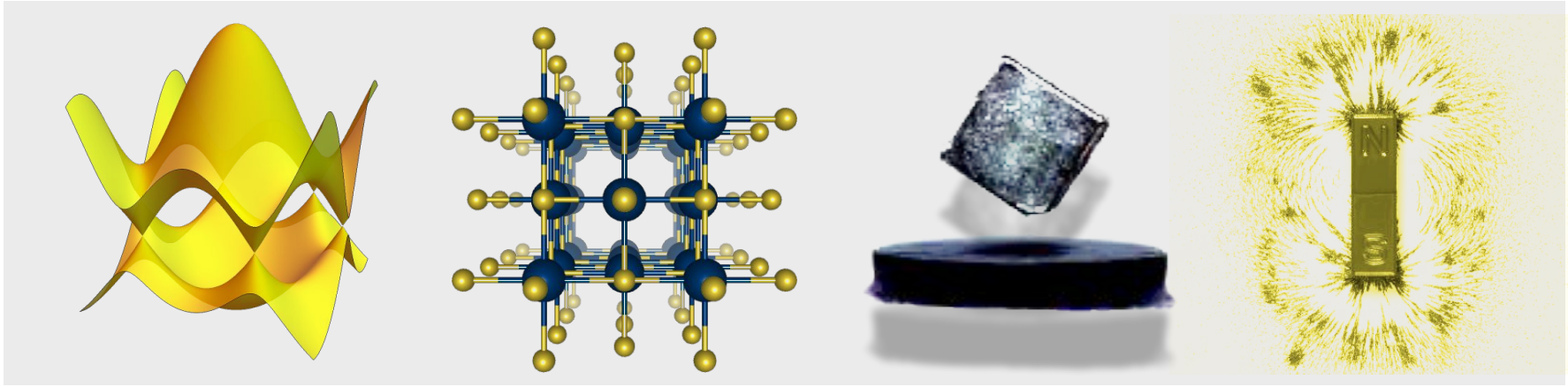
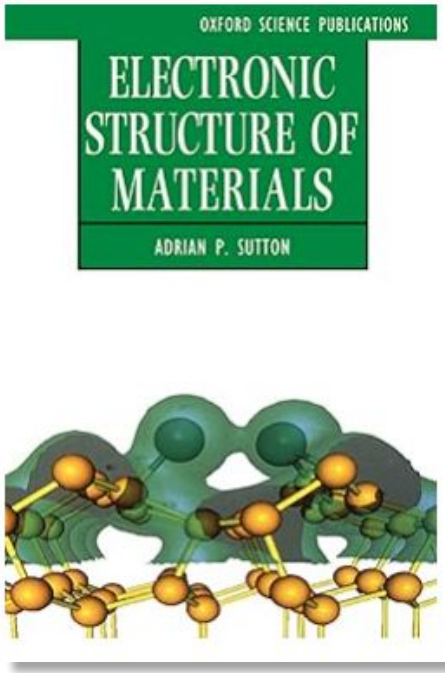
ESCOLA SÉRGIO MASCARENHAS DE FÍSICA DA MATÉRIA CONDENSADA

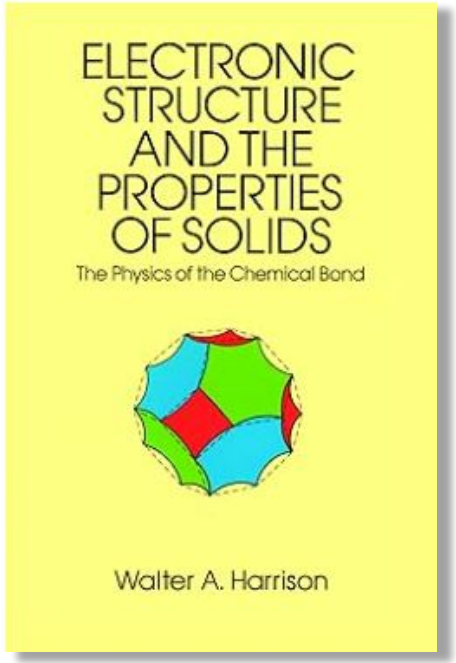
Aula 2 - 16 de Julho

Estrutura Eletrônica de Sólidos



(Algumas) Referências



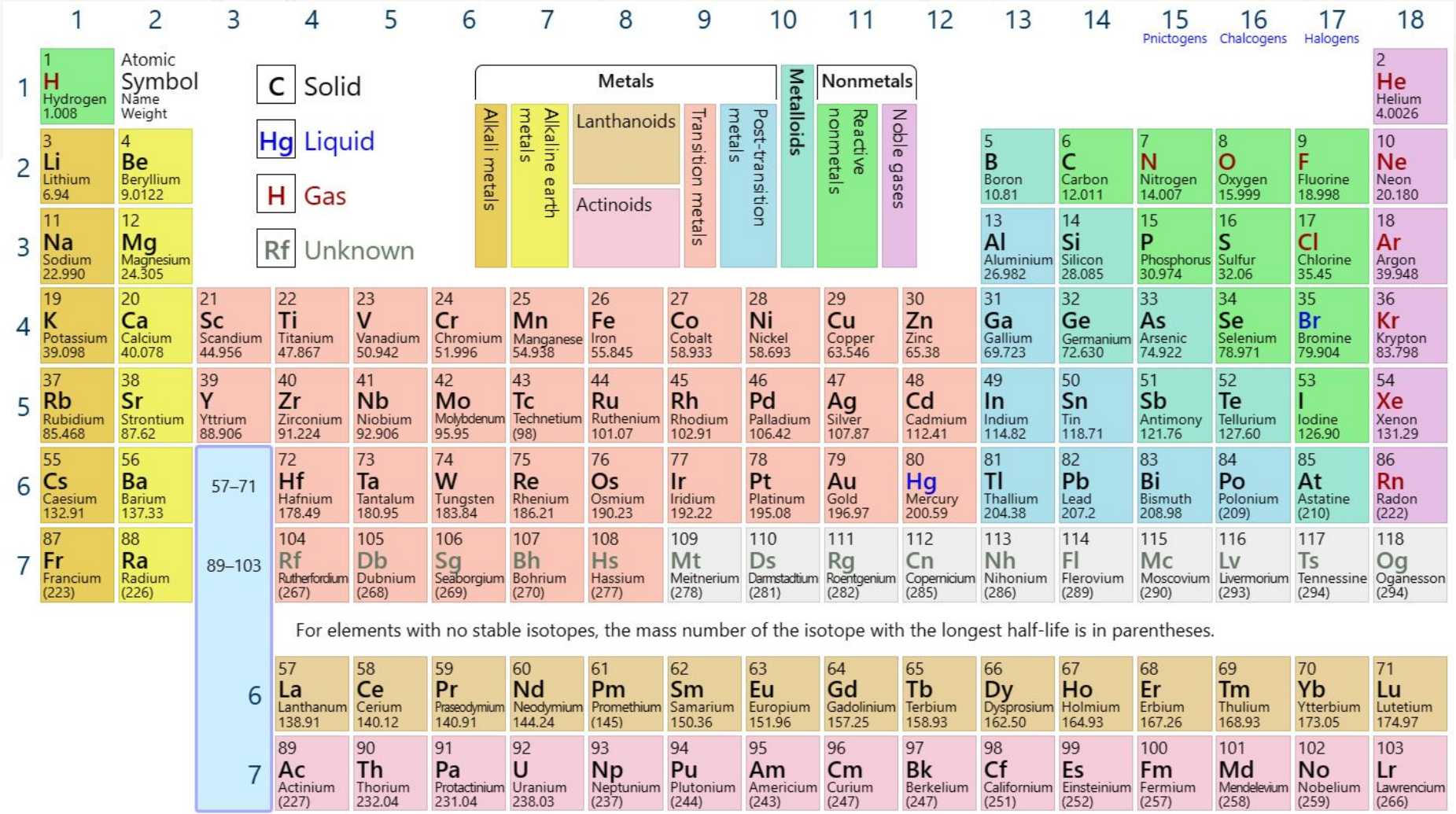


Vídeo aulas e notas de aula:
Prof. Rodrigo Capaz (UFRJ)

How Chemistry and Physics Meet in the Solid State

By Roald Hoffmann*

To make sense of the marvelous electronic properties of the solid state, chemists must learn the language of solid-state physics, of band structures. An attempt is made here to demystify that language, drawing explicit parallels to well-known concepts in theoretical chemistry. To the joint search of physicists and chemists for understanding of the bonding in extended systems, the chemist brings a great deal of intuition and some simple but powerful


1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Pnictogens
Chalcogens
Halogens
Atomic
Symbol
Name
Weight
C Solid
Hg Liquid
H Gas
Rf Unknown
Metals
Alkali metals
Alkaline earth metals
Lanthanoids
Actinoids
Transition metals
Post-transition metals
Metalloids
Nonmetals
Reactive nonmetals
Noble gases
1 H Hydrogen 1.008
2 He Helium 4.0026
3 Li Lithium 6.94
4 Be Beryllium 9.0122
5 B Boron 10.81
6 C Carbon 12.011
7 N Nitrogen 14.007
8 O Oxygen 15.999
9 F Fluorine 18.998
10 Ne Neon 20.180
11 Na Sodium 22.990
12 Mg Magnesium 24.305
13 Al Aluminium 26.982
14 Si Silicon 28.085
15 P Phosphorus 30.974
16 S Sulfur 32.06
17 Cl Chlorine 35.45
18 Ar Argon 39.948
19 K Potassium 39.098
20 Ca Calcium 40.078
21 Sc Scandium 44.956
22 Ti Titanium 47.867
23 V Vanadium 50.942
24 Cr Chromium 51.996
25 Mn Manganese 54.938
26 Fe Iron 55.845
27 Co Cobalt 58.933
28 Ni Nickel 58.693
29 Cu Copper 63.546
30 Zn Zinc 65.38
31 Ga Gallium 69.723
32 Ge Germanium 72.630
33 As Arsenic 74.922
34 Se Selenium 78.971
35 Br Bromine 79.904
36 Kr Krypton 83.798
37 Rb Rubidium 85.468
38 Sr Strontium 87.62
39 Y Yttrium 88.906
40 Zr Zirconium 91.224
41 Nb Niobium 92.906
42 Mo Molybdenum 95.95
43 Tc Technetium (98)
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.91
46 Pd Palladium 106.42
47 Ag Silver 107.87
48 Cd Cadmium 112.41
49 In Indium 114.82
50 Sn Tin 118.71
51 Sb Antimony 121.76
52 Te Tellurium 127.60
53 I Iodine 126.90
54 Xe Xenon 131.29
55 Cs Caesium 132.91
56 Ba Barium 137.33
57–71
72 Hf Hafnium 178.49
73 Ta Tantalum 180.95
74 W Tungsten 183.84
75 Re Rhenium 186.21
76 Os Osmium 190.23
77 Ir Iridium 192.22
78 Pt Platinum 195.08
79 Au Gold 196.97
80 Hg Mercury 200.59
81 Tl Thallium 204.38
82 Pb Lead 207.2
83 Bi Bismuth 208.98
84 Po Polonium (209)
85 At Astatine (210)
86 Rn Radon (222)
87 Fr Francium (223)
88 Ra Radium (226)
89–103
104 Rf Rutherfordium (267)
105 Db Dubnium (268)
106 Sg Seaborgium (269)
107 Bh Bohrium (270)
108 Hs Hassium (277)
109 Mt Meitnerium (278)
110 Ds Darmstadtium (281)
111 Rg Roentgenium (282)
112 Cn Copernicium (285)
113 Nh Nihonium (286)
114 Fl Flerovium (289)
115 Mc Moscovium (290)
116 Lv Livermorium (293)
117 Ts Tennessine (294)
118 Og Oganesson (294)
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.
6
57 La Lanthanum 138.91
58 Ce Cerium 140.12
59 Pr Praseodymium 140.91
60 Nd Neodymium 144.24
61 Pm Promethium (145)
62 Sm Samarium 150.36
63 Eu Europium 151.96
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66 Dy Dysprosium 162.50
67 Ho Holmium 164.93
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69 Tm Thulium 168.93
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71 Lu Lutetium 174.97
7
89 Ac Actinium (227)
90 Th Thorium 232.04
91 Pa Protactinium 231.04
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93 Np Neptunium (237)
94 Pu Plutonium (244)
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96 Cm Curium (247)
97 Bk Berkelium (247)
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99 Es Einsteinium (252)
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102 No Nobelium (259)
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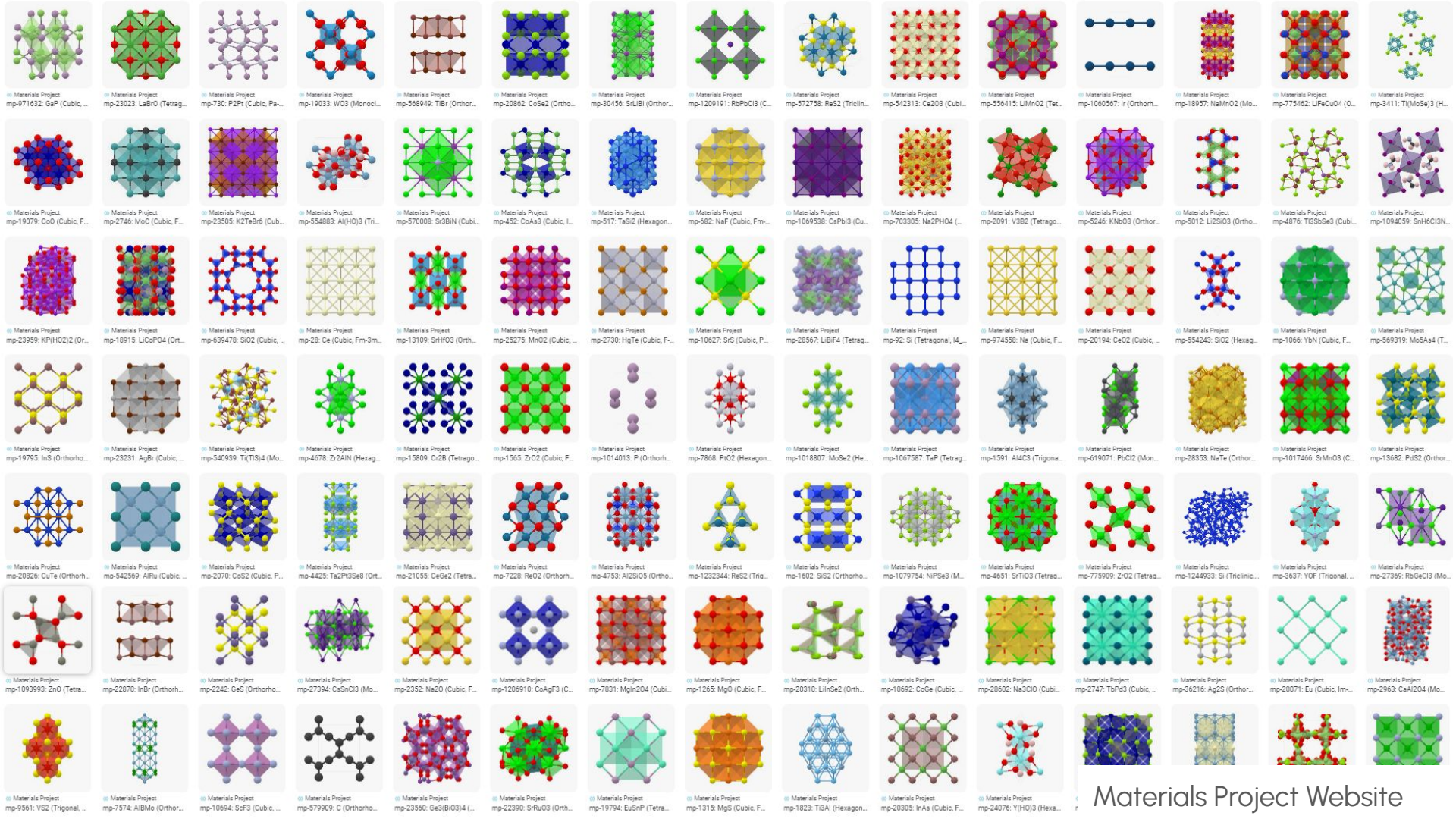
Materials Project
mp-971632: GaP (Cubic, ...
mp-23023: LaBrO (Tetrag...
mp-730: P2Pt (Cubic, Pa-...
mp-19033: WO3 (Monocl...
mp-568949: TlBr (Orthor...
mp-20862: CoSe2 (Ortho...
mp-30456: SrLiBi (Orthor...
mp-1209191: RbPbCl3 (C...
mp-572758: ReS2 (Triclin...
mp-542313: Ce2O3 (Cubi...
mp-556415: LiMnO2 (Tet...
mp-1060567: Ir (Orthorh...
mp-18957: NaMnO2 (Mo...
mp-775462: LiFeCuO4 (O...
mp-3411: Ti(MoSe)3 (H...
mp-19079: CoO (Cubic, F...
mp-2746: MoC (Cubic, F...
mp-23505: K2TeBr6 (Cub...
mp-554883: Al(HO)3 (Tri...
mp-570008: Sr3BiN (Cubi...
mp-452: CoAs3 (Cubic, I...
mp-517: TaSi2 (Hexagon...
mp-682: NaF (Cubic, Fm-...
mp-1069538: CaPbI3 (Cu...
mp-703305: Na2PHO4 (...
mp-2091: V3B2 (Tetrago...
mp-5246: KNbO3 (Orthor...
mp-5012: Li2SiO3 (Ortho...
mp-4876: Ti3SbSe3 (Cubi...
mp-1094059: SnH6Cl3N...
mp-23959: KP(HO2)2 (Or...
mp-18915: LiCoPO4 (Ort...
mp-639478: SiO2 (Cubic, ...
mp-28: Ce (Cubic, Fm-3m...
mp-13109: SrHfO3 (Orth...
mp-25275: MnO2 (Cubic, ...
mp-2730: HgTe (Cubic, F-...
mp-10627: SrS (Cubic, P...
mp-28567: LiBiF4 (Tetrag...
mp-92: Si (Tetragonal, I4_...
mp-974558: Na (Cubic, F...
mp-20194: CeO2 (Cubic, ...
mp-554243: SiO2 (Hexag...
mp-1066: YbN (Cubic, F...
mp-569319: MoSbs4 (T...
mp-19795: InS (Orthorho...
mp-23231: AgBr (Cubic, ...
mp-540939: Ti(TlS)4 (Mo...
mp-4678: Zr2AlN (Hexag...
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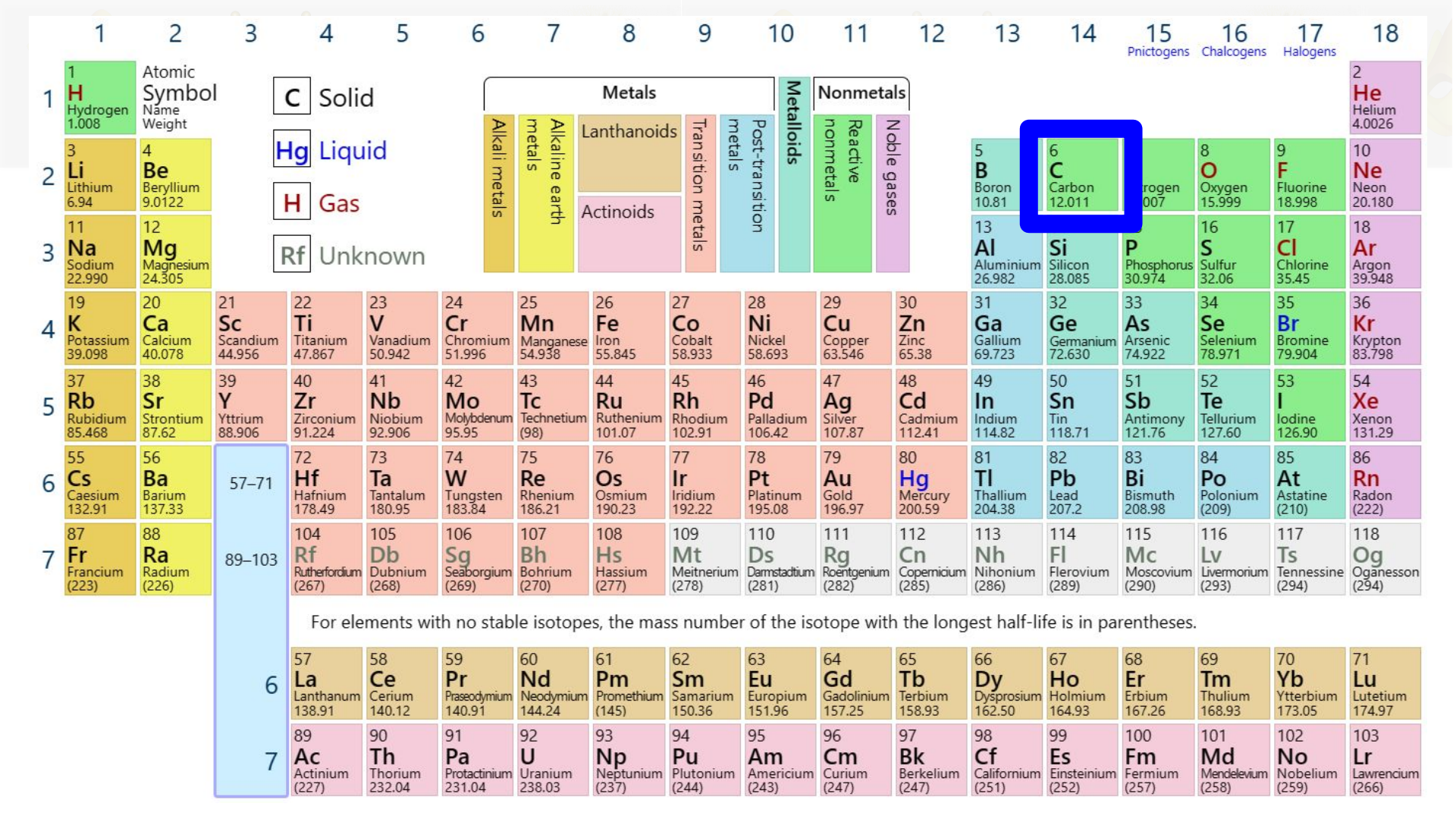
mp-1823: TiSAl (Hexagon...
mp-20305: InAs (Cubic, F...
mp-24076: Y(HO)3 (Hexa...
Materials Project Website


