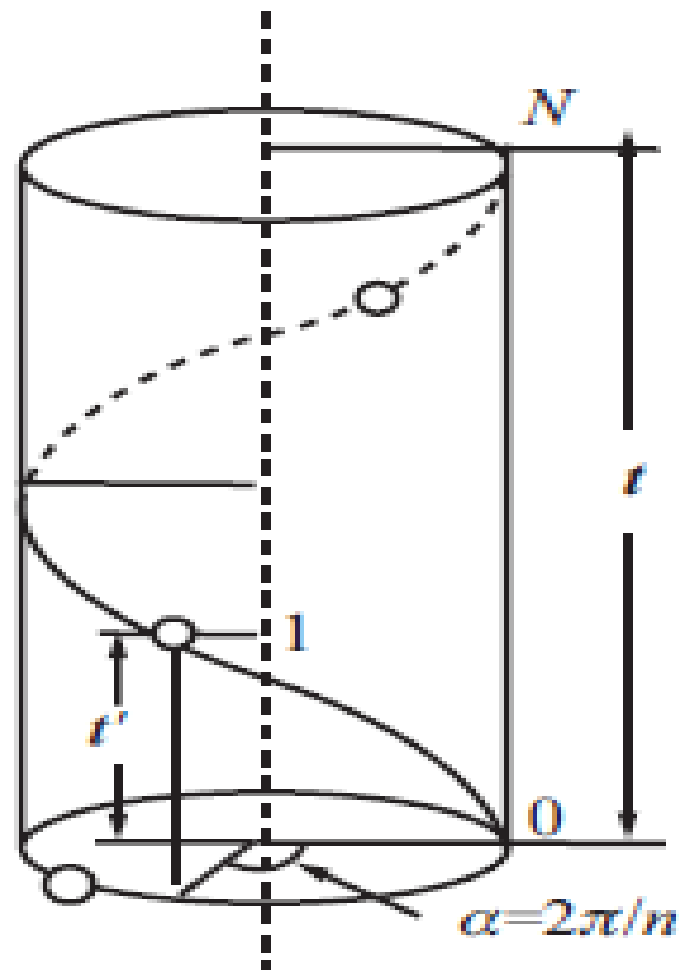
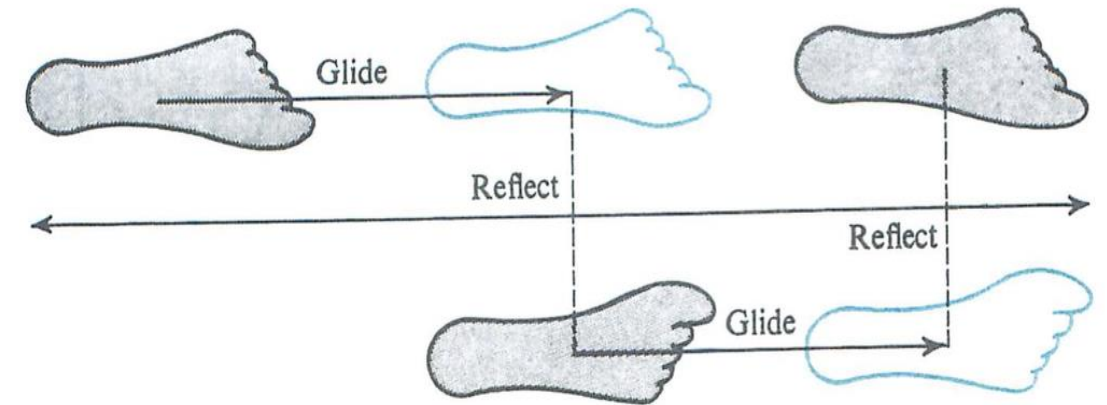
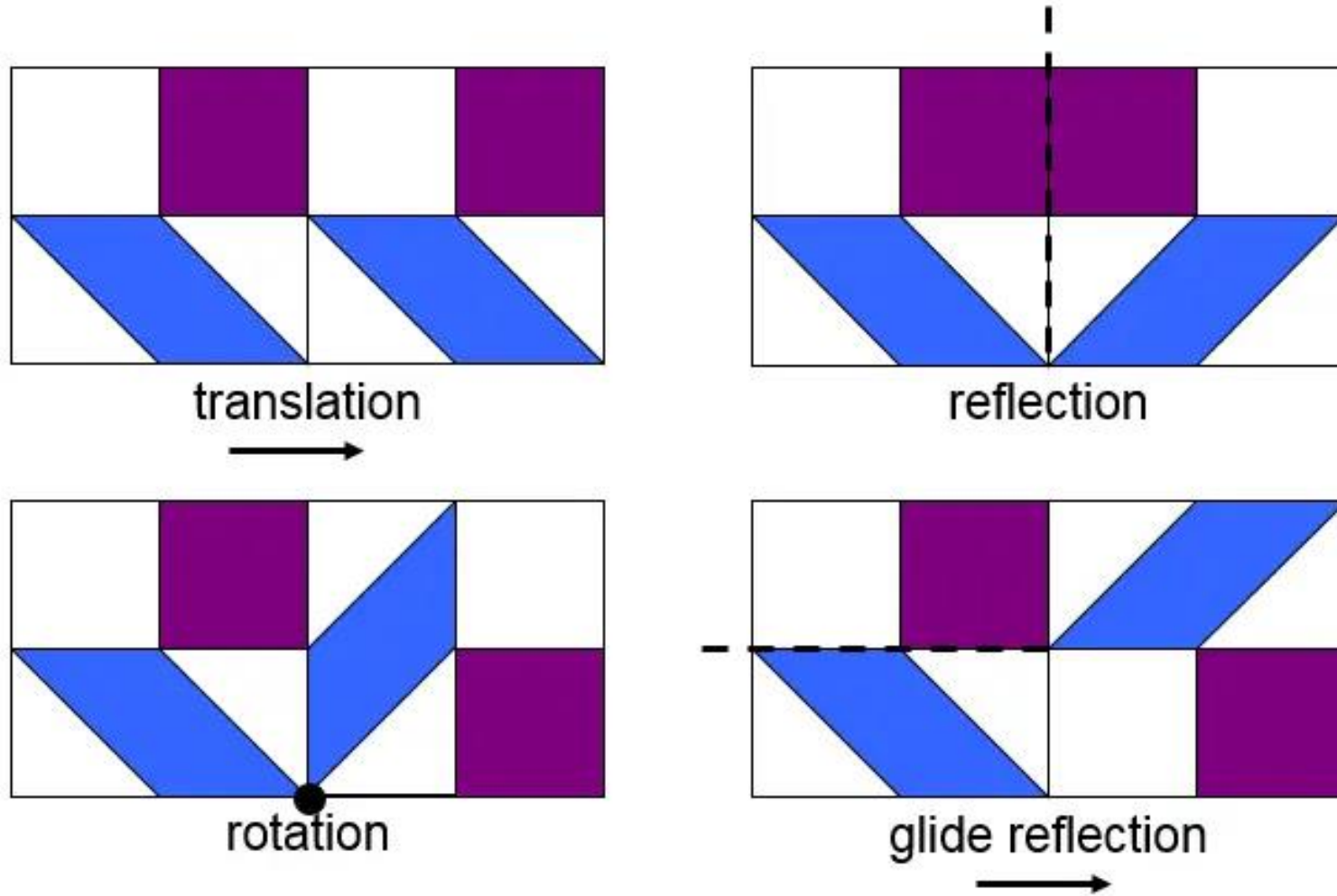
