

Structure électronique des matériaux

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De l'atome au cristal:
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Structure électronique et cohésion des solides p.58

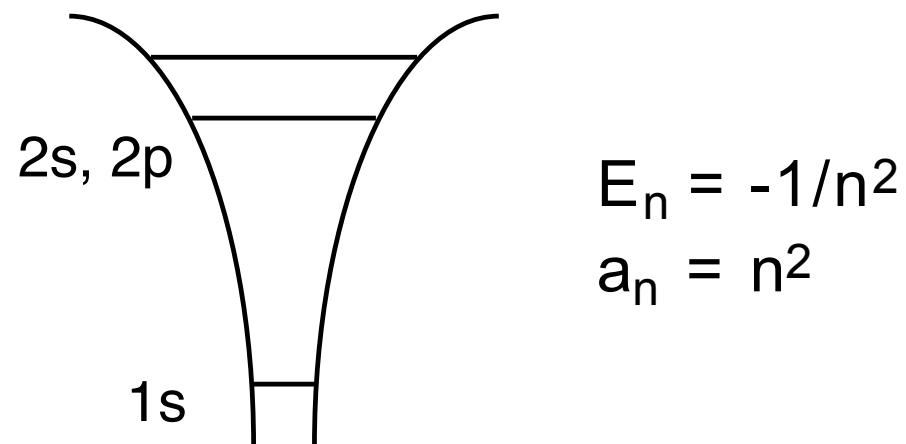
Alliages p.96

De l'atome au cristal

Visite du tableau de Mendeleiev

L'atome

Hydrogène



Unités atomiques

$$\hbar = m = e = 1$$

$$\text{Rydberg} = 13.6 \text{ eV} = 1/2 \text{ Hartree}$$

$$\text{Longueur} = 0.53 \text{ Ang}$$

Mécanique quantique

$$-\frac{\hbar^2}{2m} \Delta \Psi(\vec{r}) + V(\vec{r}) \Psi(\vec{r}) = E \Psi(\vec{r})$$

$$H|\Psi\rangle = E|\Psi\rangle \quad ; \quad \Psi(\vec{r}) = \langle \vec{r} | \Psi \rangle$$