1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Pnictogens
Chalcogens
Halogens
Atomic
Symbol
Name
Weight
C Solid
Hg Liquid
H Gas
Rf Unknown
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Alkali metals
Alkaline earth metals
Lanthanoids
Actinoids
Transition metals
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Grafite X Diamante

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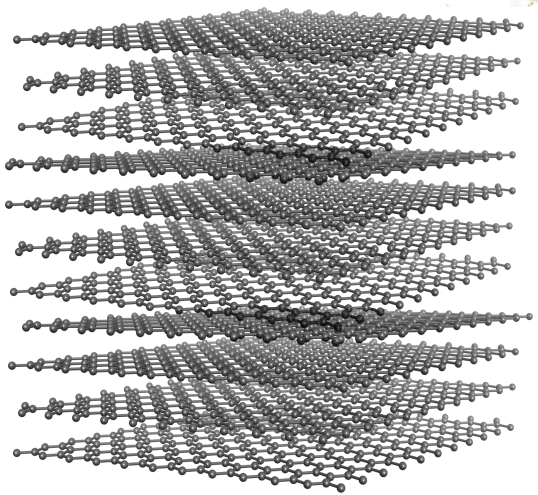
Grafite X Diamante



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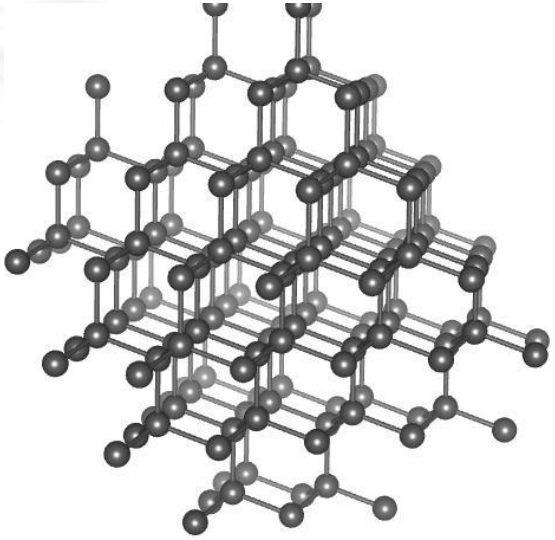

Problema de muitos corpos

Schrödinger Equation

$H\Psi = E\Psi$

Energia cinética dos núcleos.

Energia cinética dos elétrons.

Interação elétron-núcleo

$$\hat{H} = -\sum_a \frac{\hbar^2}{2M_a}\nabla^2_{\vec{R}_a} - \frac{\hbar^2}{2m}\sum_i \nabla^2_{\vec{r}_i} - \sum_a \sum_i \frac{Z_a e^2}{4\pi\epsilon_0 |\vec{R}_a - \vec{r}_i|} + \frac{1}{2}\sum_a \sum_{b\neq a} \frac{Z_a Z_b e^2}{4\pi\epsilon_0 |\vec{R}_a - \vec{R}_b|} + \frac{1}{2}\sum_i \sum_{j\neq i} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$

Interação núcleo-núcleo

Interação elétron-elétron

Aproximação de Born-Oppenheimer

Schrödinger Equation

$H\Psi = E\Psi$

Energia cinética dos núcleos.

Energia cinética dos elétrons.

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Interação núcleo-núcleo

Interação elétron-elétron

~Constante

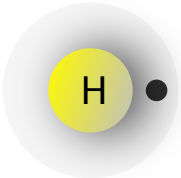
Aproximação de Born-Oppenheimer: nos permite desacoplar o Hamiltoniano eletrônico do nuclear.

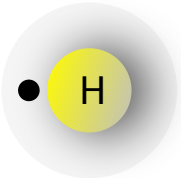
Bonding States: H_2 molecule

$1s^1$

E = -13.6 eV

$1s^1$





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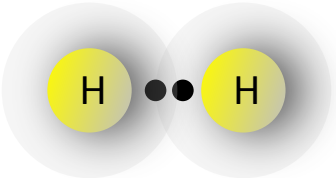
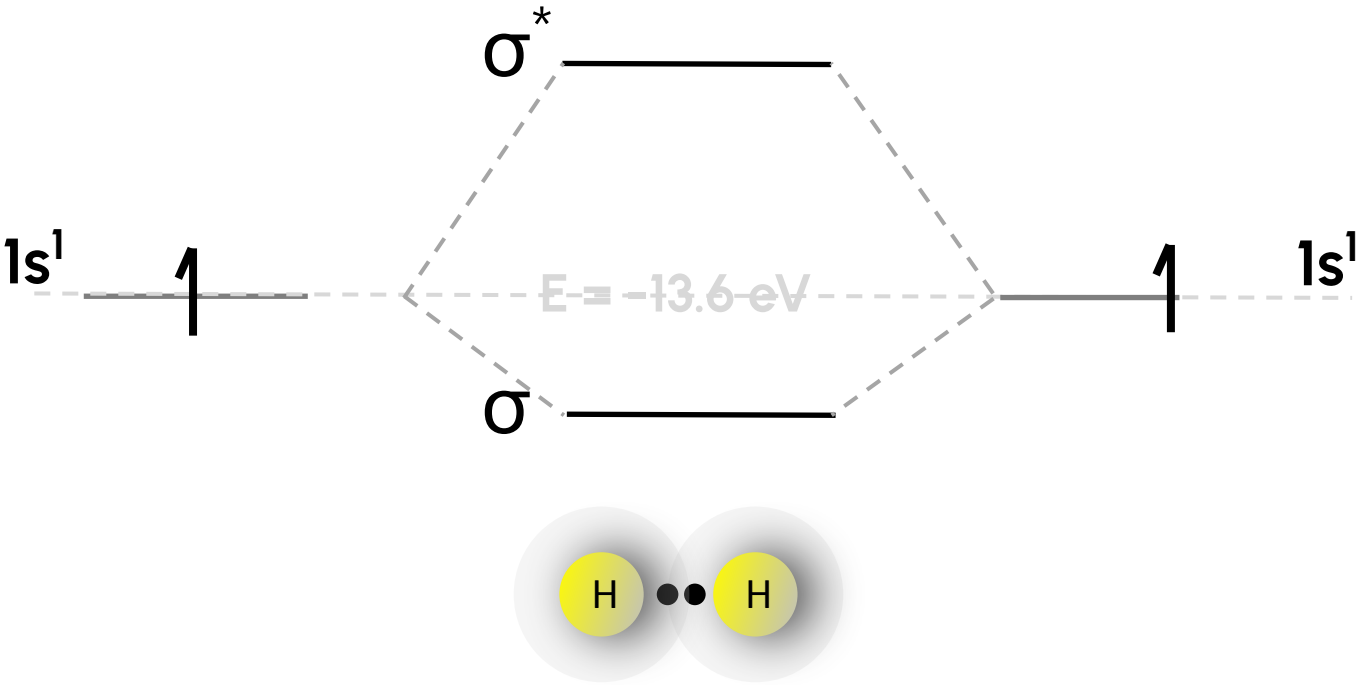
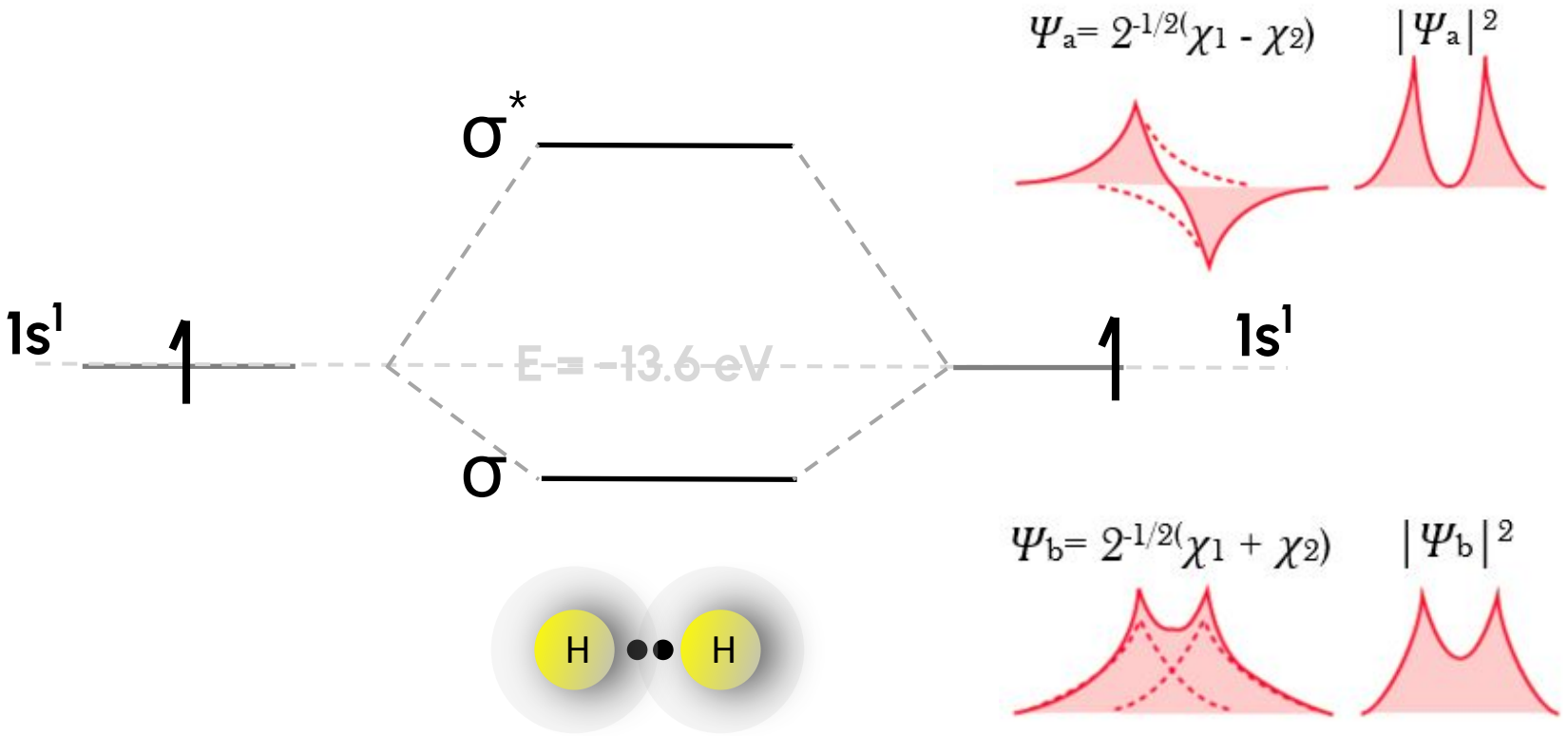
$1s^1$  E = -13.6 eV  $1s^1$



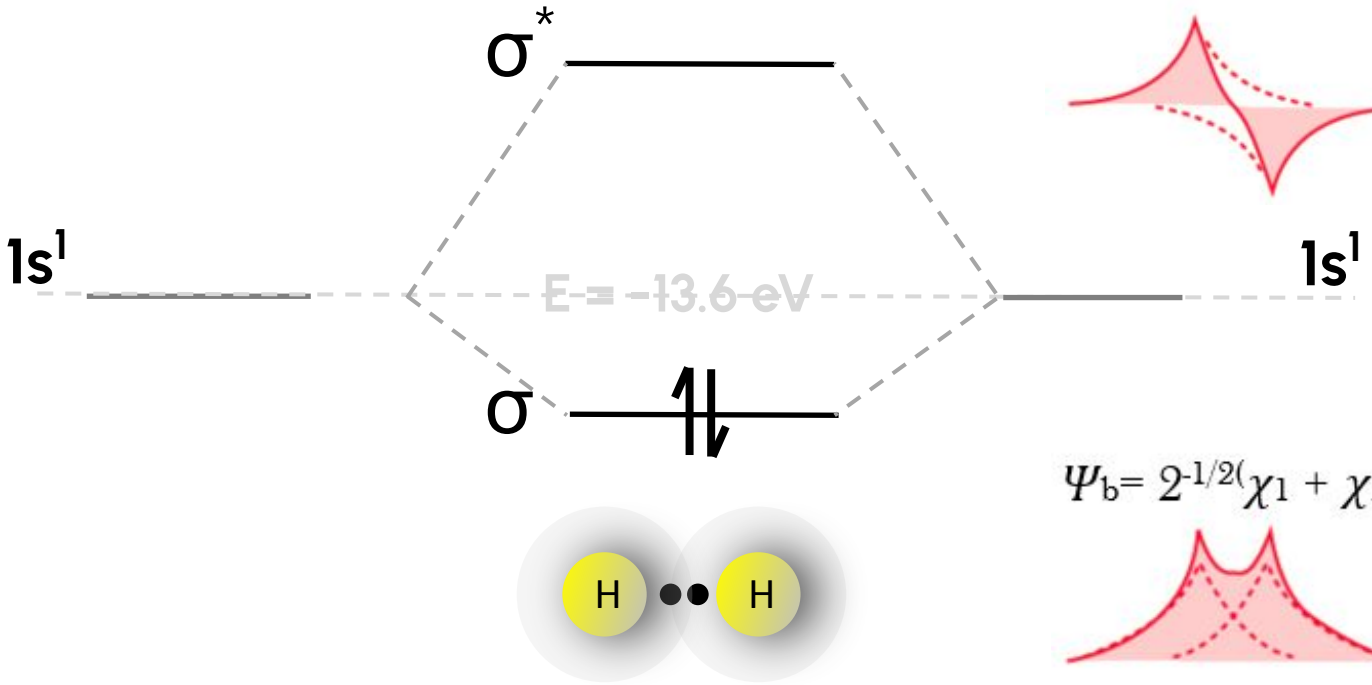
Bonding States: H_2 molecule



Bonding States: H_2 molecule



Bonding States: H_2 molecule



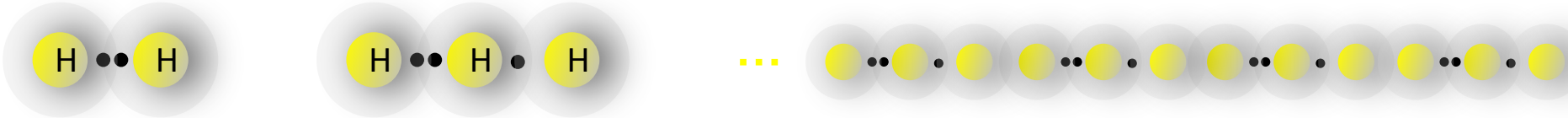
$\Psi_a = 2^{-1/2}(\chi_1 - \chi_2)$

$|\Psi_a|^2$

$\Psi_b = 2^{-1/2}(\chi_1 + \chi_2)$

$|\Psi_b|^2$

Cadeia infinita de átomos de H



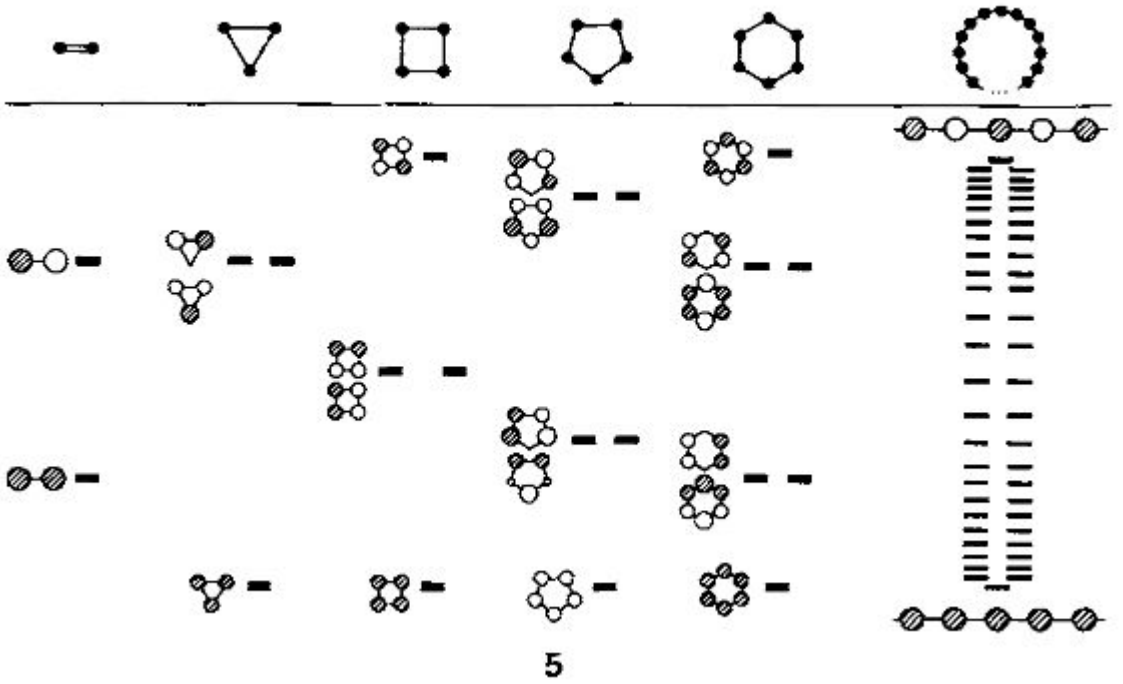
N = 2

N = 3

...