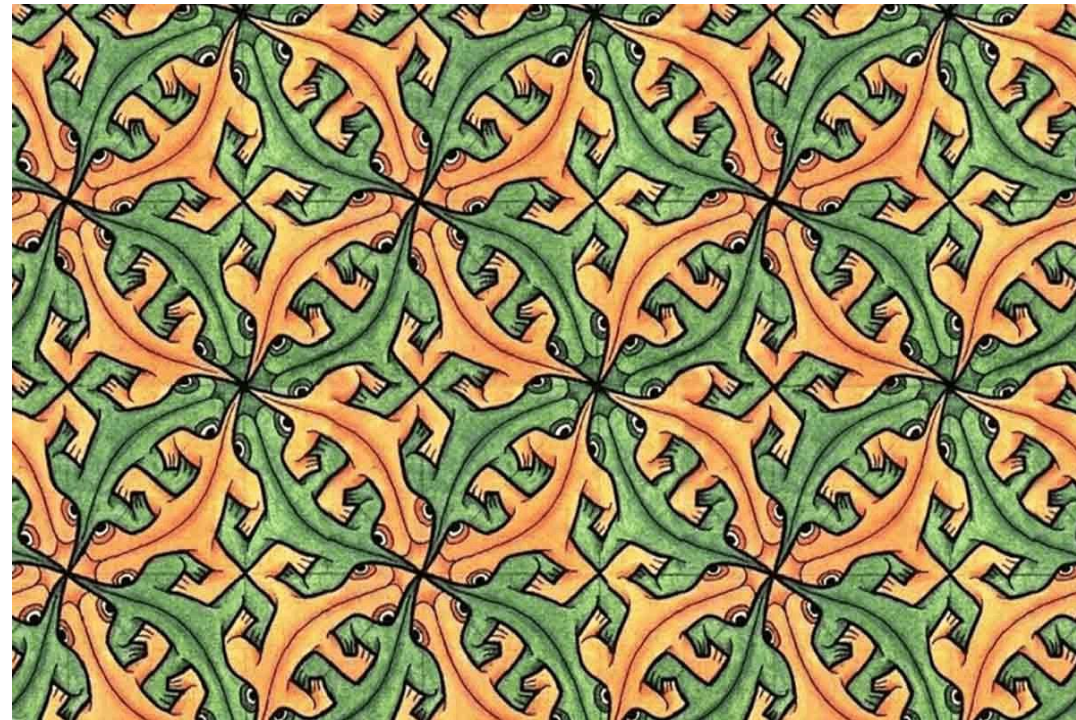
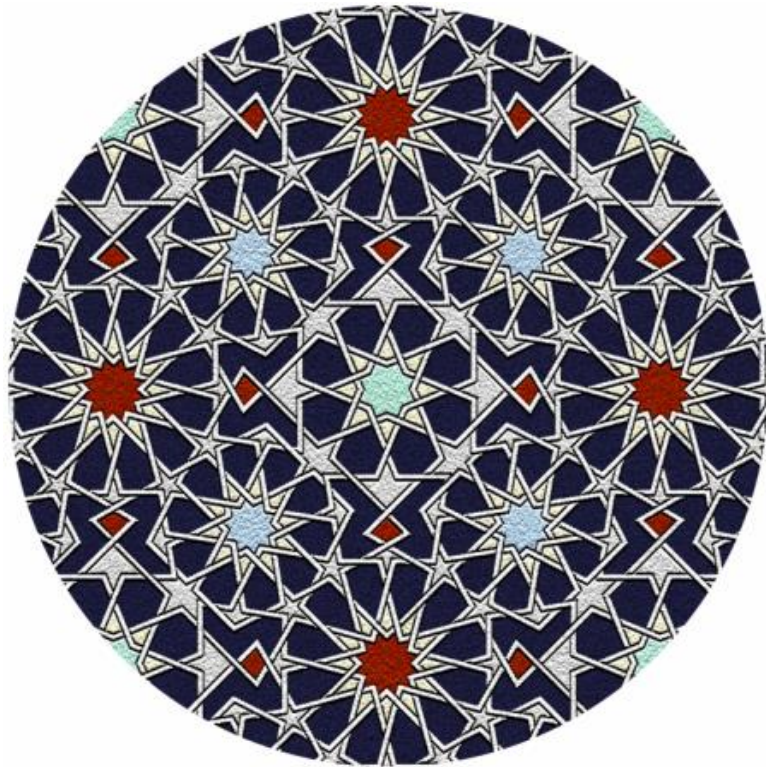