$$\Psi_{n\ell m}(\vec{r}) = R_{n\ell}(r) Y(\theta, \varphi)$$

► Schrödinger

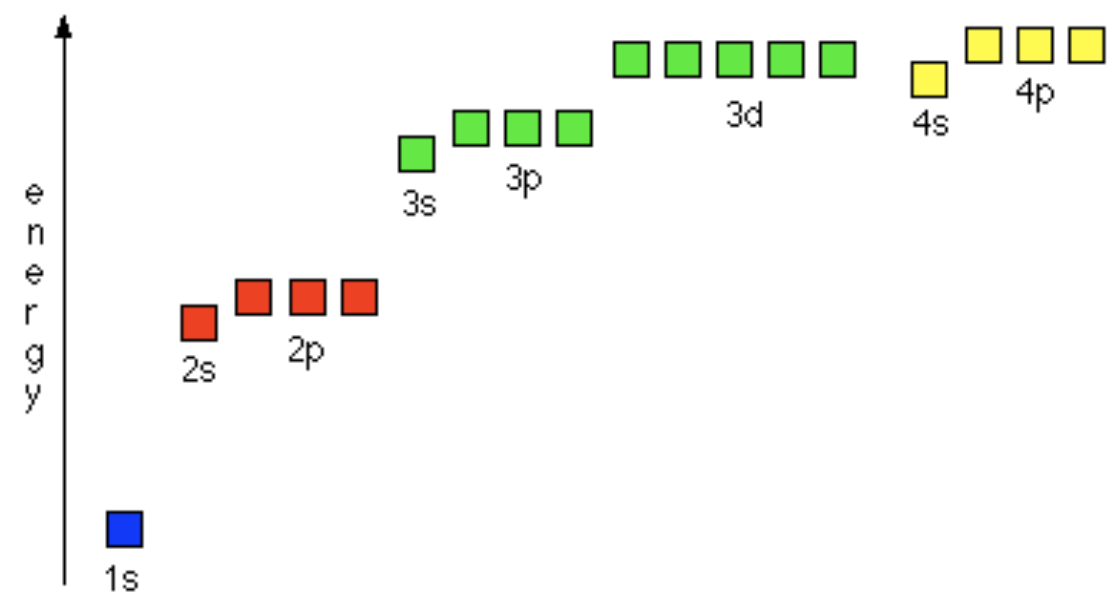
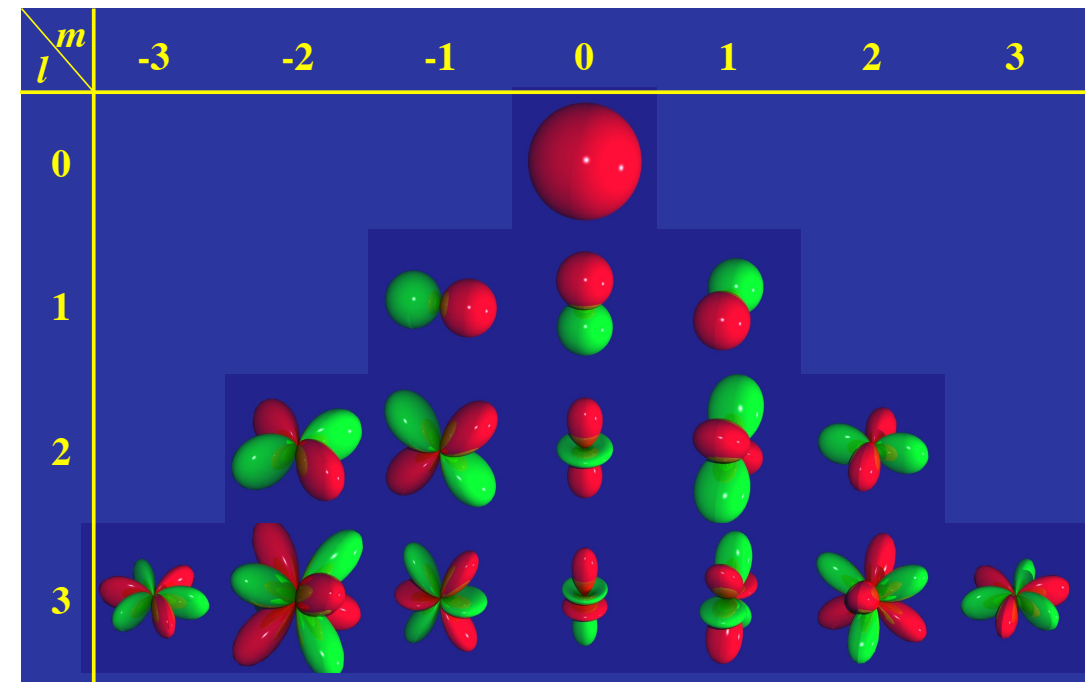
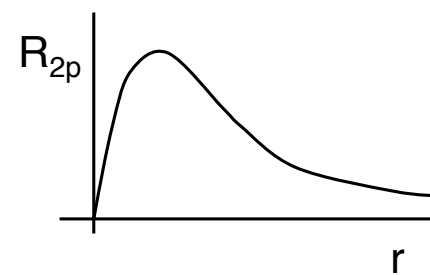
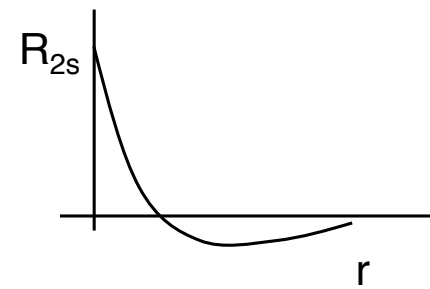
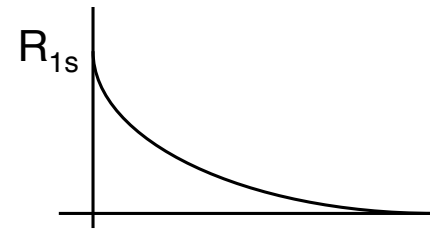
► symétrie sphérique