N = ∞ (~10^{23})

Cadeia infinita de átomos de H



5

Problema de muitos corpos

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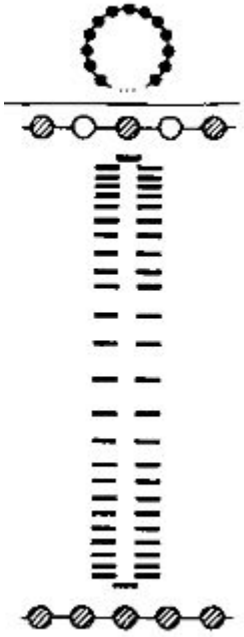
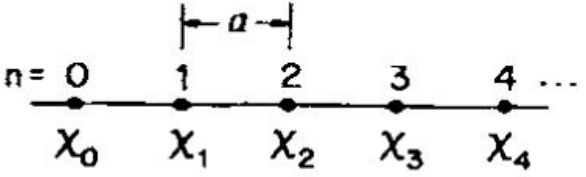
Interação núcleo-núcleo

Interação elétron-elétron

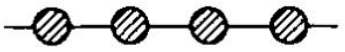
Elétrons num potencial cristalino 1D



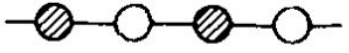


$$\psi_k = \sum_n e^{ikna} \chi_n$$

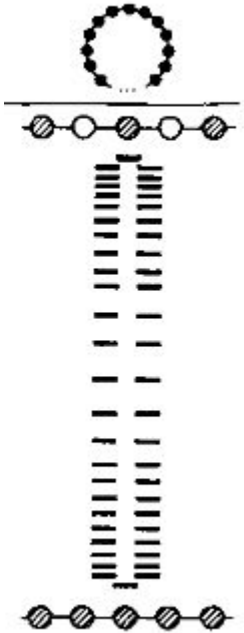
$k = 0 \qquad \psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 + \cdots$



$k = \frac{\pi}{a} \qquad \psi_{\frac{\pi}{a}} = \sum_n e^{\pi i n} \chi_n = \sum_n (-1)^n \chi_n = \chi_0 - \chi_1 + \chi_2 - \chi_3 + \cdots$



Elétrons num potencial cristalino 1D



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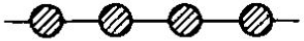

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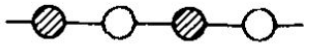
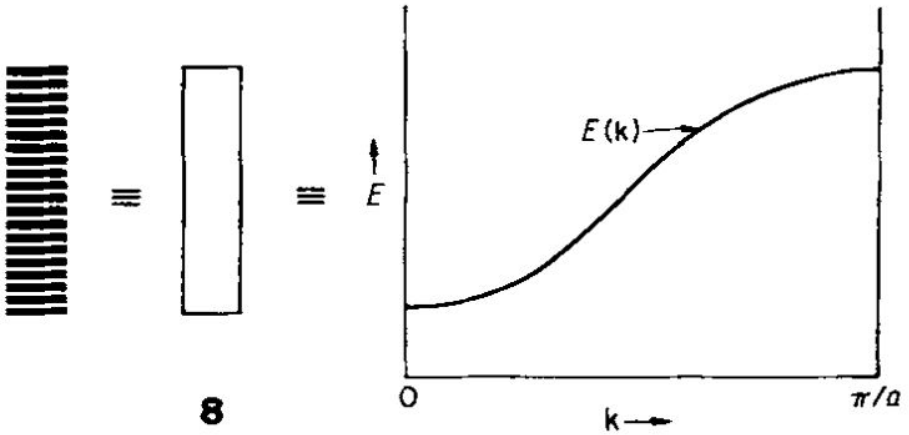
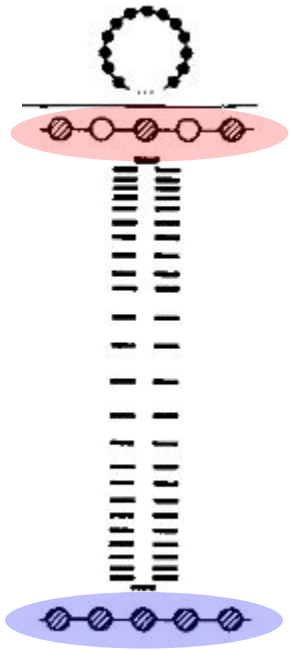




Elétrons num potencial cristalino 1D



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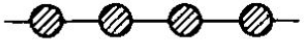

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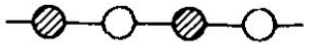
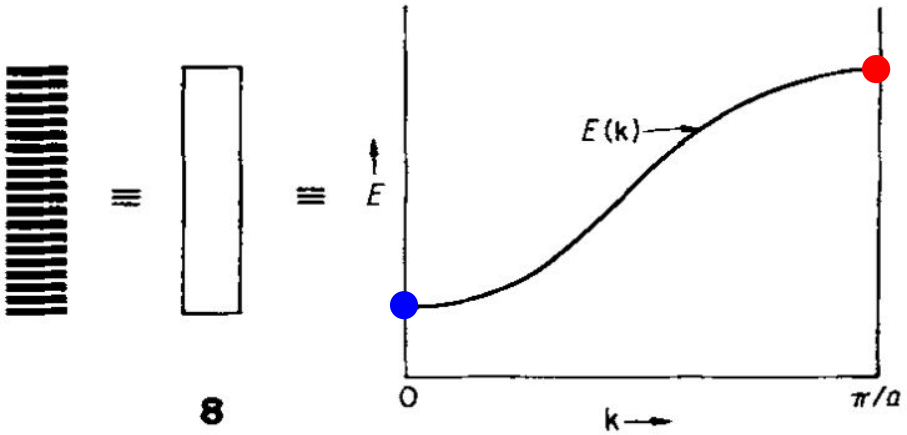
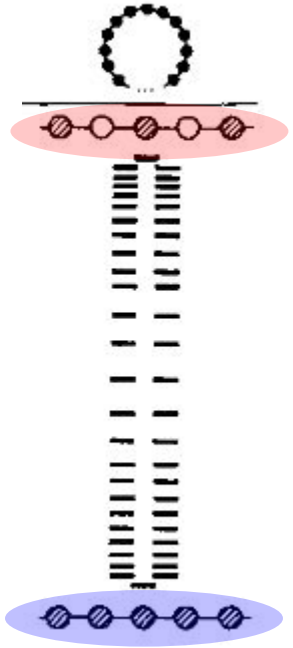




Elétrons num potencial cristalino 1D



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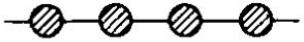

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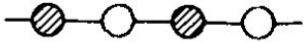
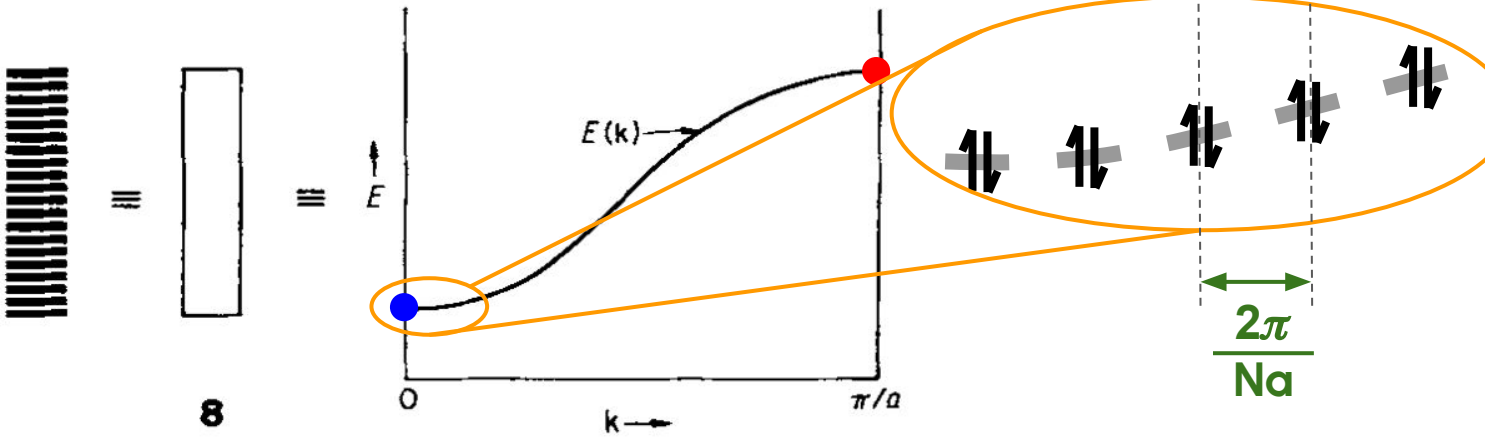
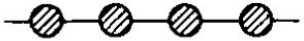




8

Estrutura de Bandas

$k = 0 \qquad \psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 + \cdots$



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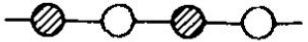

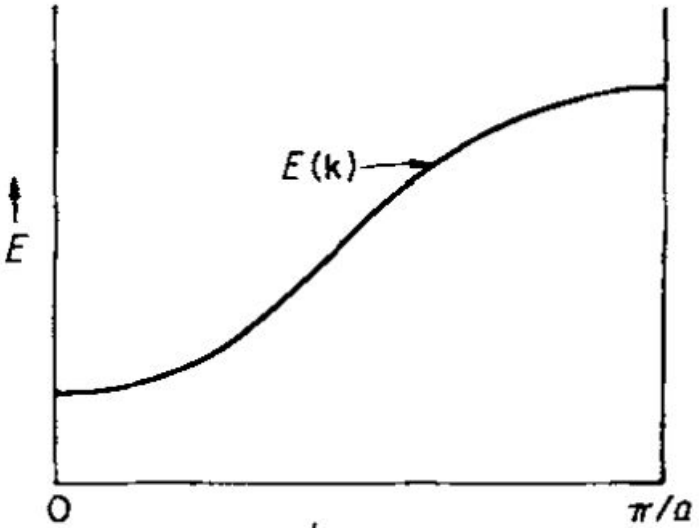

Estrutura de Bandas

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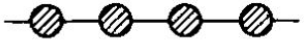

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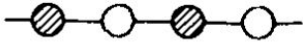
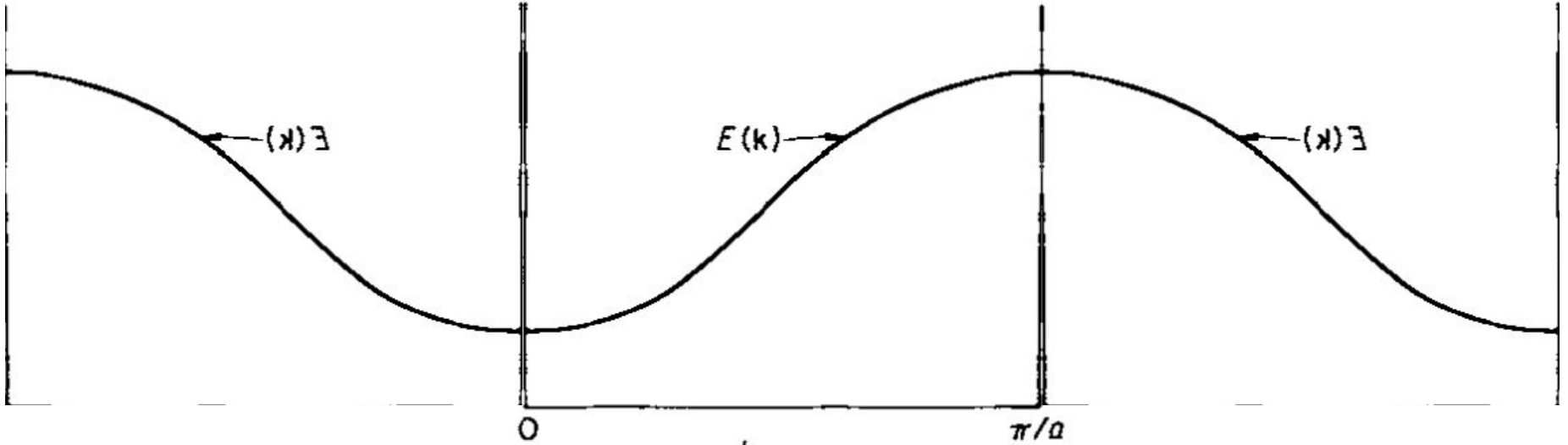
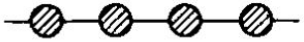


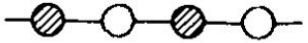


Zona de Brillouin

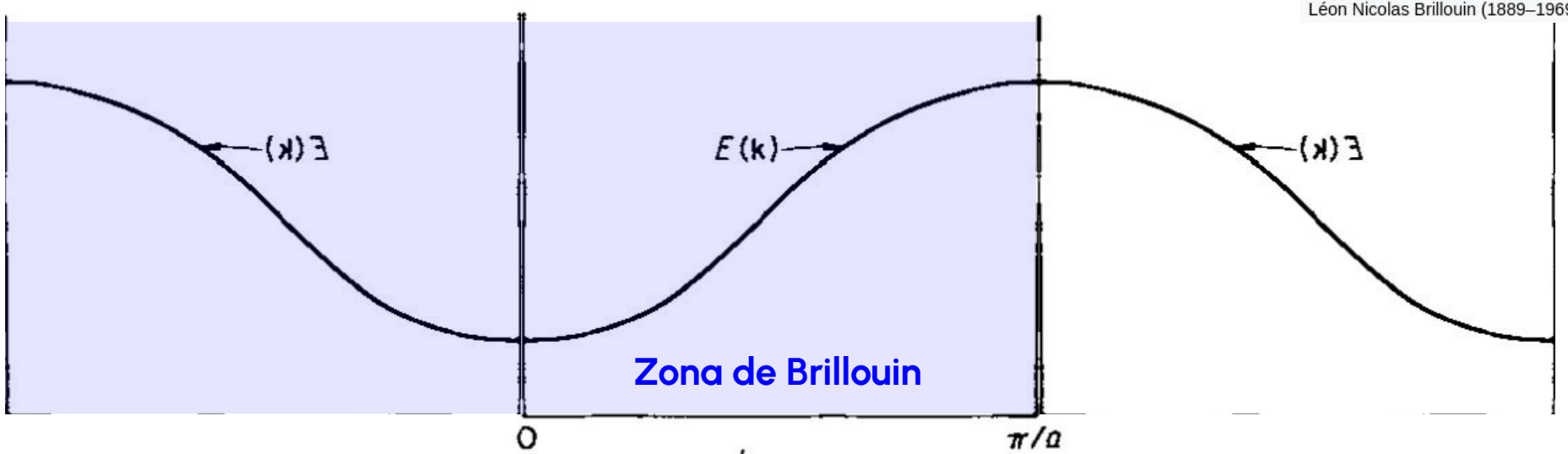
$$k = 0 \qquad \psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 + \cdots$$



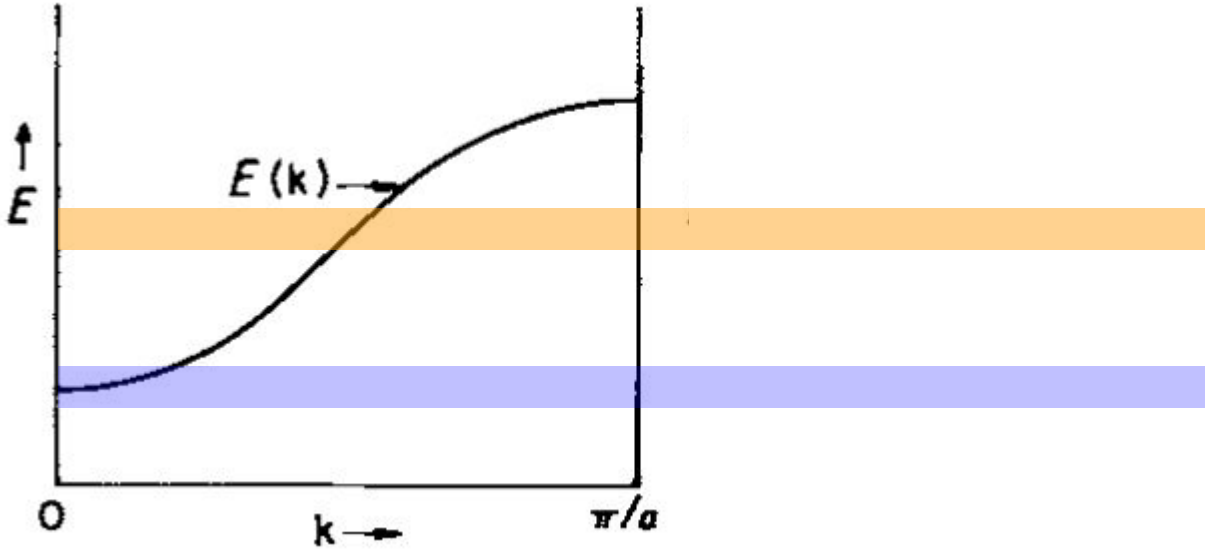
$$k = \frac{\pi}{a} \qquad \psi_{\frac{\pi}{a}} = \sum_n e^{\pi i n} \chi_n = \sum_n (-1)^n \chi_n = \chi_0 - \chi_1 + \chi_2 - \chi_3 + \cdots$$