Figure 1.3.5 The schematic diagram of a screw axis.

Operações em simetria

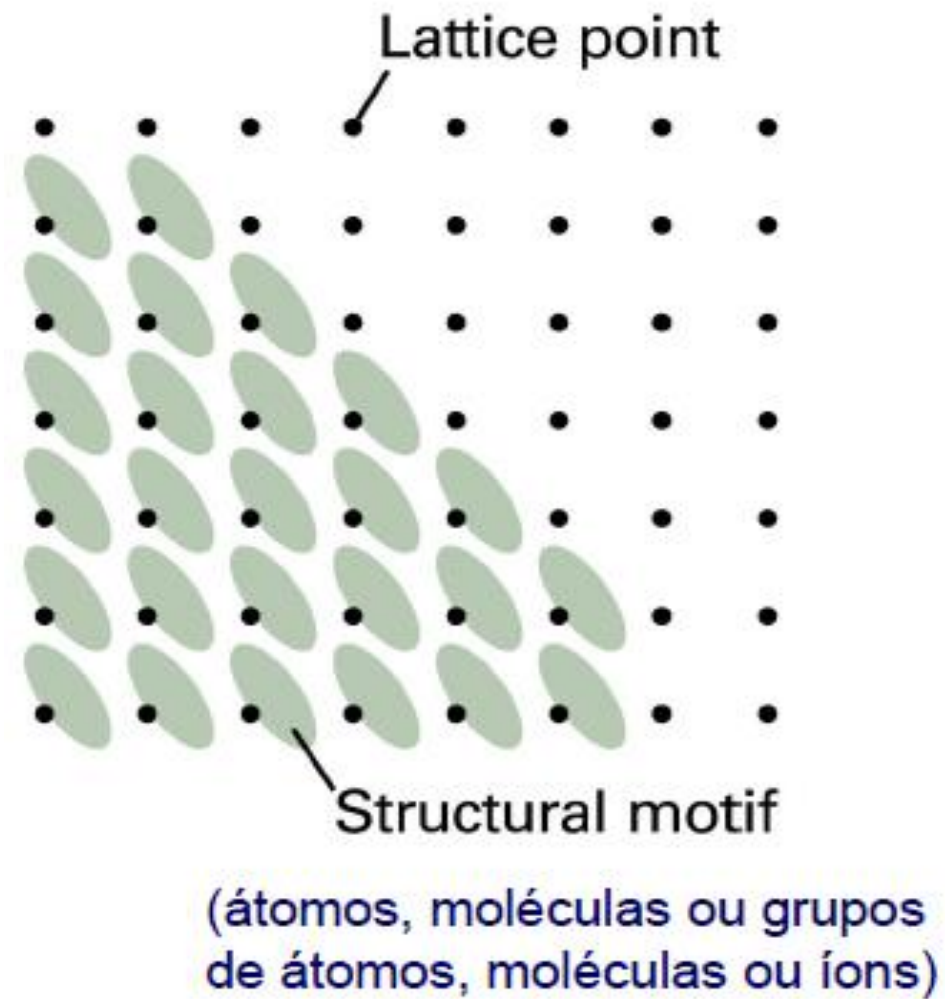


Descubra as simetrias

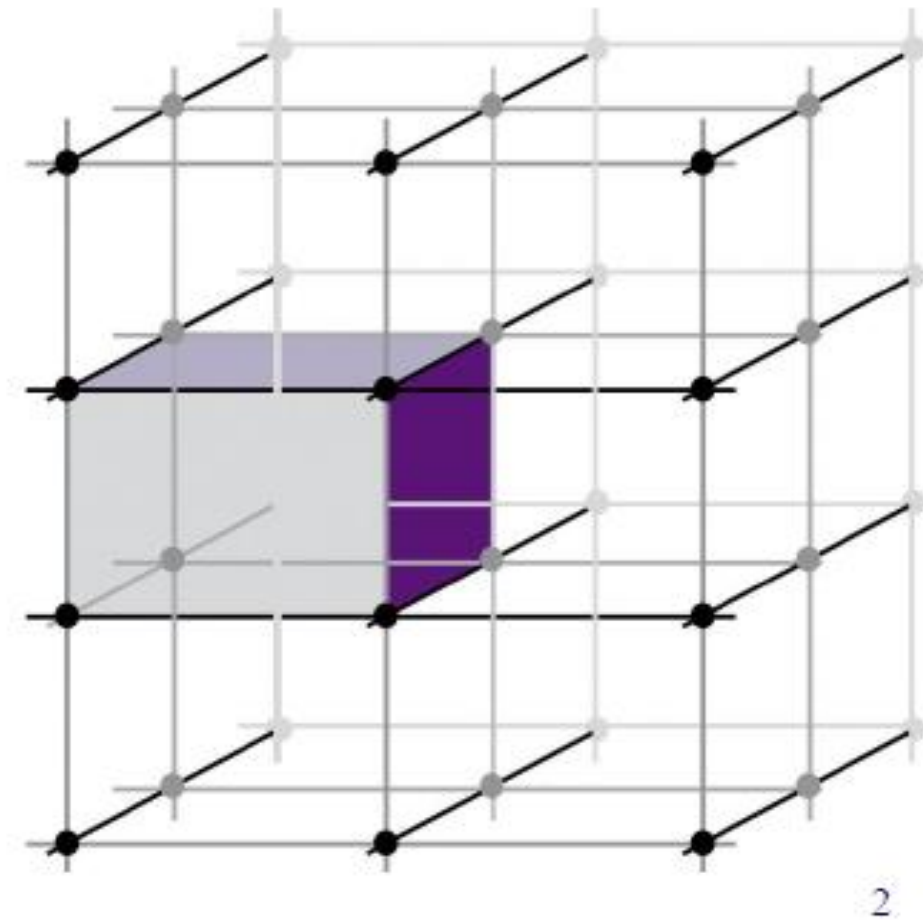


Redes Cristalinas

- Redes Espaciais



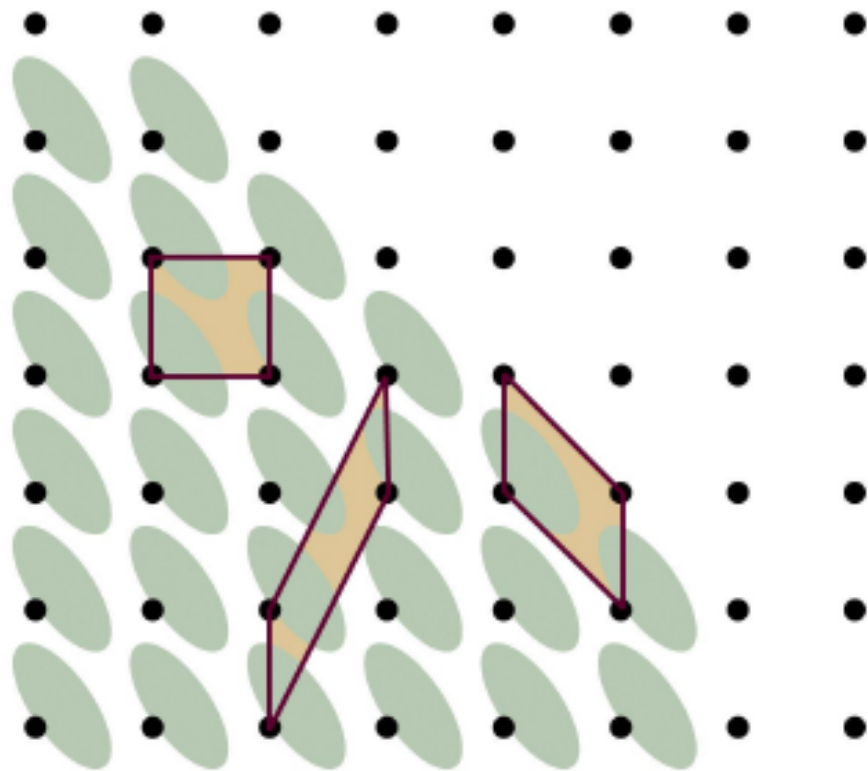
- Células Unitárias



Redes Cristalinas

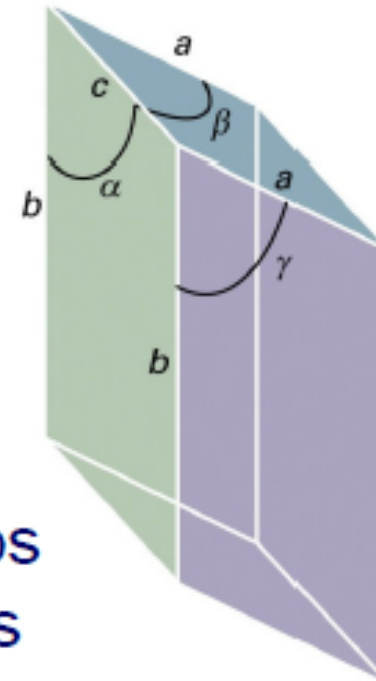
- Células Unitárias

(em geral mesma simetria que a rede cristalina)



- usualmente escolhem-se as que têm menores arestas e cujas faces sejam aproximadamente perpendiculares entre si.