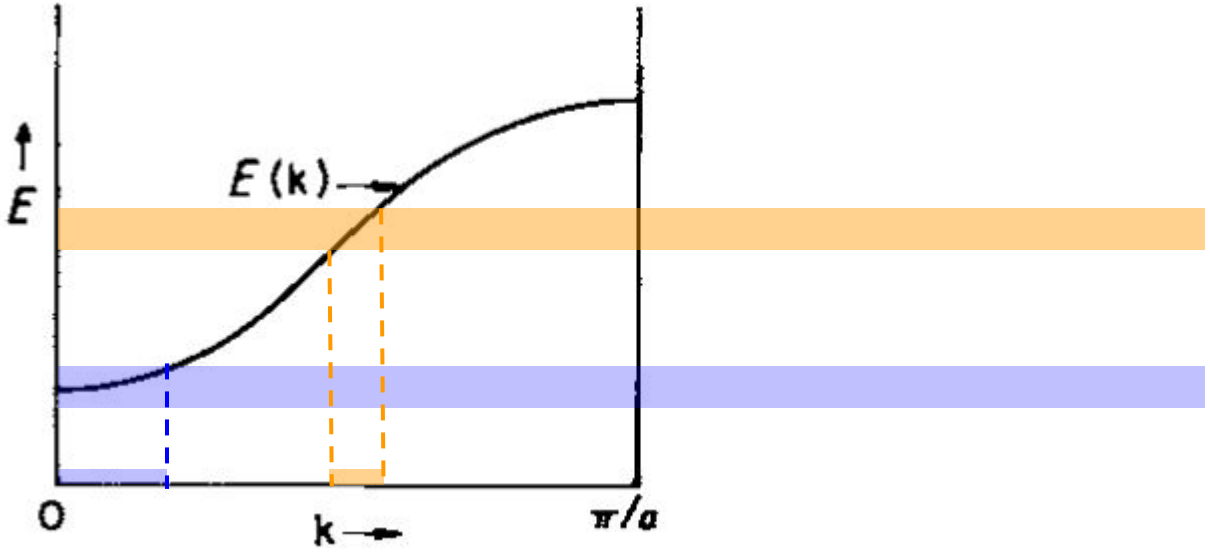
Léon Nicolas Brillouin (1889–1969)



Densidade de estados

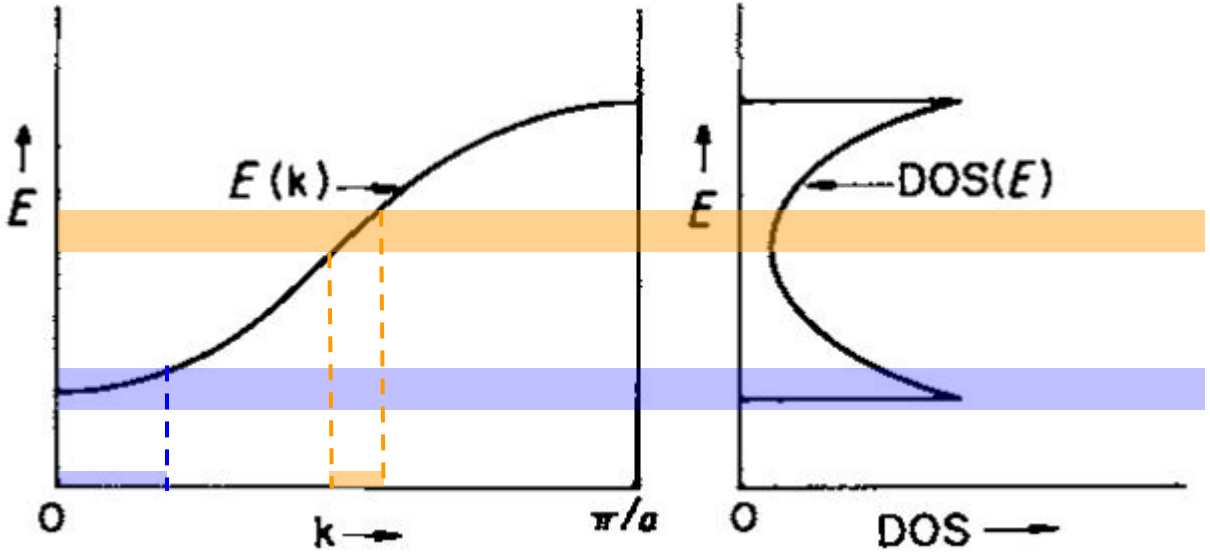


Densidade de estados



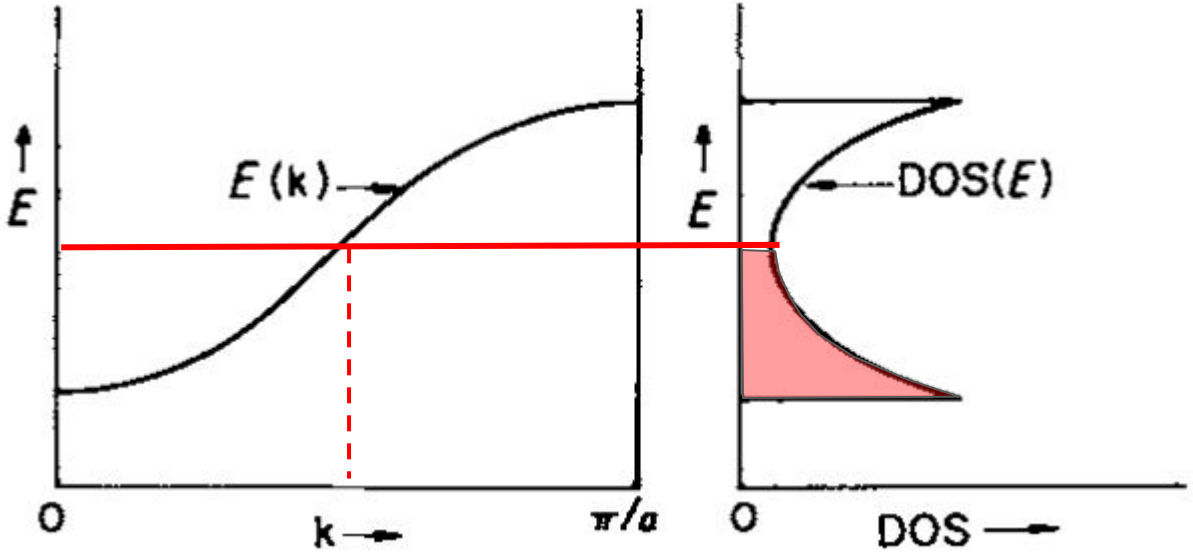
Densidade de estados

$\mathrm{DOS}(E)\,dE$ = number of levels between E and $E+dE$

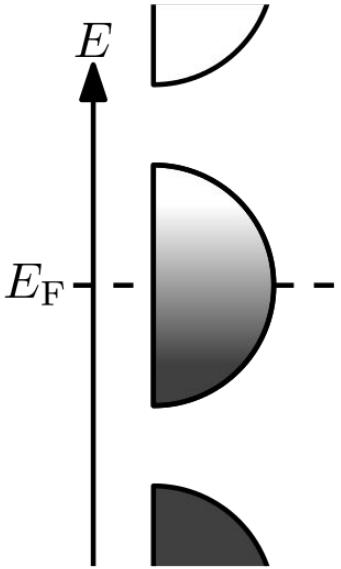


Densidade de estados e Nível de Fermi

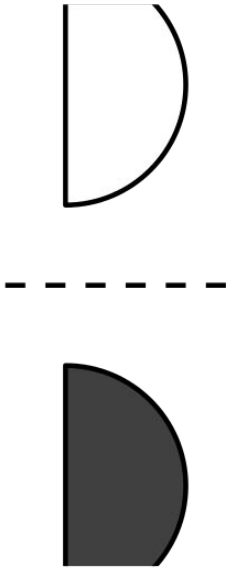
$\mathrm{DOS}(E)\,dE$ = number of levels between E and $E+dE$



Densidade de estados e Nível de Fermi

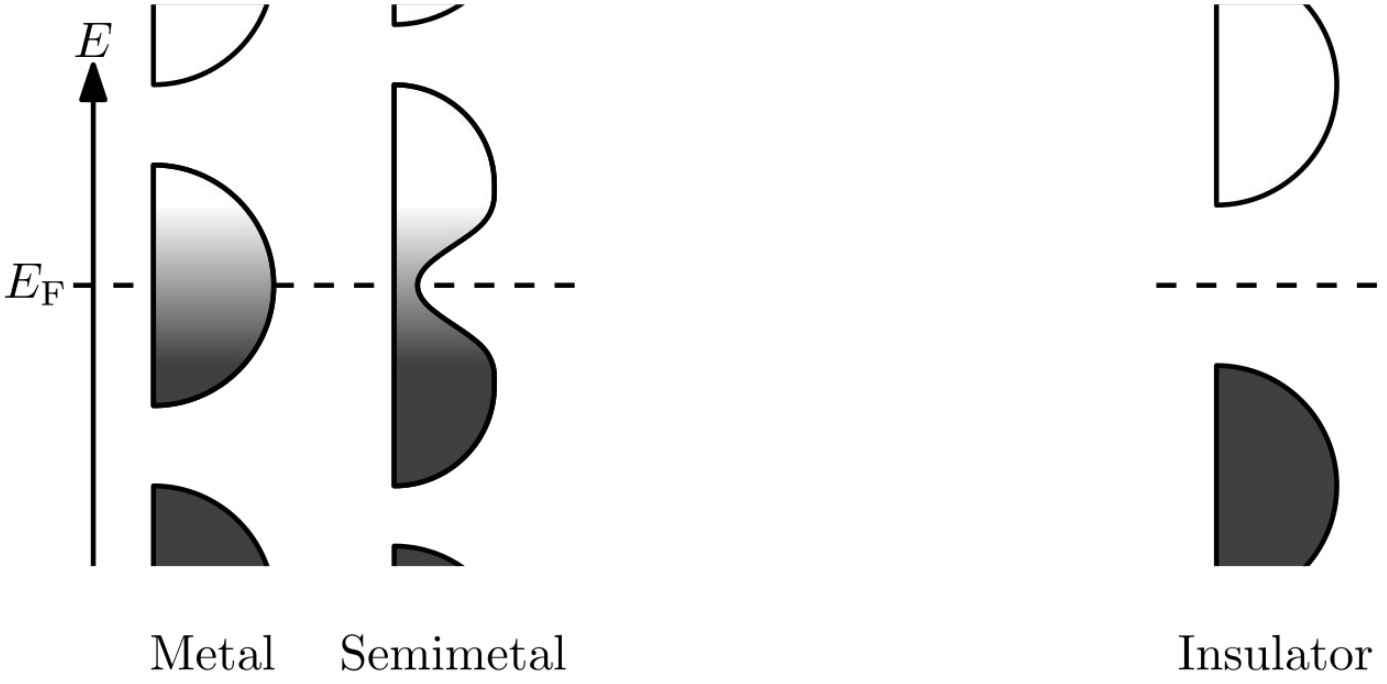


Metal

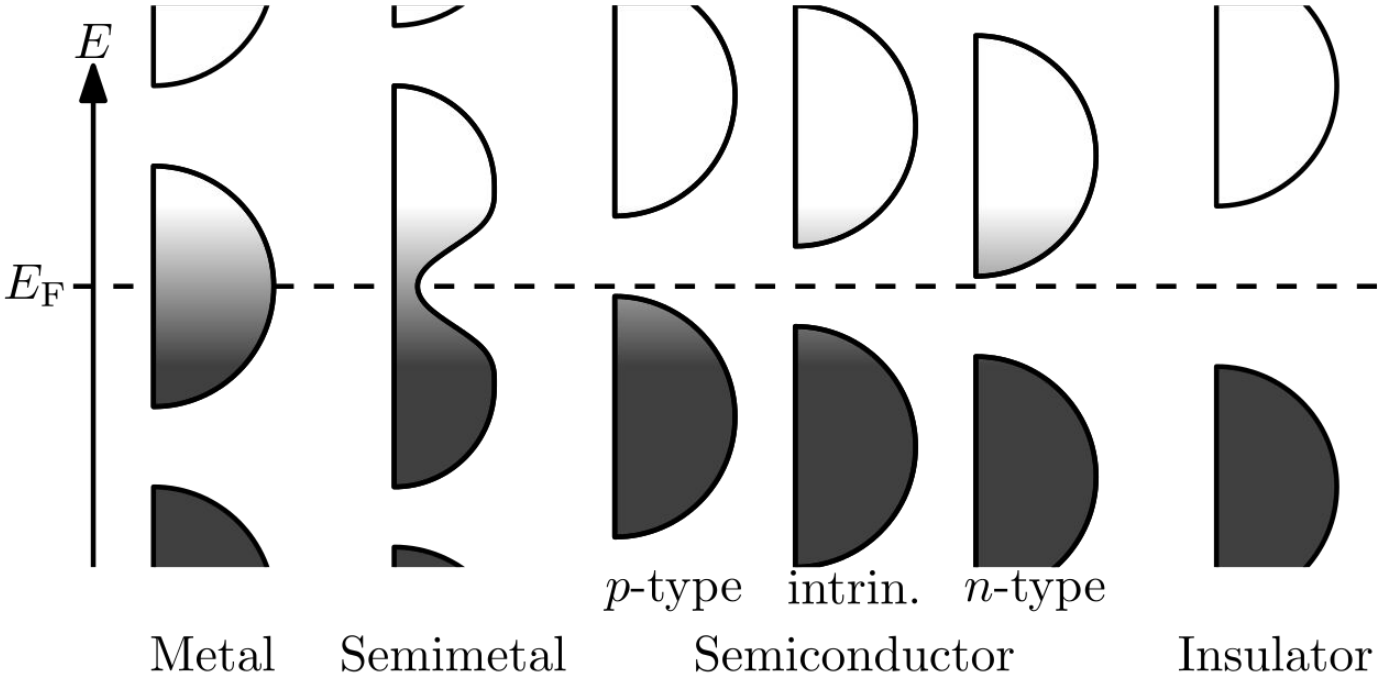


Insulator

Densidade de estados e Nível de Fermi



Densidade de estados e Nível de Fermi



Largura de banda

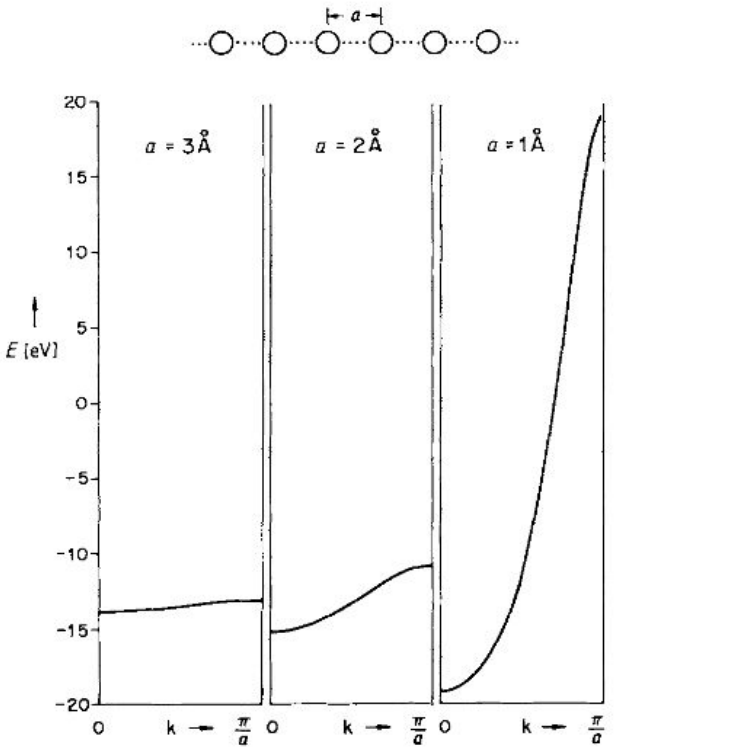
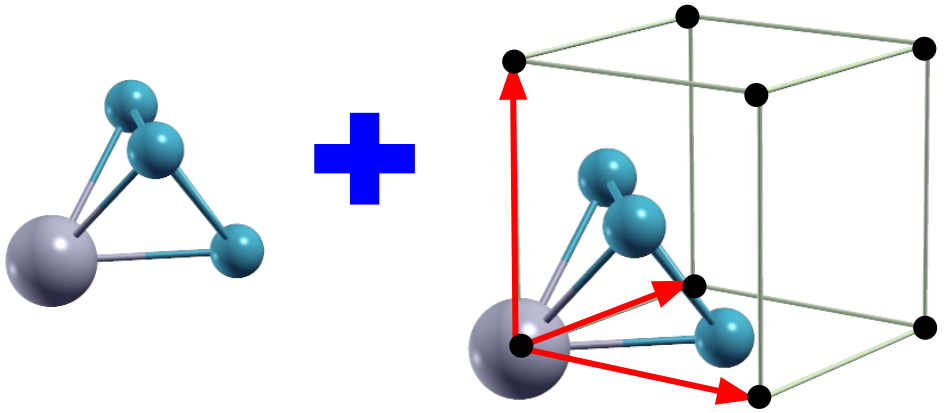


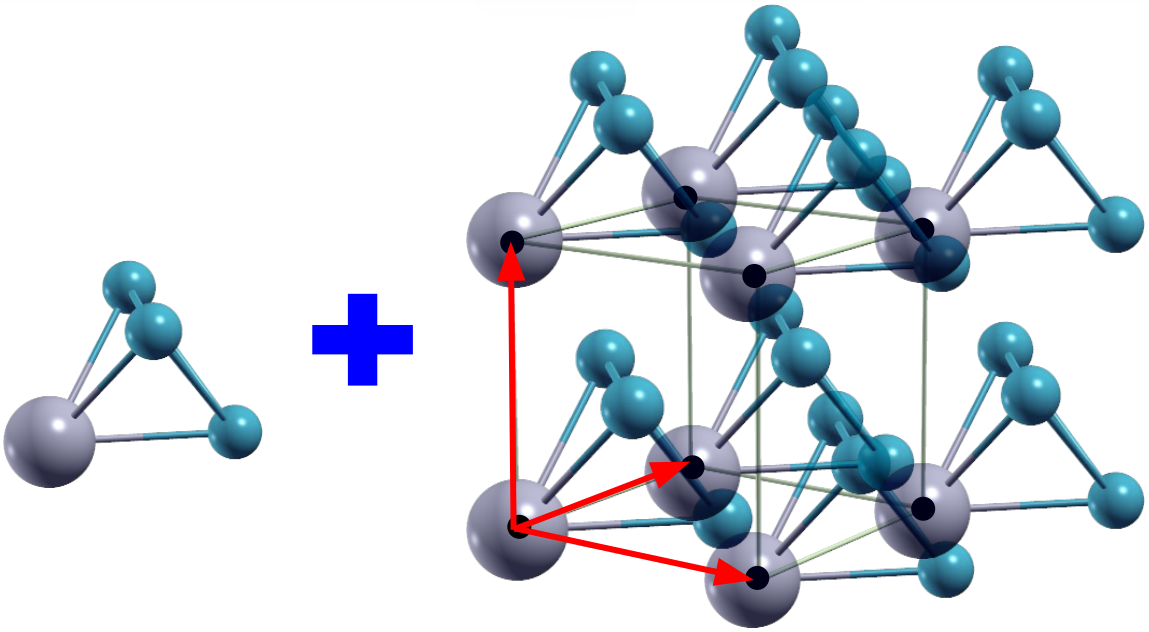
Fig. 1. The band structure of a chain of H atoms spaced 3, 2, and 1 Å apart. The energy of an isolated H atom is −13.6 eV.

$$E = \alpha + 2\beta \cos ka$$

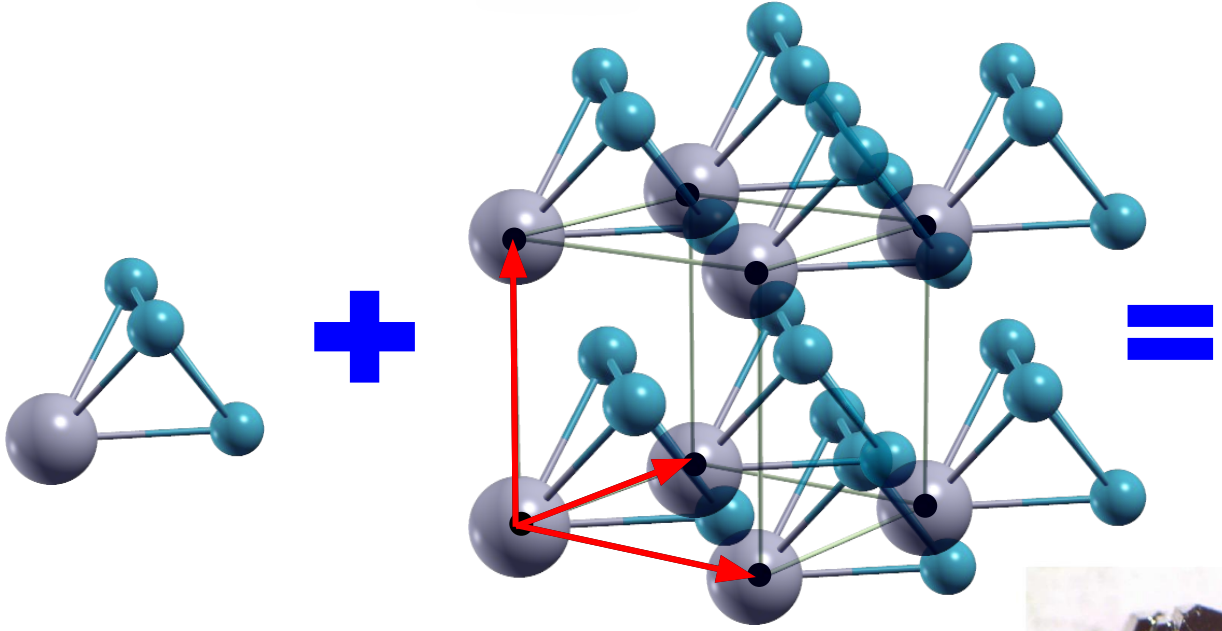
Cristais 3D

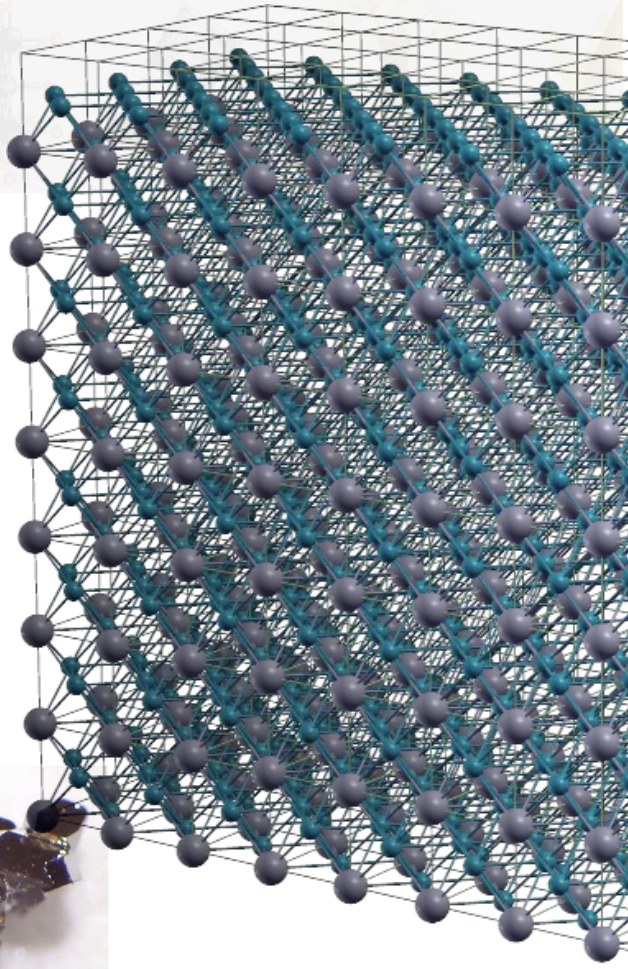


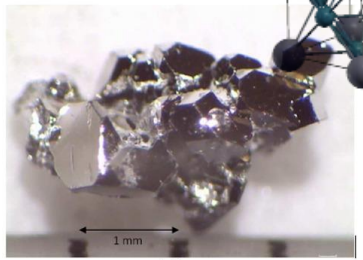
Cristais 3D



Cristais 3D







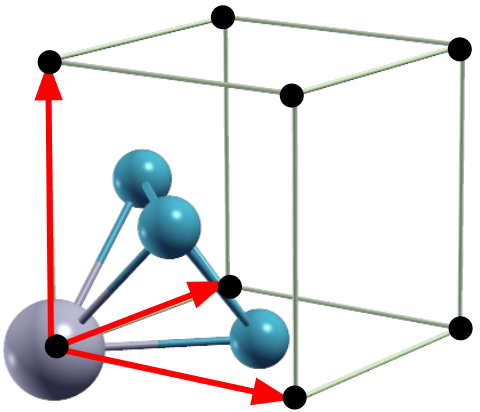
YIn_3

Elétrons num potencial cristalino 3D

Num sólido periódico, o potencial U(***r***) sentido pelos elétrons obedece:

$$U(\boldsymbol{r}) = U(\boldsymbol{r}+\boldsymbol{R})$$

com ***R*** um vetor da rede de Bravais: $\boldsymbol{R} = n_1\boldsymbol{a_1} + n_2\boldsymbol{a_2} + n_3\boldsymbol{a_3}$



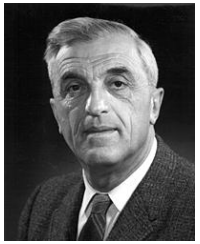
Teorema de Bloch

A solução da equação de Schrödinger correspondentes a elétrons num potencial periódico, U(***r***) = U(***r*** + ***R***),

$$H\psi = \left[\frac{-\hbar^2\nabla^2}{2m} + U(\mathbf{r})\right]\psi = \varepsilon\psi$$

podem ser escolhidas da forma:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$$



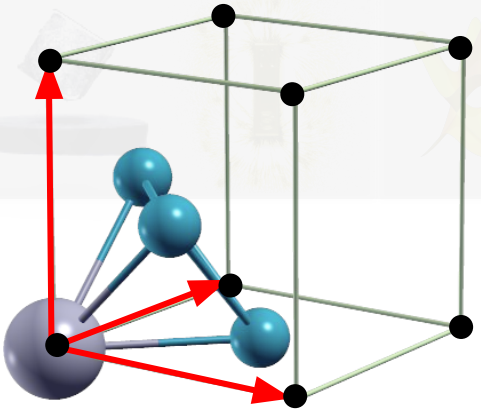
Felix Bloch
(1905-1983)

Onda plana com vetor de onda ***k***

Função com a mesma periodicidade da rede

$$u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R})$$

Rede Recíproca



Considere $\boldsymbol{R}$ o conjunto de pontos que constitui uma rede de Bravais:

$$\boldsymbol{R} = n_1\boldsymbol{a_1} + n_2\boldsymbol{a_2} + n_3\boldsymbol{a_3}$$

Uma onda plana $e^{i\boldsymbol{k}\,.\,\boldsymbol{r}}$ terá a mesma periodicidade da rede para um determinado conjunto de vetores $\boldsymbol{K}$ que obedeçam:

$$e^{i\boldsymbol{K}\,.\,(\boldsymbol{r}+\boldsymbol{R})} = e^{i\boldsymbol{K}\,.\,\boldsymbol{r}}$$

$$e^{i\boldsymbol{K}\,.\,\boldsymbol{R}} = 1$$

O conjunto de todos os vetores de onda $\boldsymbol{K}$ que resultam em ondas planas com a periodicidade de uma dada rede de Bravais é conhecida como sua ***rede recíproca***.

Rede Recíproca

Sejam $\boldsymbol{b_1}$, $\boldsymbol{b_2}$ e $\boldsymbol{b_3}$ os vetores primitivos que formam uma base na rede recíproca. Assim, qualquer vetor $\boldsymbol{k} \in \boldsymbol{K}$, pode ser escrito:

$$\boldsymbol{k} = k_1\boldsymbol{b_1} + k_2\boldsymbol{b_2} + k_3\boldsymbol{b_3}$$

Assim, para que tenhamos:

$$e^{i\boldsymbol{K}\,.\,\boldsymbol{R}} = 1$$

devemos ter:

$$\boldsymbol{k}\,.\,\boldsymbol{R} = 2\pi N = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

$$\mathbf{b}_1 = \frac{2\pi}{V}\,\mathbf{a}_2 \times \mathbf{a}_3 \qquad \mathbf{b}_2 = \frac{2\pi}{V}\,\mathbf{a}_3 \times \mathbf{a}_1 \qquad \mathbf{b}_3 = \frac{2\pi}{V}\,\mathbf{a}_1 \times \mathbf{a}_2$$

$$V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$$

Rede Cúbica.

$$\mathbf{b}_1 = \frac{2\pi}{V}\,\mathbf{a}_2 \times \mathbf{a}_3 \qquad \mathbf{b}_2 = \frac{2\pi}{V}\,\mathbf{a}_3 \times \mathbf{a}_1 \qquad \mathbf{b}_3 = \frac{2\pi}{V}\,\mathbf{a}_1 \times \mathbf{a}_2$$

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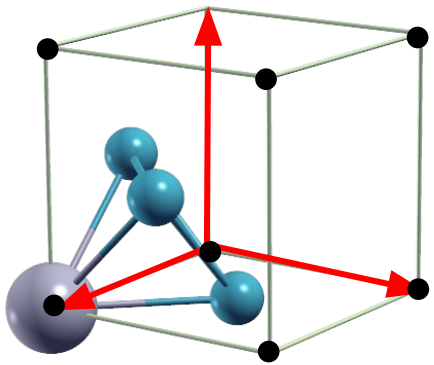


Rede real

$a_1 = a\,\hat{i}$

$a_2 = a\,\hat{j}$

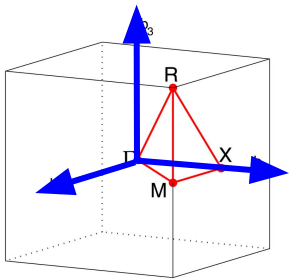
$a_3 = a\,k$

Rede recíproca

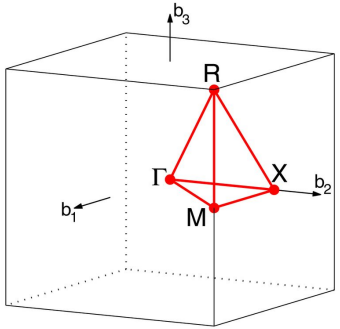
$b_1 = \frac{2\pi}{a}\,\hat{i}$

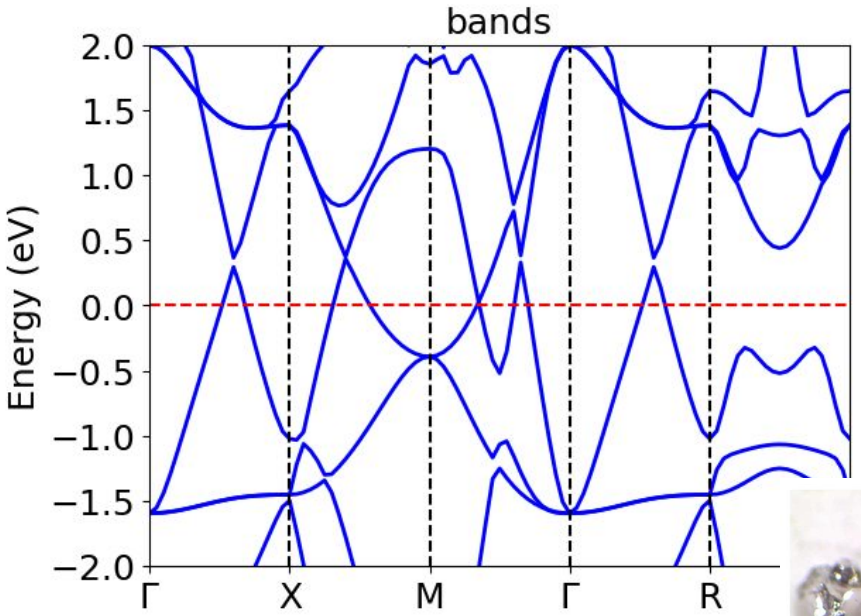
$b_2 = \frac{2\pi}{a}\,\hat{j}$

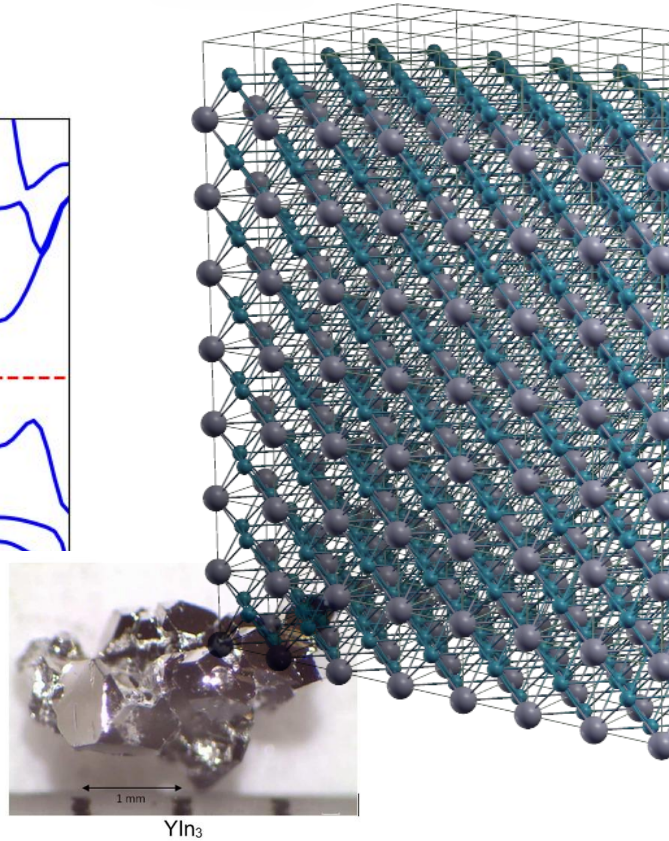
$b_3 = \frac{2\pi}{a}\,k$



Rede Cúbica: YIn_3







Estrutura de Bandas

Significado de *k*: Número de onda, associado ao momento cristalino $\boldsymbol{p} = \hbar\boldsymbol{k}$.

Número de *k*'s permitidos: O número de ***k***'s permitidos é igual ao número de células primitivas N contidas no cristal

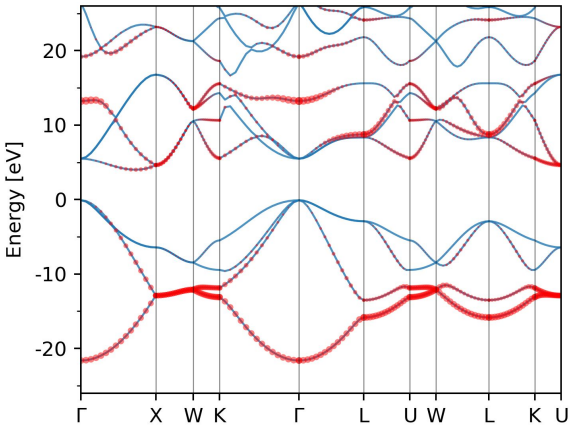
Cristal macroscópico, N → ∞ e então $\boldsymbol{k} \rightarrow \infty$.

Índice de banda: Para cada ***k*** na 1ª ZB, há diversas soluções ψ_{nk} possíveis da equação de Schrödinger, cada qual indexada por um número inteiro **n**, conhecido como índice de banda.

$$\left[\frac{-\hbar^2(i\mathbf{k}+\vec{\nabla})^2}{2m}+U(\mathbf{r})\right]u_{\mathbf{k}}(\mathbf{r})=\varepsilon_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r}).$$