ângulos e lados



Redes primitivas

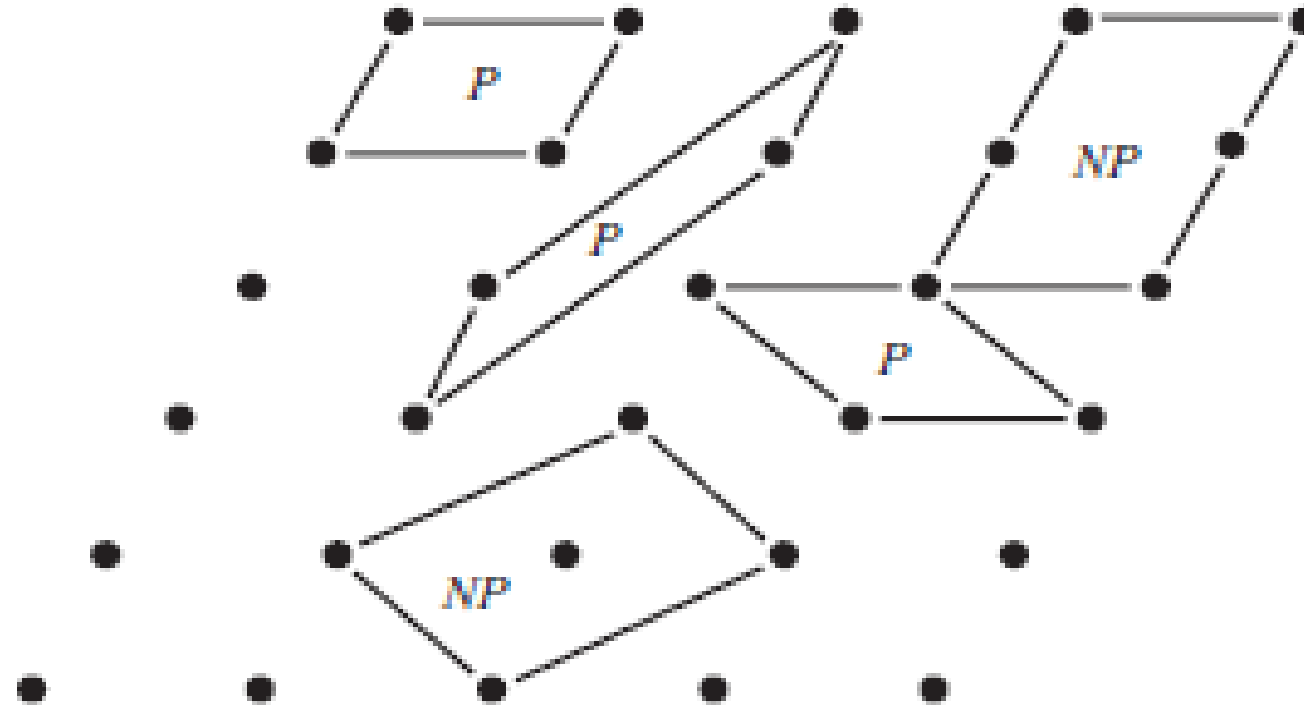


Figure 1.3.2 The different choices of unit cells in 2D lattice (P = primitive, NP = nonprimitive).

Redes de Bravais

(a) Um conjunto infinito de pontos com arranjo e orientação que parecem exatamente os mesmos quando vistos de qualquer ponto da rede.

(b) Todos os pontos cujas posições \mathbf{R} têm a forma

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 ,$$

onde \mathbf{a}_1 , \mathbf{a}_2 e \mathbf{a}_3 são três vetores não coplanares e n_1 , n_2 e n_3 são inteiros.

Redes de Bravais – 2D

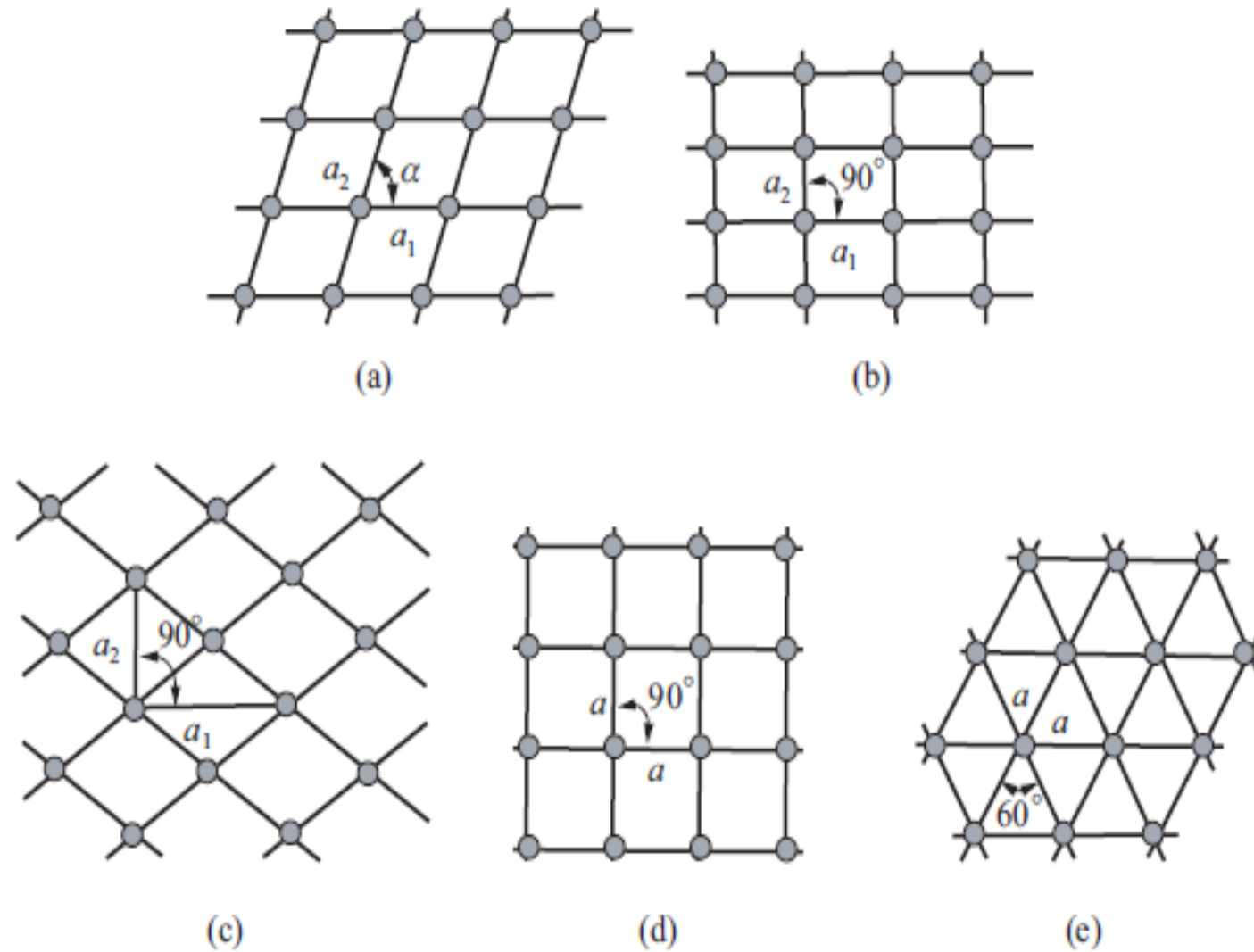
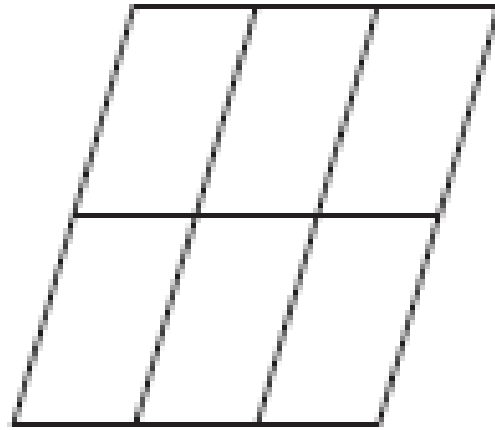
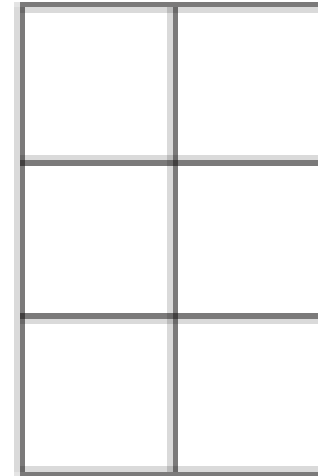