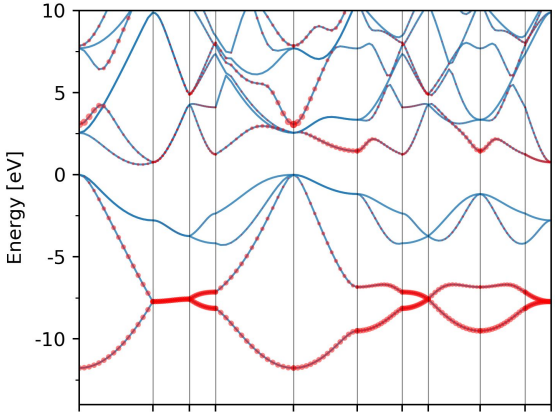
C

$d_{C-C} \sim 1.5$ Å



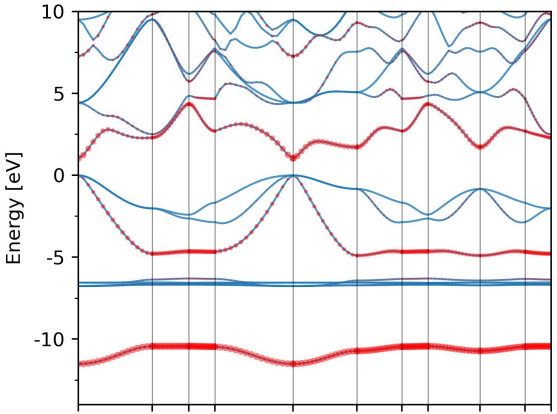
Si

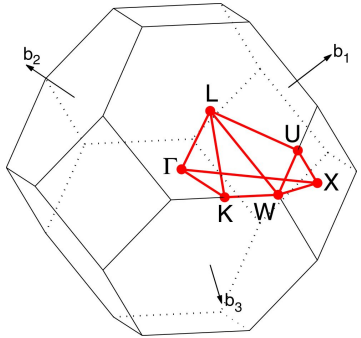
$d_{Si-Si} \sim 2.3$ Å



ZnTe

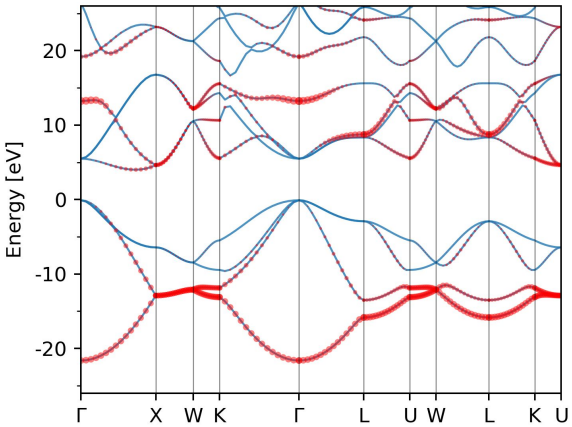
$d_{Zn-Te} \sim 2.6$ Å

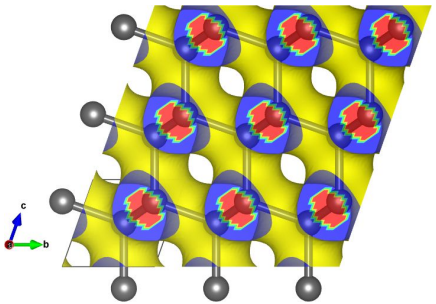




C

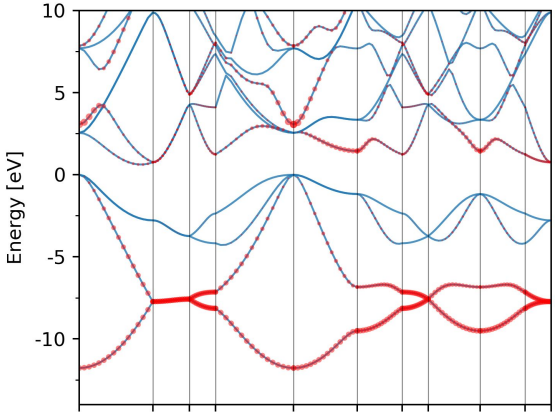
$d_{C-C} \sim 1.5$ Å

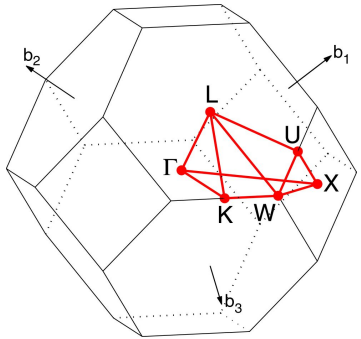




Si

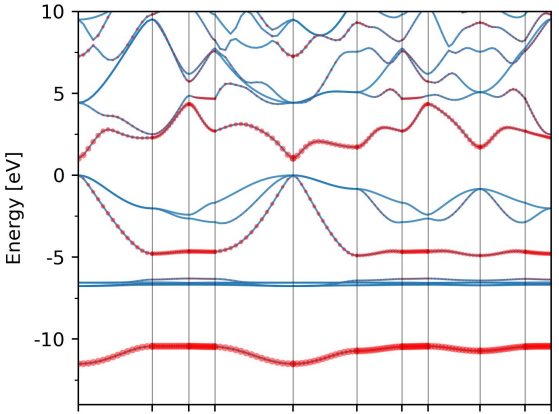
$d_{Si-Si} \sim 2.3$ Å

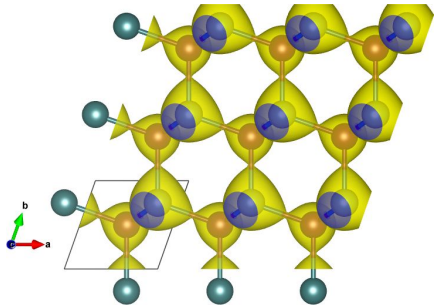




ZnTe

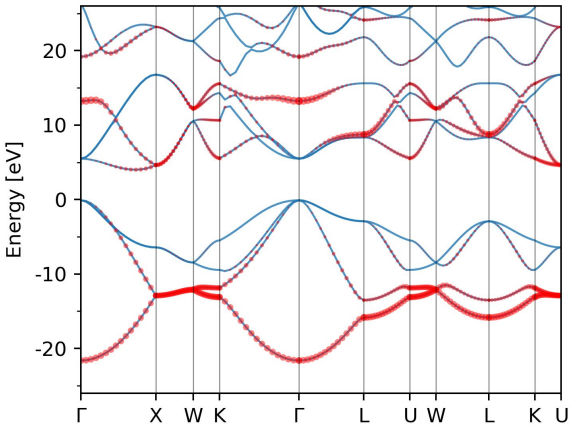
$d_{Zn-Te} \sim 2.6$ Å

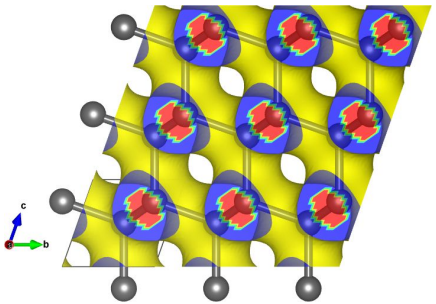




C

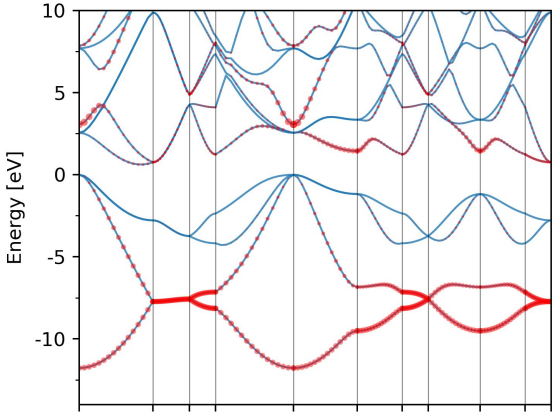
$d_{C-C} \sim 1.5$ Å

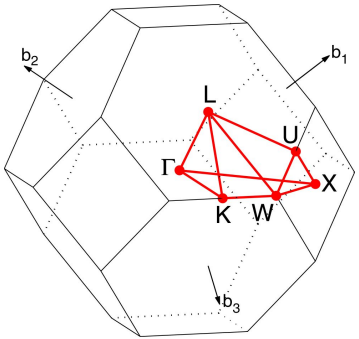




Si

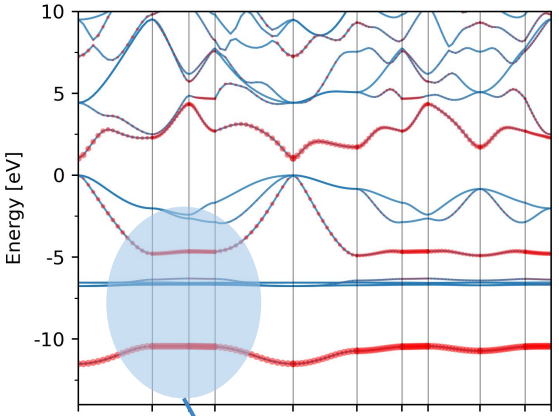
$d_{Si-Si} \sim 2.3$ Å





ZnTe

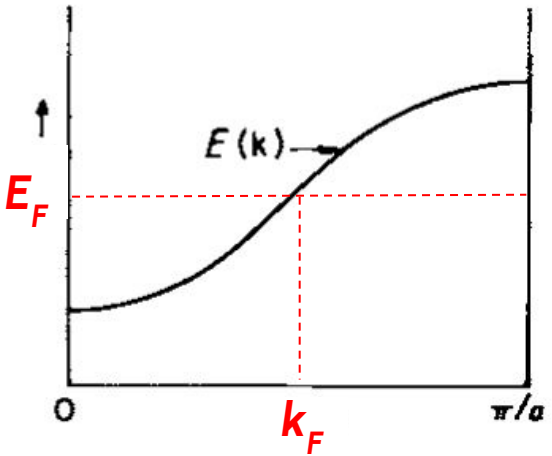
$d_{Zn-Te} \sim 2.6$ Å



Abertura de gap:
quebra de simetria.

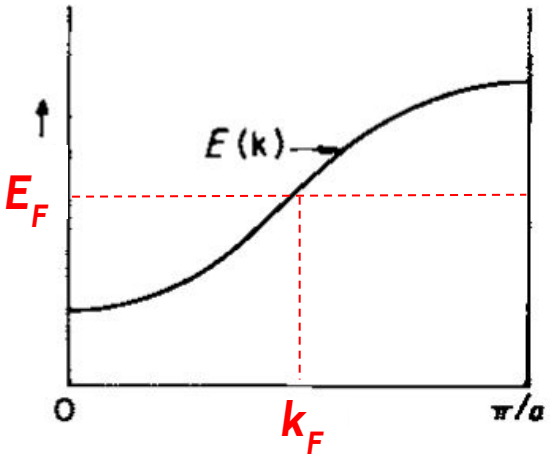
Instabilidade de Peierls

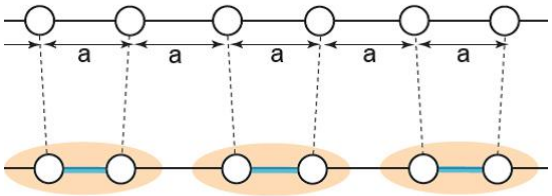
Sistema 1D metálico:
Instável!



Instabilidade de Peierls

Sistema 1D metálico:
Instável!

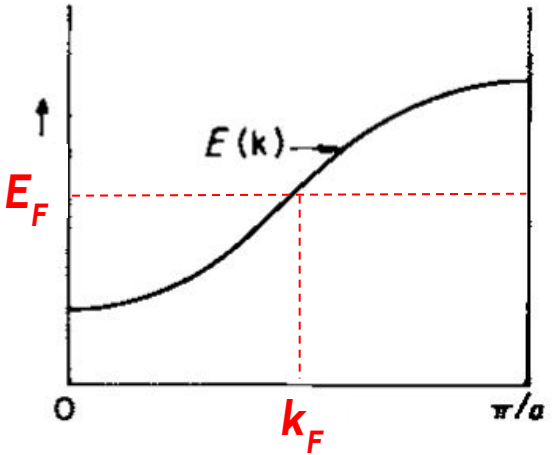


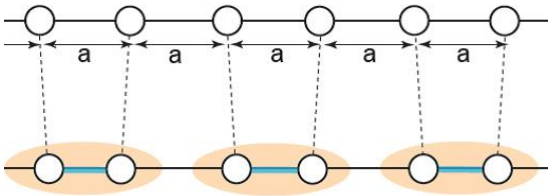


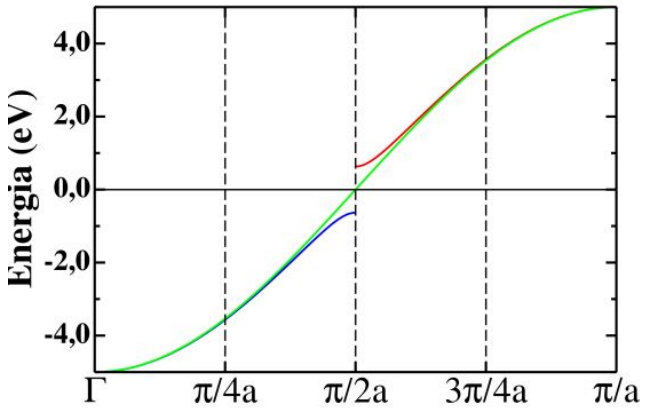
Instabilidade de Peierls

Sistema 1D metálico:
Instável!

$$E_{\pm} = \frac{1}{2}(E_k^0 + E_{k-K}^0) \pm \sqrt{\left(\frac{E_k^0 - E_{k-K}^0}{2}\right)^2 + |V_K^2|}$$



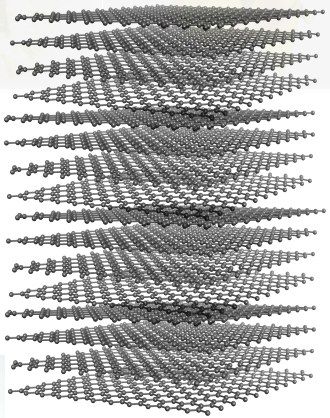


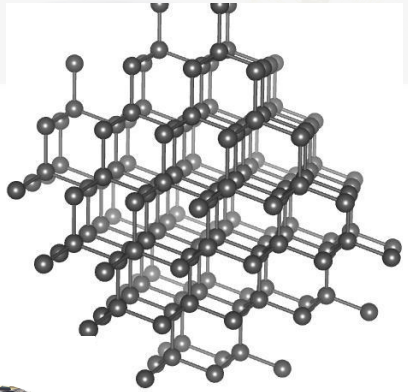


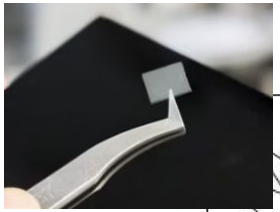
Grafeno

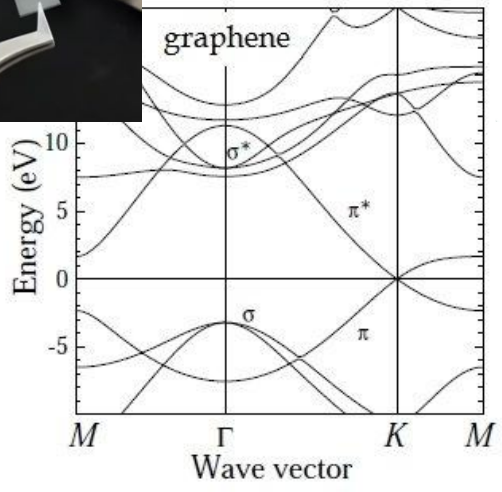
Grafite

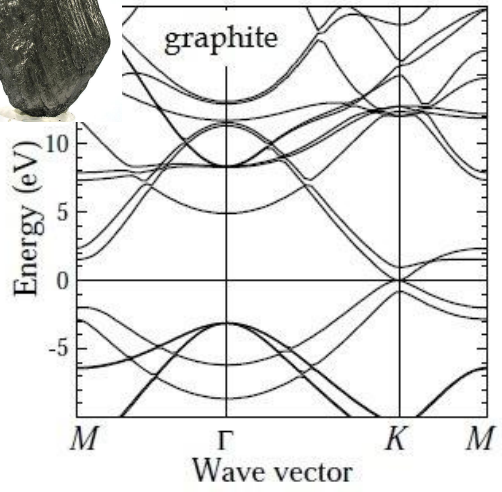
Diamante

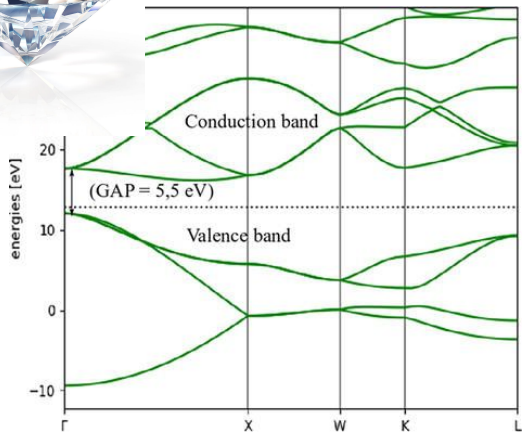






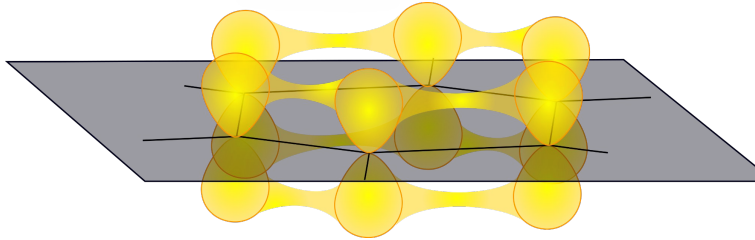


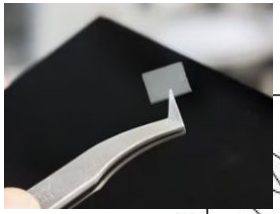


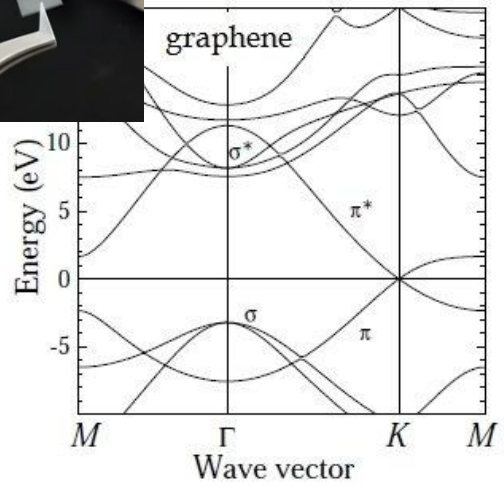


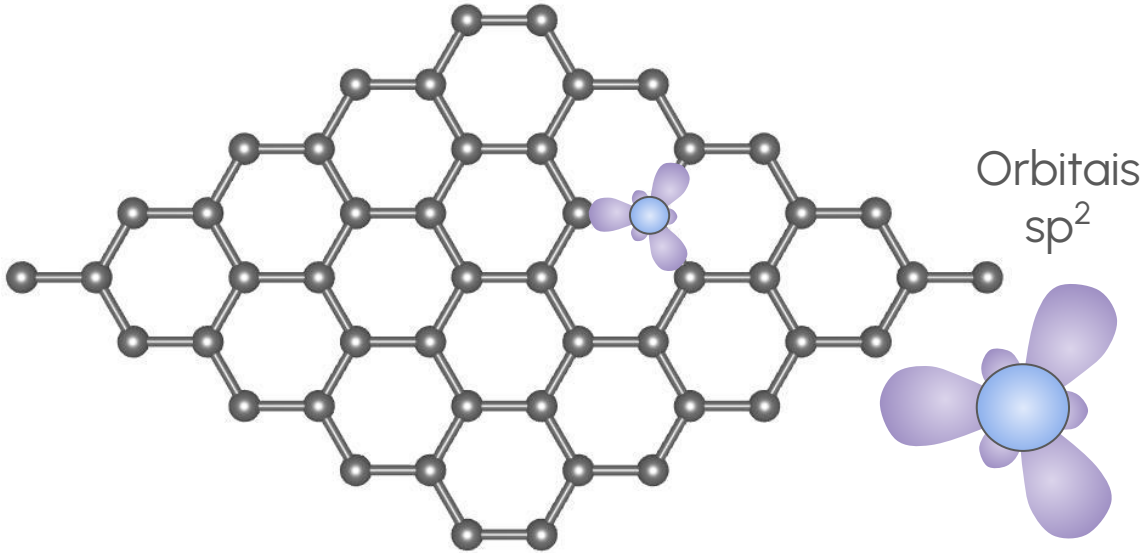
https://www.intechopen.com/chapters/86

Grafeno





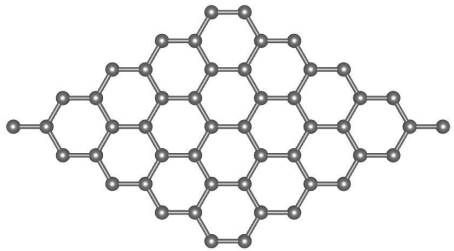


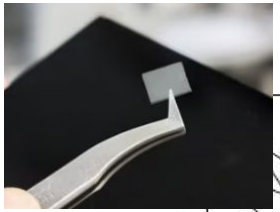


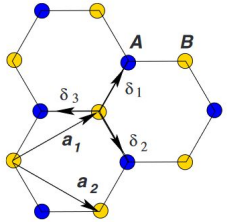
Orbitais sp^2

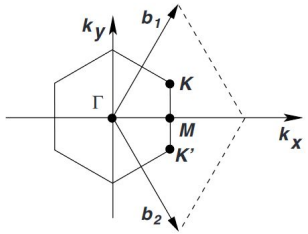
Grafeno

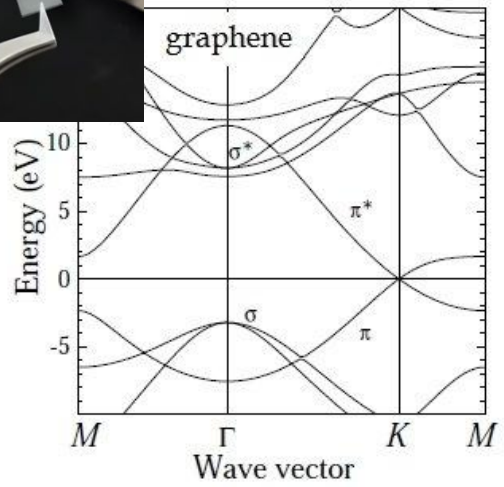
" One of the most interesting aspects of the graphene problem is that its low-energy excitations are massless, chiral, Dirac fermions. "

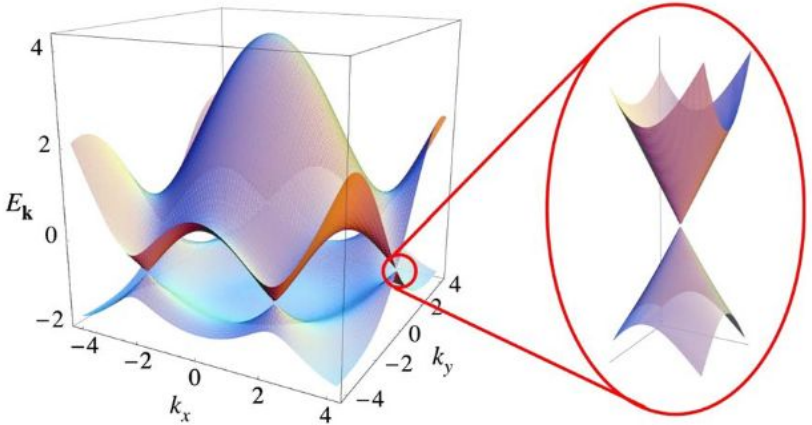






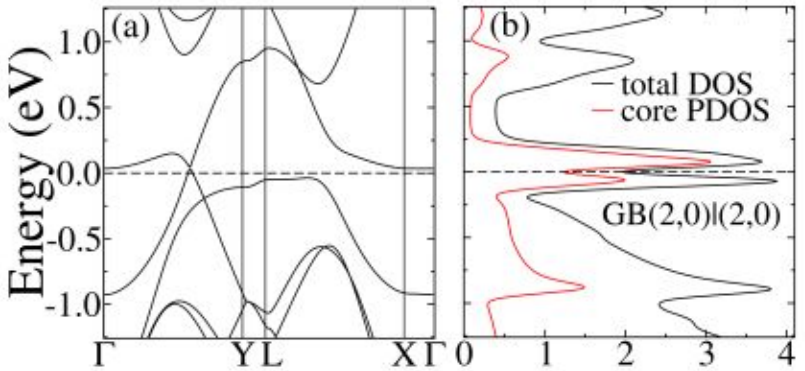


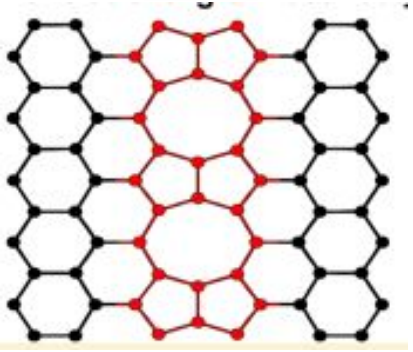




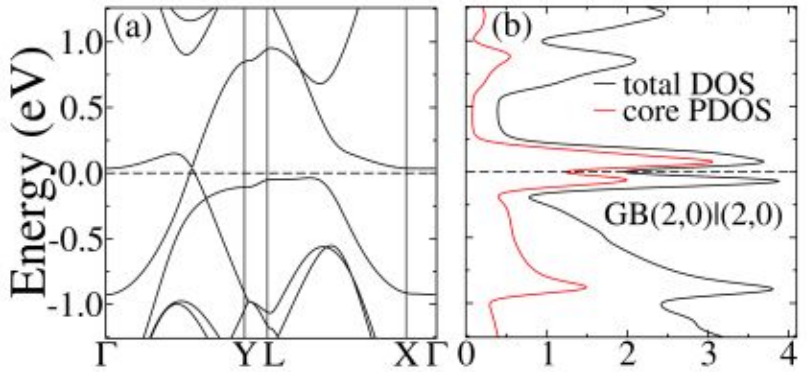
Castro Neto et al, Rev. Mod. Phys., 81, 2009

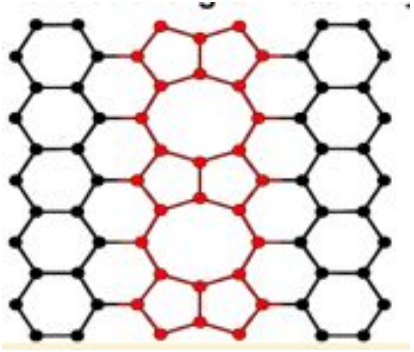
Instabilidades Magnéticas

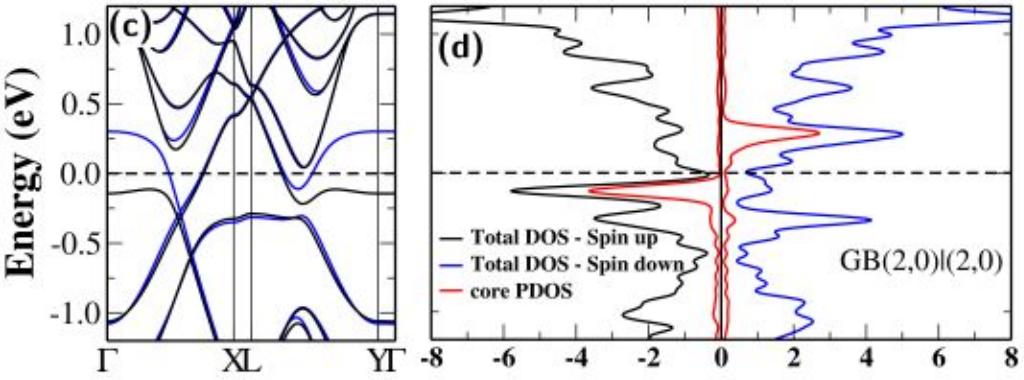




Instabilidades Magnéticas







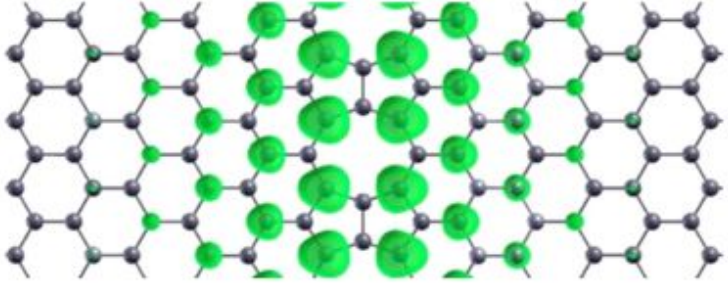
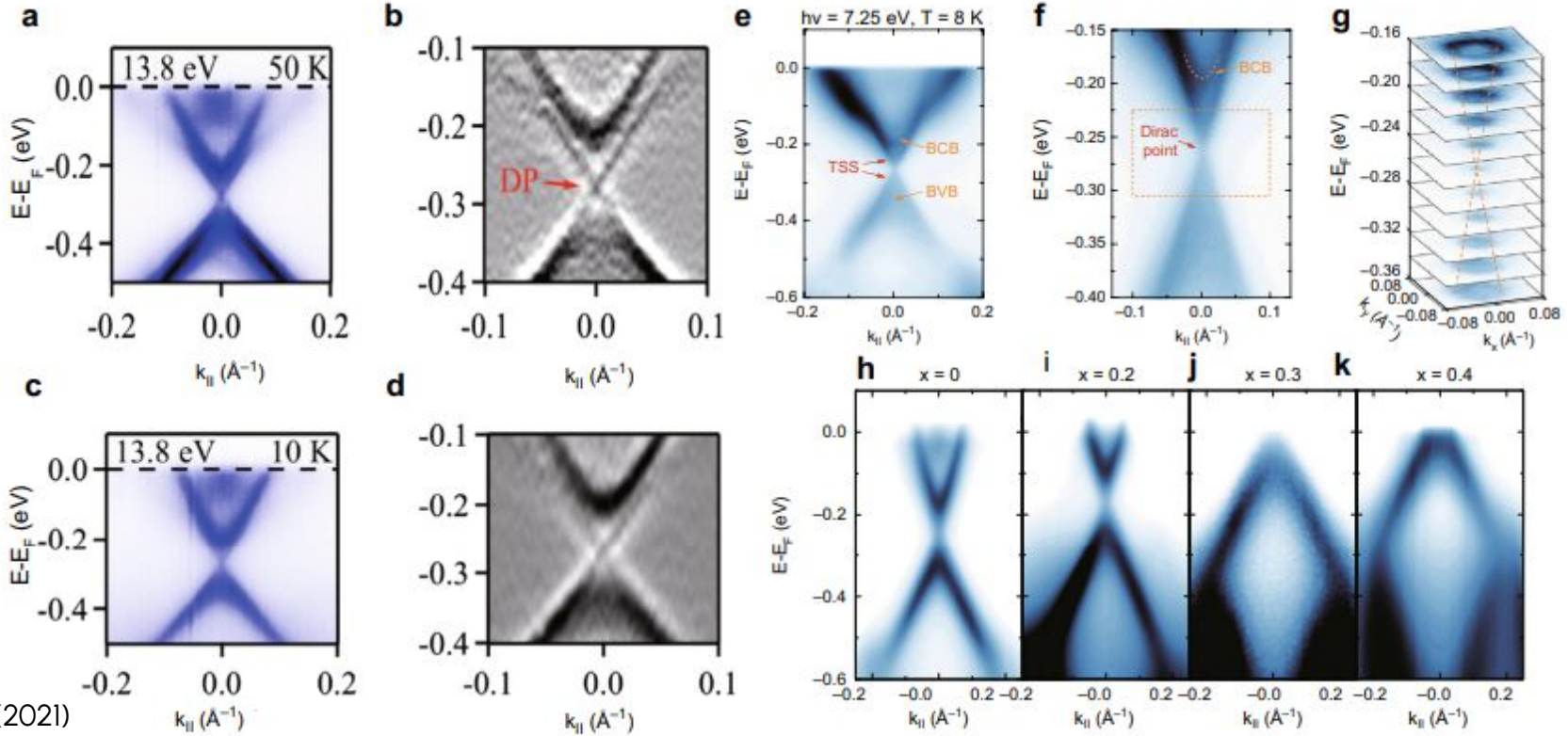


Figure 4. Isosurface of spin polarization density for the domain-boundary magnetic state.

Angle-resolved photoemission spectroscopy (ARPES)



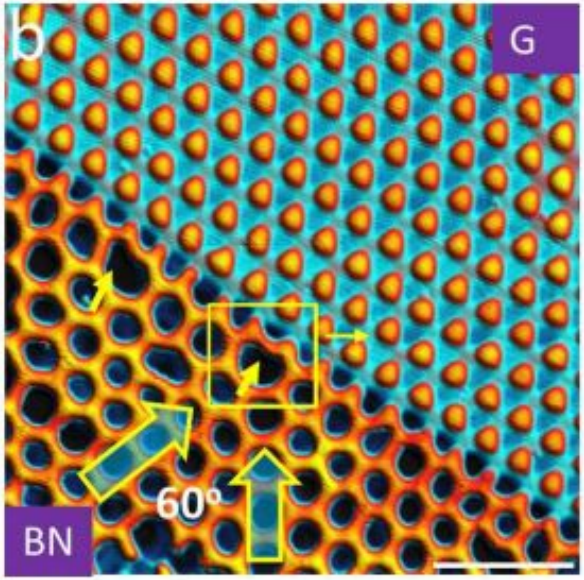
Nucl Sci Tech (2021)

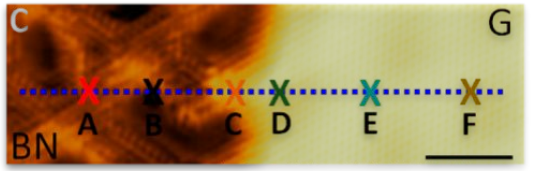
Local DOS e Curva dV/dI
(LDOS)

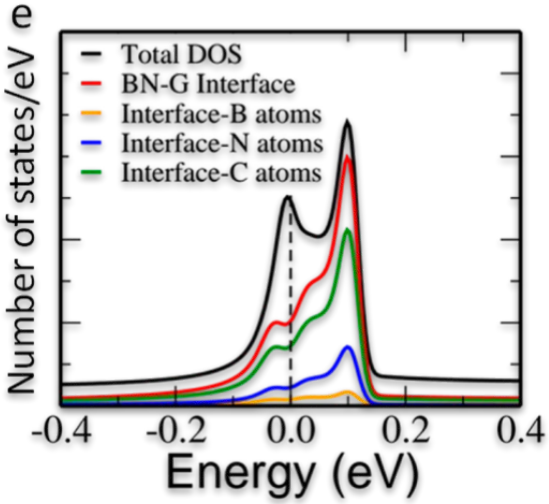
NANO LETTERS
Letter
pubs.acs.org/NanoLett

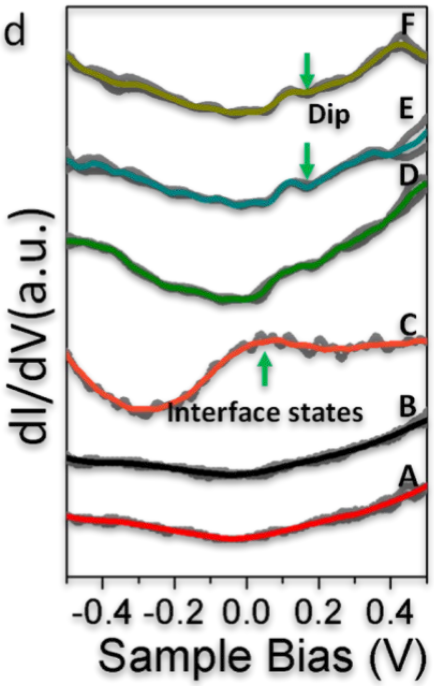
Lattice Relaxation at the Interface of Two-Dimensional Crystals: Graphene and Hexagonal Boron-Nitride

Jiong Lu,[†,‡,#] Lídia C. Gomes,[‡,§,#] Ricardo W. Nunes,[§] A. H. Castro Neto,[‡,∥] and Kian Ping Loh*[,†,‡]









Local DOS e Curva dV/dI
(LDOS)

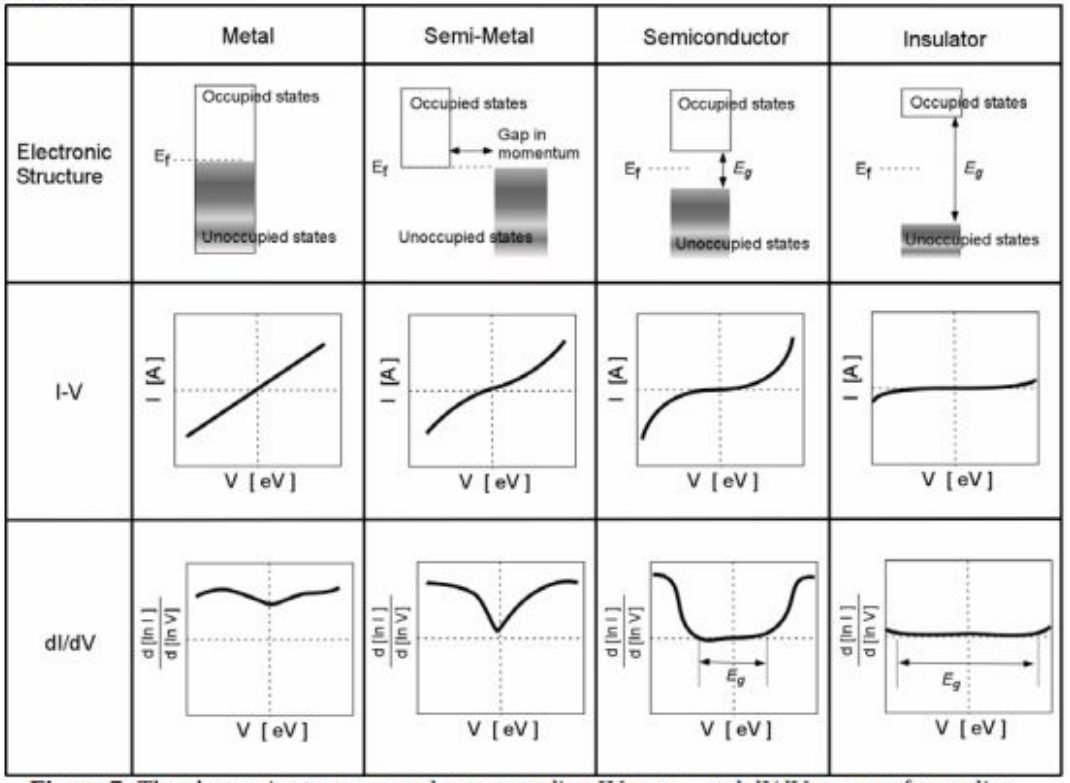
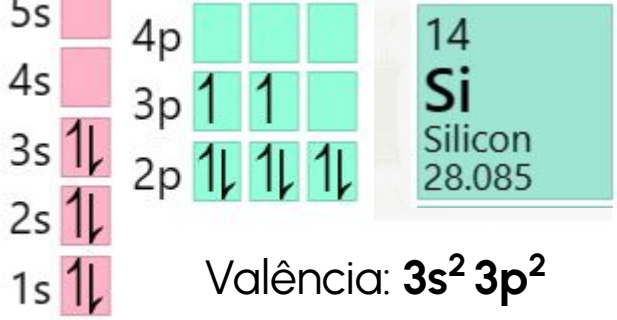


Figure 7: The electronic structures and corresponding IV curves and dI/dV curves of tunneling spectroscopy.