Figure 1.3.6 The 2D Bravais lattices: (a) Oblique; (b) rectangular; (c) rhombic; (d) square; (e) hexagonal.

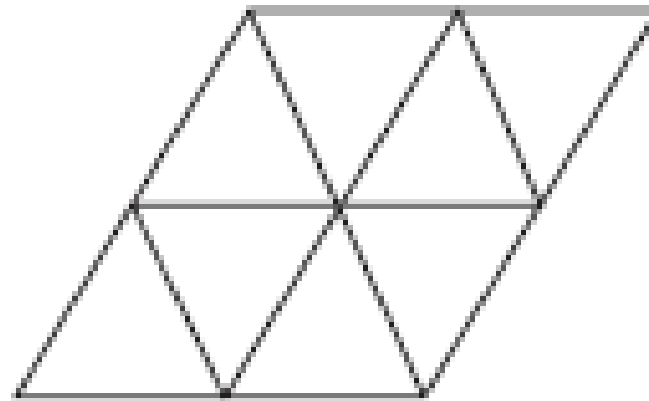
Simetrias permitidas em 2D



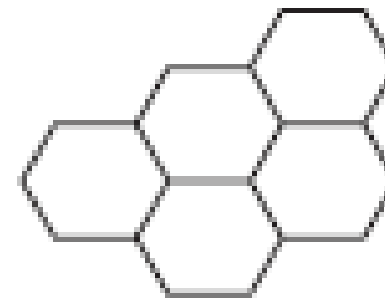
2-Fold (180°)



4-Fold (90°)

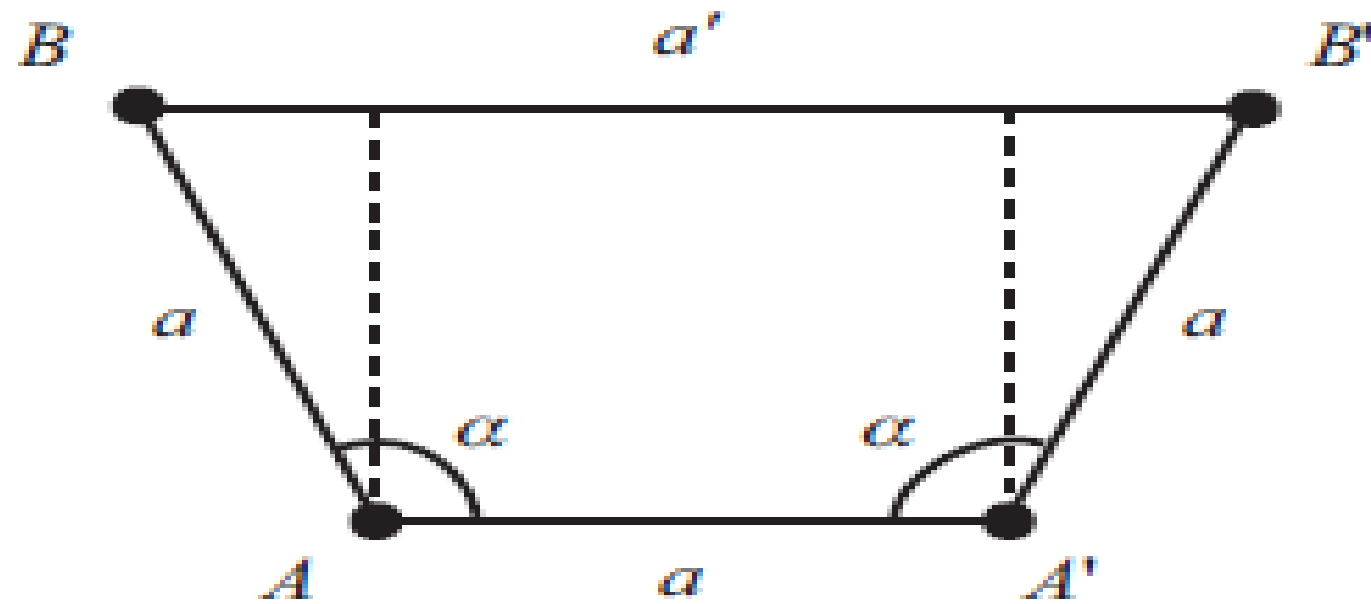


3-Fold (120°)



6-Fold (60°)