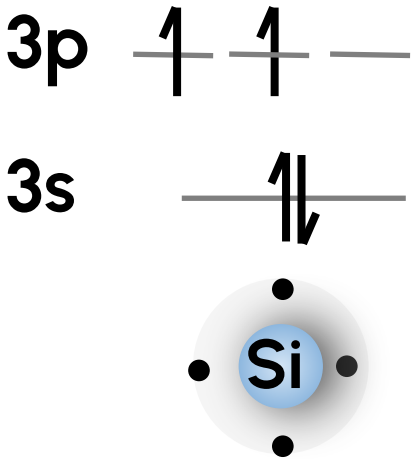
Isolantes Topológicos

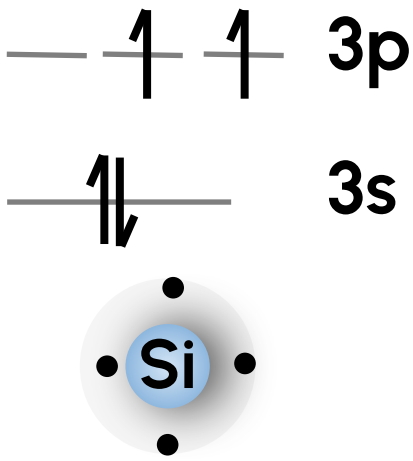
Spin Splitting

Electronic Band Structure: Si crystal



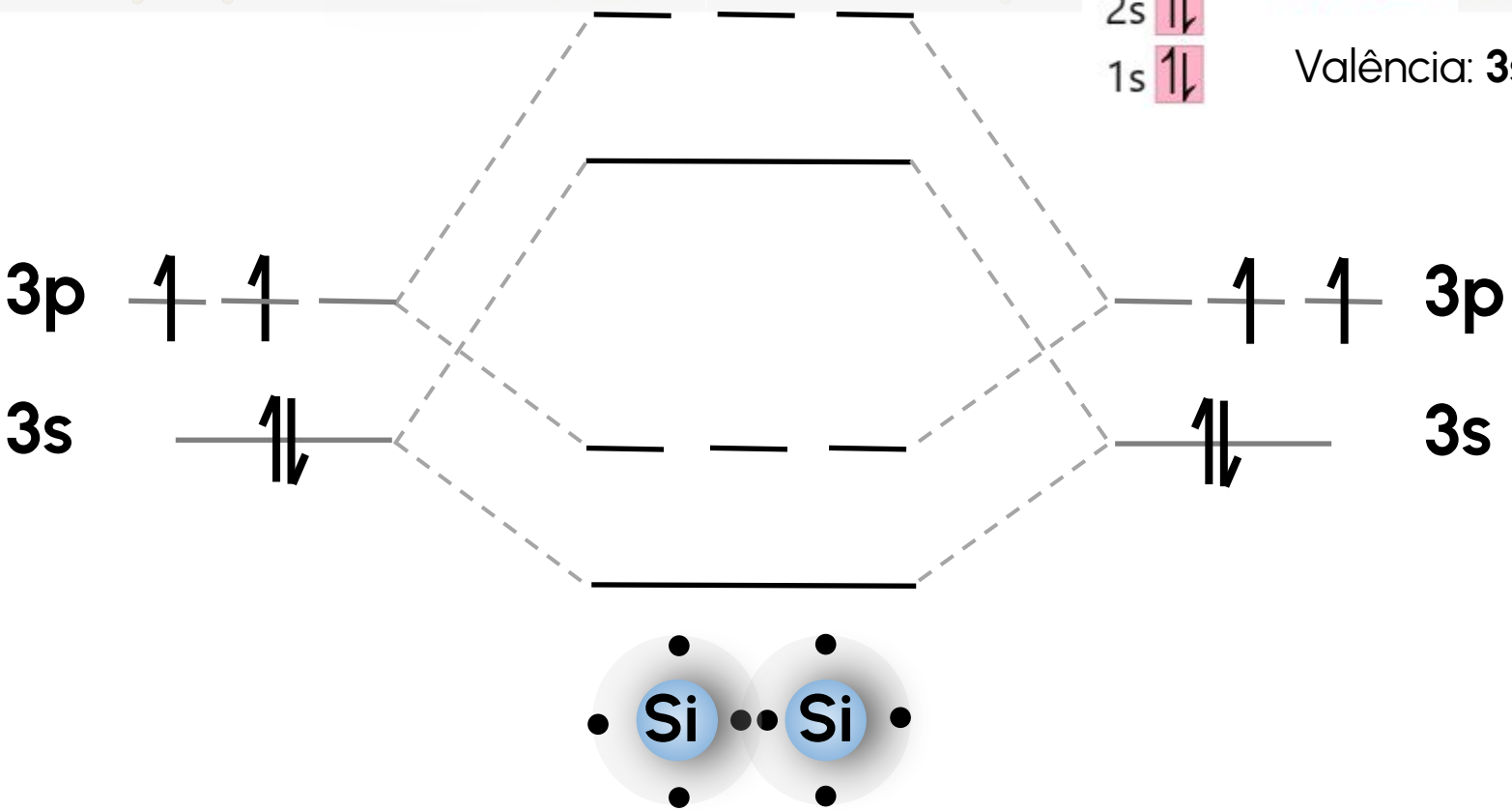
Valência: $3s^2\ 3p^2$





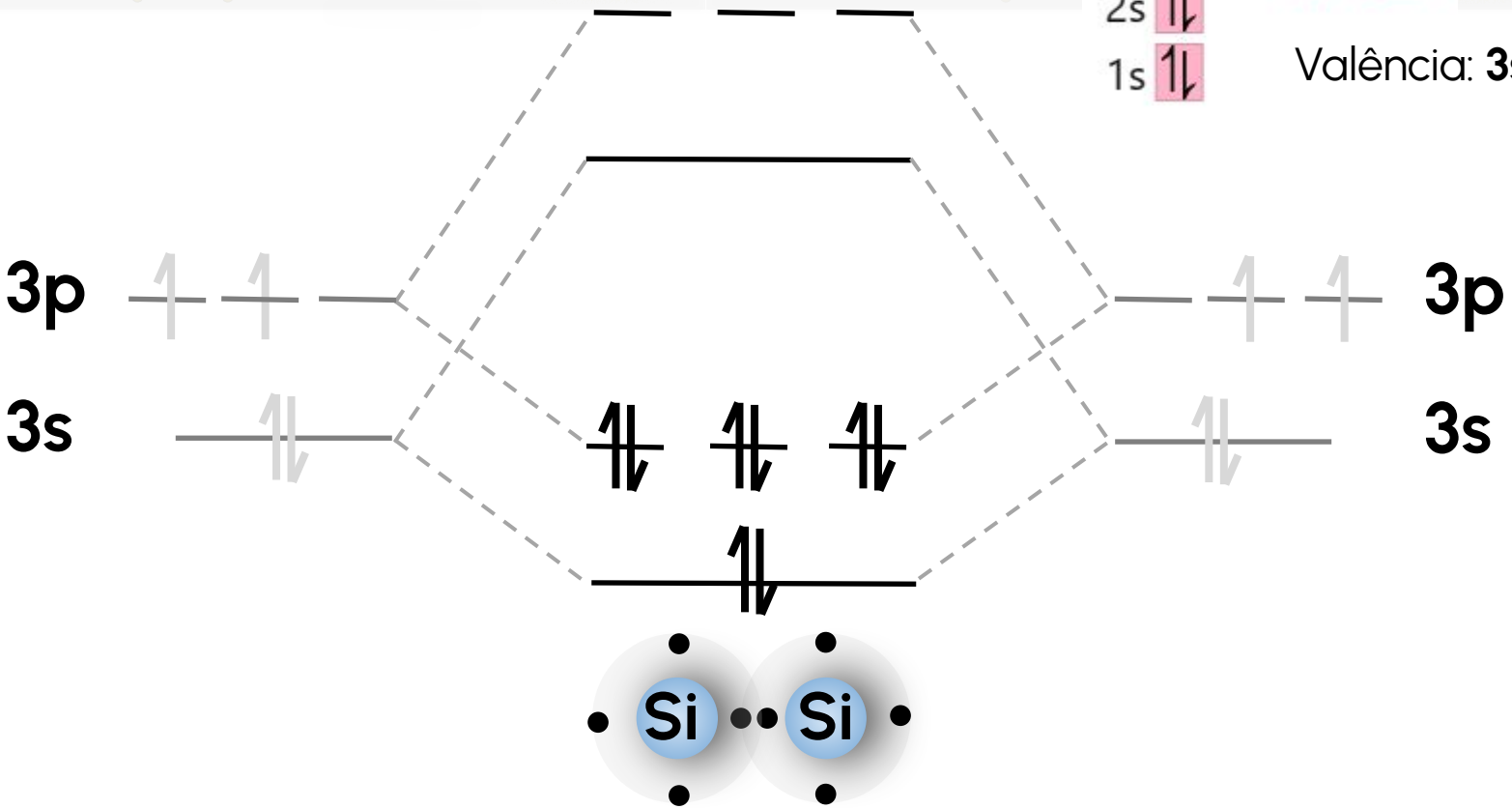
Electronic Band Structure: Si crystal

Valência: $3s^2\ 3p^2$



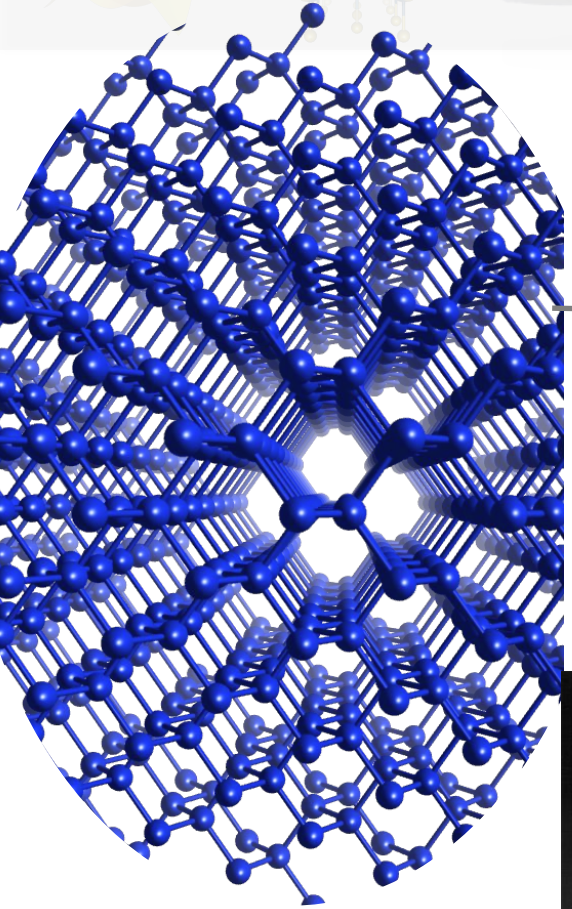
Electronic Band Structure: Si crystal

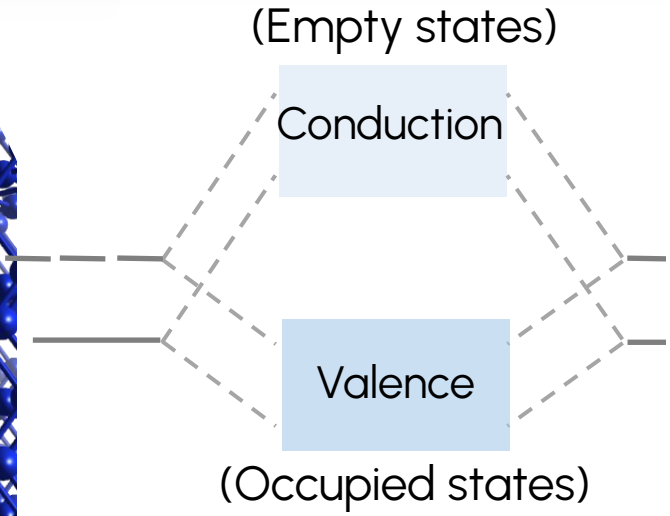
Valência: $3s^2\ 3p^2$

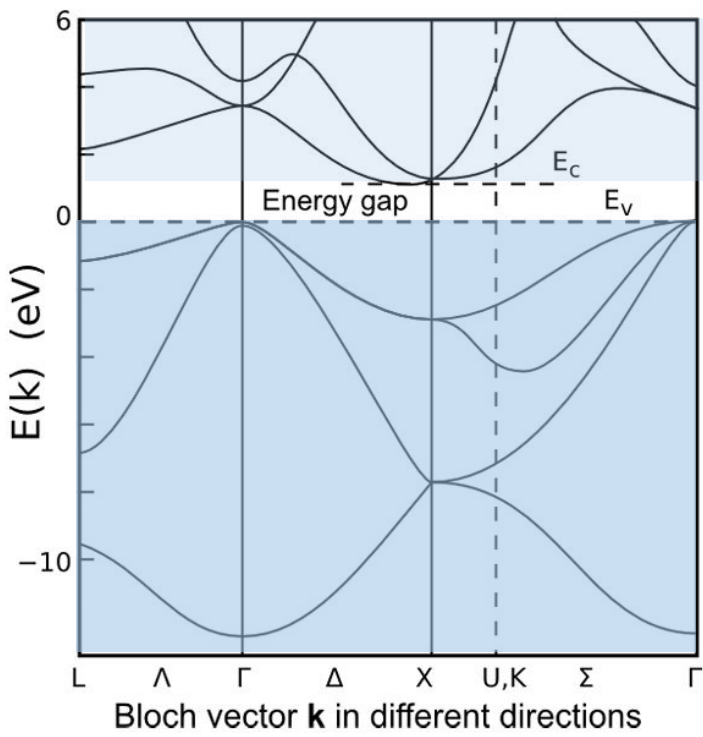


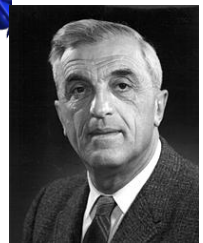
Electronic Band Structure: Si crystal

If we have **a lot of** atoms? (~ 10^{23})









Felix Bloch
(1905-1983)

Bloch's Theorem

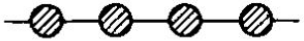
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$

Andreas Wacker Notes (2018)

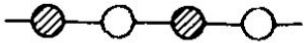
Elétrons livres X Elétrons num potencial cristalino

Rede Recíproca

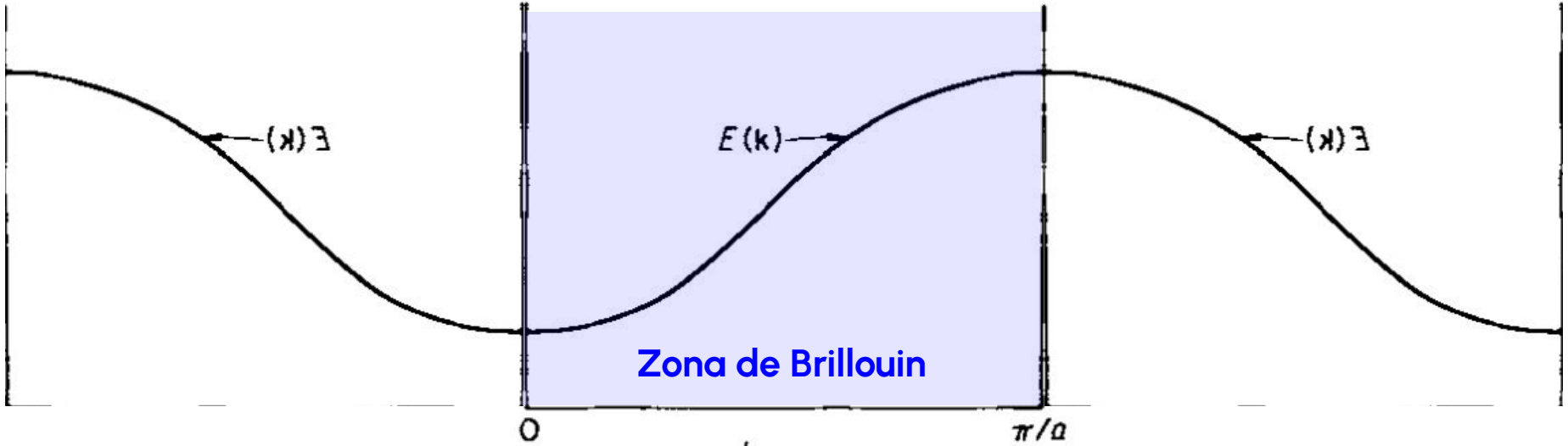
$k = 0 \qquad \psi_0 = \sum_n e^0 \chi_n = \sum_n \chi_n = \chi_0 + \chi_1 + \chi_2 + \chi_3 + \cdots$



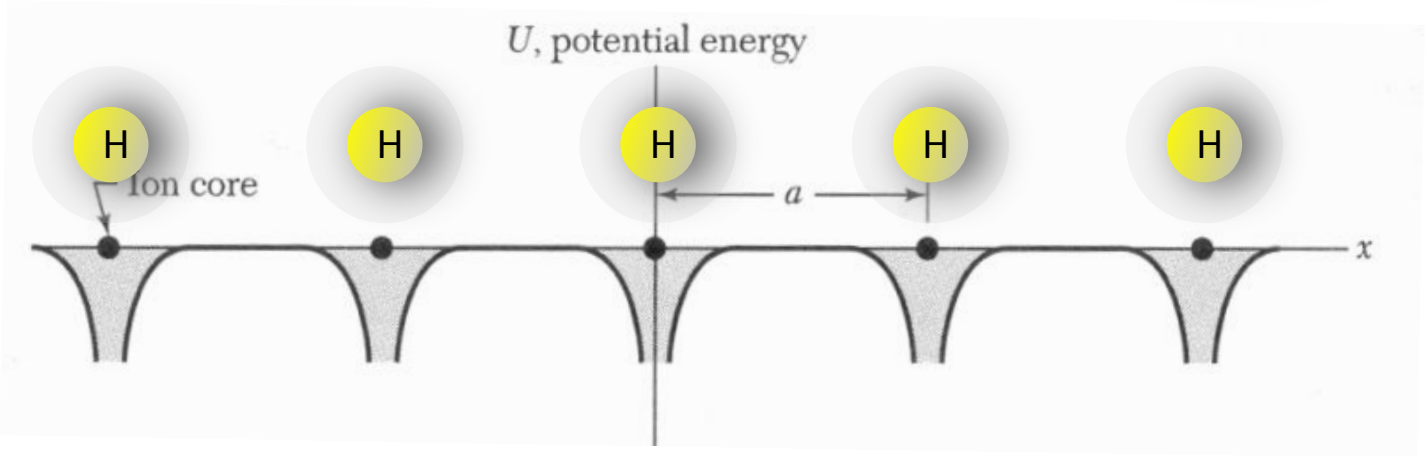
$k = \frac{\pi}{a} \qquad \psi_{\frac{\pi}{a}} = \sum_n e^{\pi i n} \chi_n = \sum_n (-1)^n \chi_n = \chi_0 - \chi_1 + \chi_2 - \chi_3 + \cdots$



$\boldsymbol{R} = n\boldsymbol{a}$



Elétrons num potencial cristalino 1D

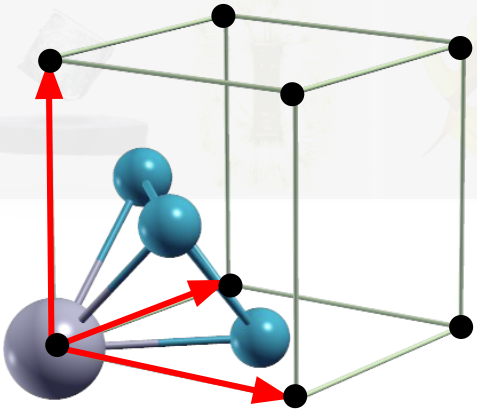


Num sólido periódico, o potencial U(***r***) sentido pelos elétrons obedece:

$$U(\boldsymbol{r}) = U(\boldsymbol{r}+\boldsymbol{R})$$

com ***R*** um vetor da rede de Bravais.

Rede Recíproca



Considere ***R*** o conjunto de pontos que constitui uma rede de Bravais:

$$\boldsymbol{R} = n_1\boldsymbol{a_1} + n_2\boldsymbol{a_2} + n_3\boldsymbol{a_3}$$