Simetrias de rotação



$$\alpha = 2\pi / n$$

$$a' = a + 2a \cos(\alpha) = j \cdot a$$

j , inteiro

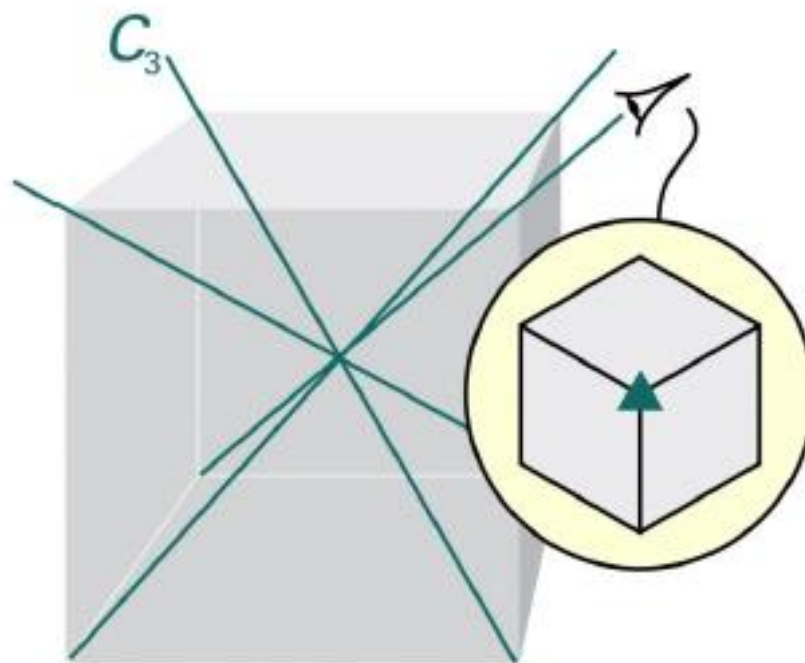
$$\cos(\alpha) = (j - 1)/2 = i/2$$

Figure 1.3.3 The compatibility of the N -fold rotation with periodicity.

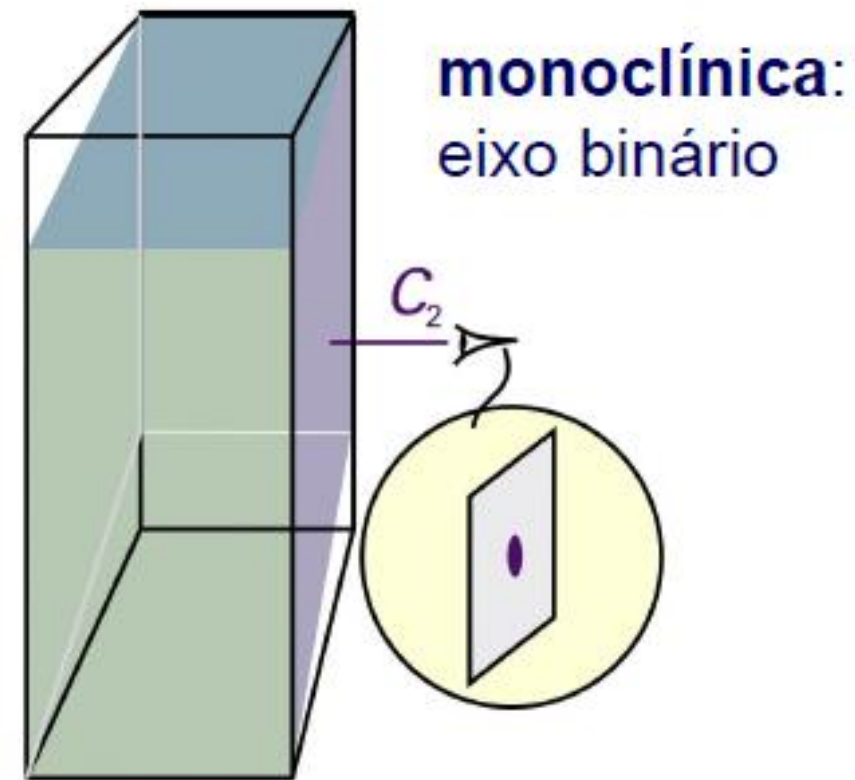
i	$\cos \alpha$	α	$N = 2\pi/\alpha$	b
-2	-1	π	2	-a
-1	$-\frac{1}{2}$	$2\pi/3$	3	0
0	0	$\pi/2$	4	a
1	$\frac{1}{2}$	$\pi/3$	6	2a
2	1	0	=1	3a

Redes de Bravais – 3D

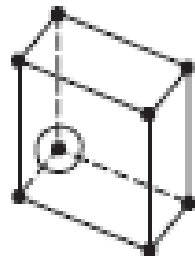
- Células Unitárias: sete sistemas cristalinos (elementos de simetria de rotação)



cúbica: 4 eixos ternários dispostos em um arranjo tetraédrico

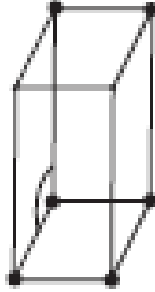
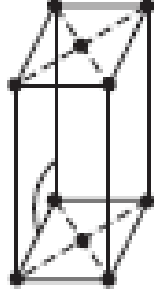


Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90$						$1, \bar{1}$

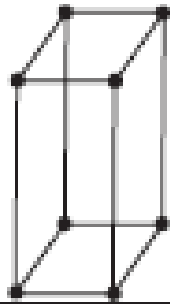
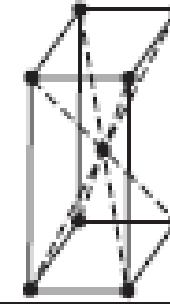
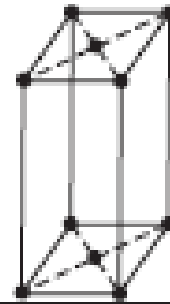
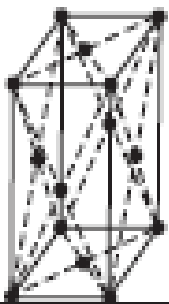
P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombhedron)

Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group	
	P	I	C	F	R		
Monoclinic $a \neq b \neq c$ $\alpha = \gamma = 90$ $\beta \neq 90$							$2, m, \frac{2}{m}$

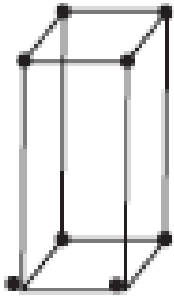
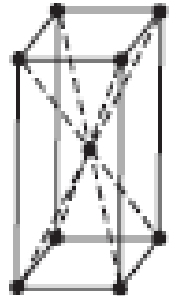
P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombhedron)

Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Orthorhombic $a \neq b \neq c$ $\alpha = \beta = \gamma = 90$						$222, 2mm,$ $\frac{2}{m} \frac{2}{m} \frac{2}{m} (mmm)$

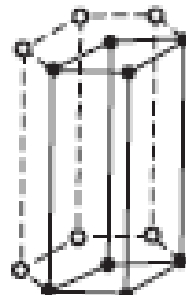
P (Primitive), I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombhedron)

Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90$						$4, \bar{4}, \frac{4}{m} 422,$ $4mm, \bar{4} 2m,$ $\frac{4}{m} \frac{2}{m} \frac{2}{m} (4/mmm)$

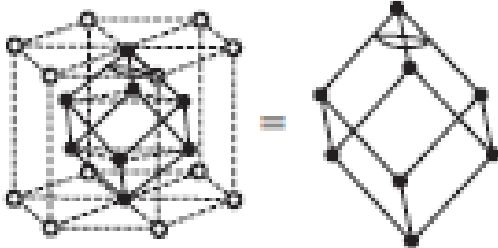
P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombohedron)

Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Hexagonal $a = b \neq c$ $\alpha = \beta = 90$ $\gamma = 120$						$6, \frac{3}{m}, \frac{6}{m}, 622,$ $6mm, \overline{6} 2 m,$ $\frac{6}{m} \frac{2}{m} \frac{2}{m} (6/mmm)$

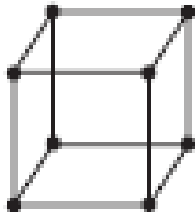
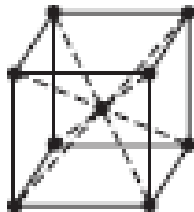
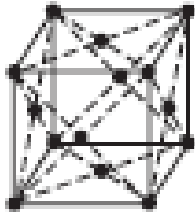
P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombohedron)

Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Rhombohedral $a = b = c$ $\alpha = \beta = \gamma \neq 90$						$\bar{3}, \bar{3}, 32, 3m,$ $\bar{3} \frac{2}{m} (\bar{3}m)$

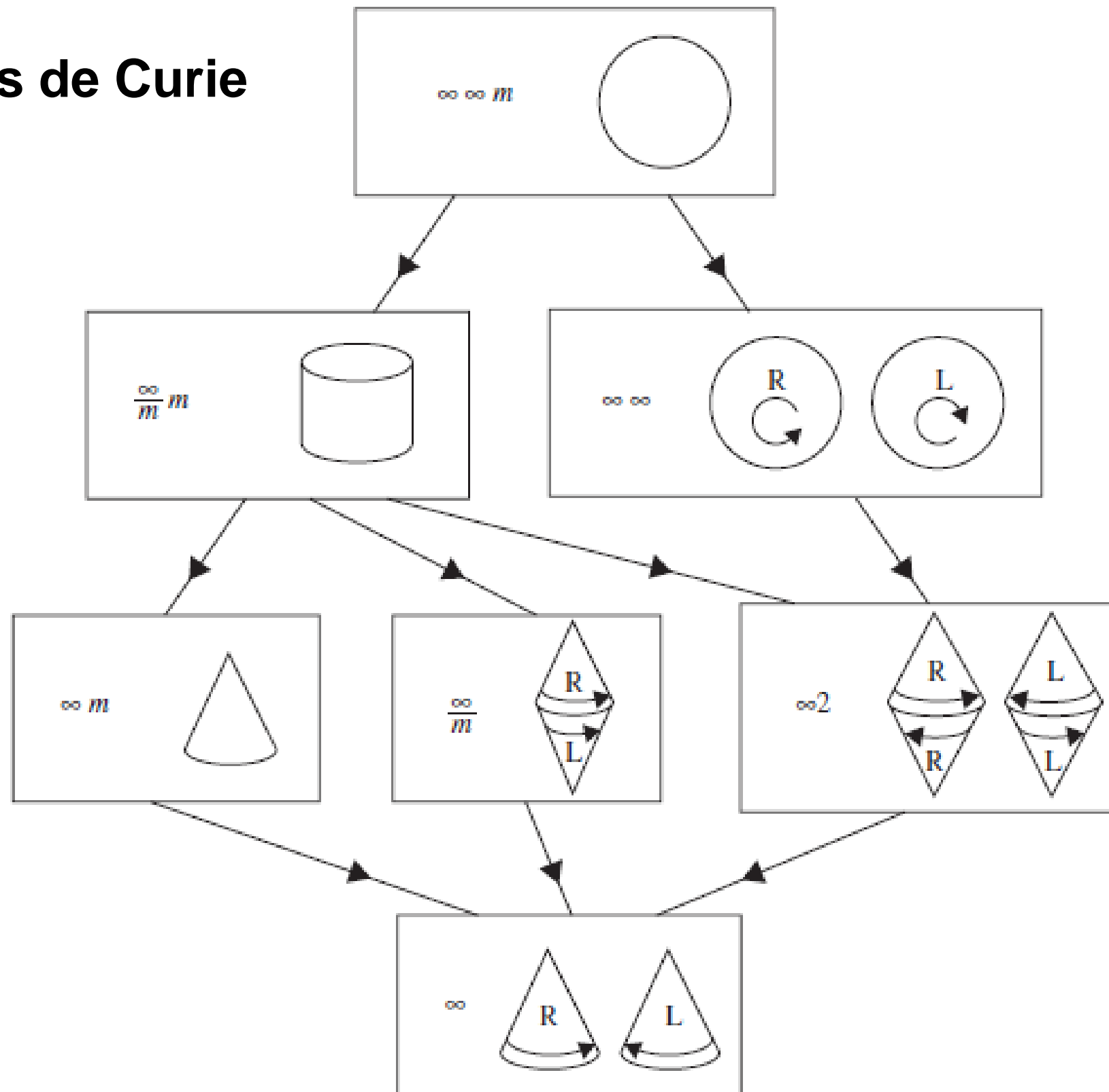
P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombohedron)

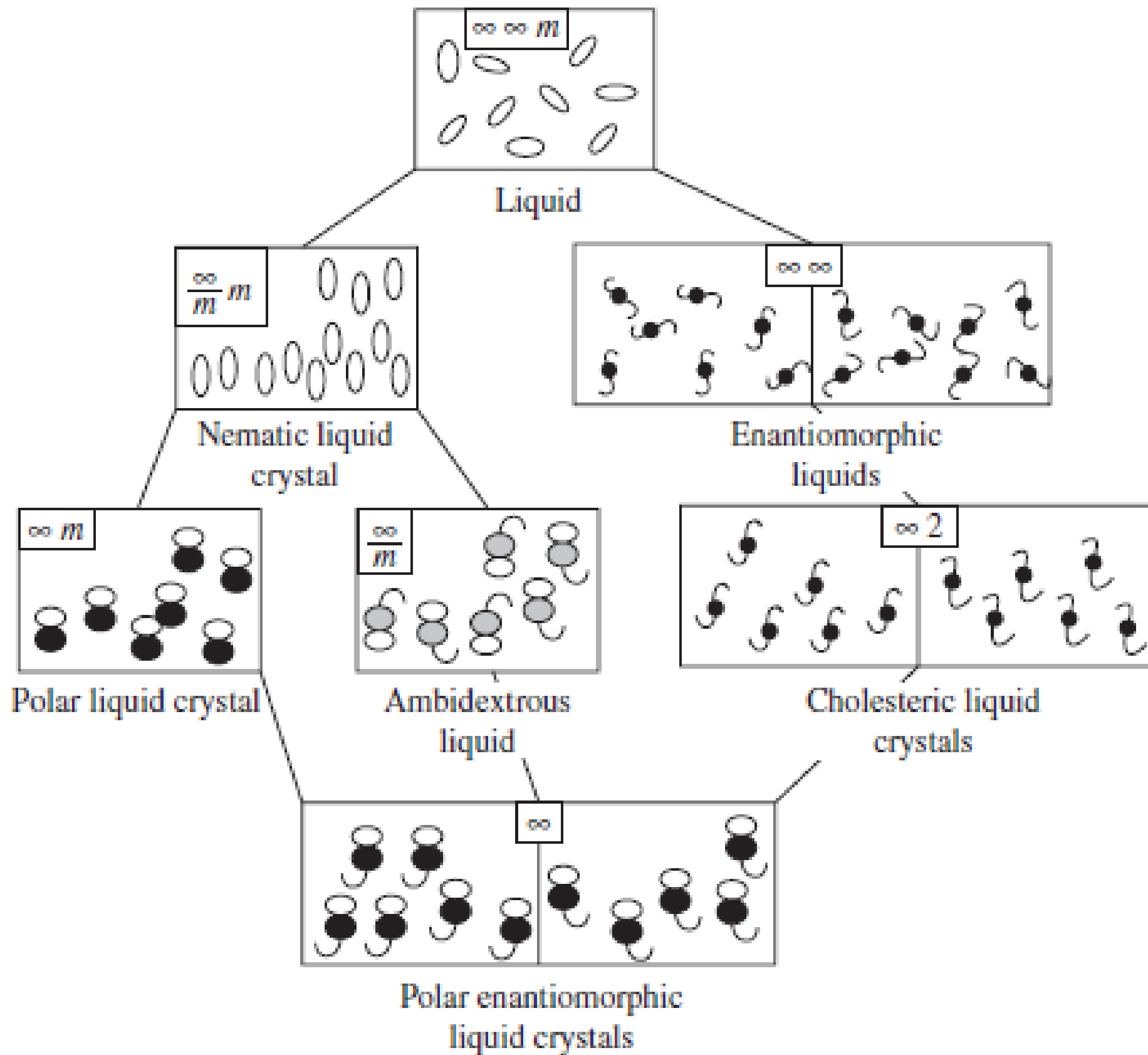
Redes de Bravais – 3D

Crystal System	Type of Lattices					Related Point Group
	P	I	C	F	R	
Cubic $a = b = c$ $\alpha = \beta = \gamma = 90$						$23, \frac{2}{m}\bar{3}(3m),$ $432, 43m,$ $\frac{4}{m}\bar{3}\frac{2}{m}(m\bar{3}m)$

P (Primitive) , I (Body Center) , C (Bottom Center), F (Face Center), R (Rhombohedron)

Grupos de Curie





Simetrias e nanoestruturas

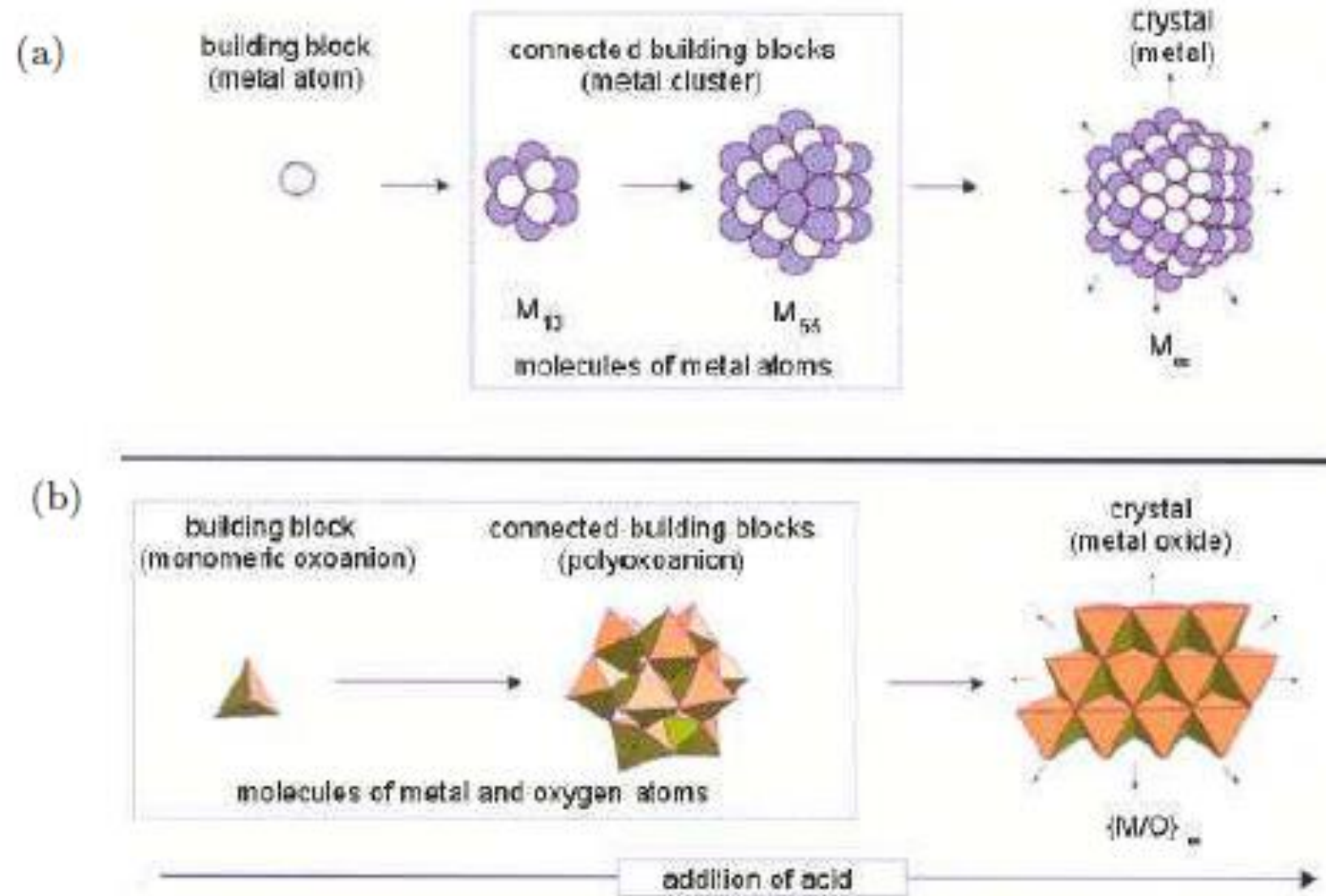


Fig. 57. Molecular self-organization of complex crystals with symmetric atoms