► nombres quantiques n, l, m

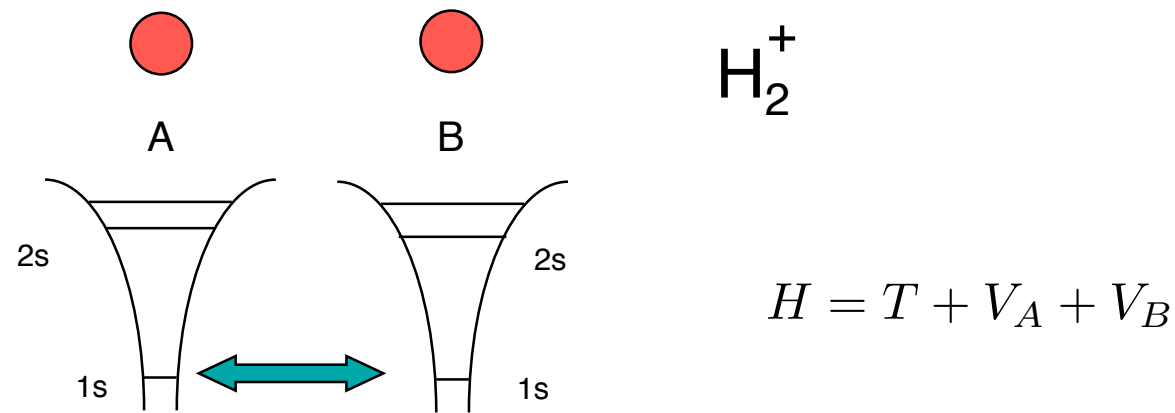
- principal, orbital, magnétique
- couches K, L, M
- électrons s, p, d, f

► et le spin 1/2 !

Orbitales atomiques



Molécule diatomique



Orbitales moléculaires
liaisons fortes, Hückel

$$\Psi(\vec{r}) \simeq a \Psi_{1s}(\vec{r} - \vec{r}_A) + b \Psi_{1s}(\vec{r} - \vec{r}_B)$$

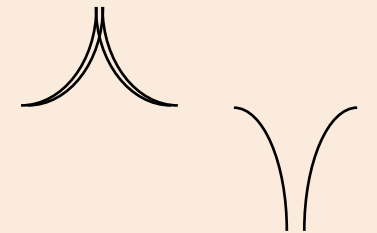
$$|\Psi\rangle \simeq a|A\rangle + b|B\rangle \quad ; \quad \langle \vec{r} | A \rangle = \Psi_{1s}(\vec{r} - \vec{r}_A)$$

$$H = \begin{pmatrix} E_{1s} + \alpha & t \\ t & E_{1s} + \alpha \end{pmatrix}$$

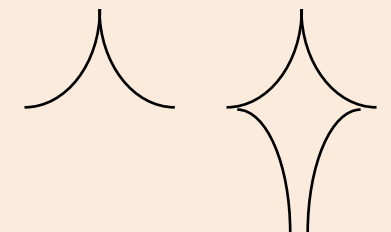
$$\alpha = \int d\vec{r} |\Psi_{1s}(\vec{r} - \vec{r}_A)|^2 V(\vec{r} - \vec{r}_B)$$

$$t = \int d\vec{r} \Psi_{1s}(\vec{r} - \vec{r}_A) \Psi_{1s}(\vec{r} - \vec{r}_B) V(\vec{r} - \vec{r}_B)$$

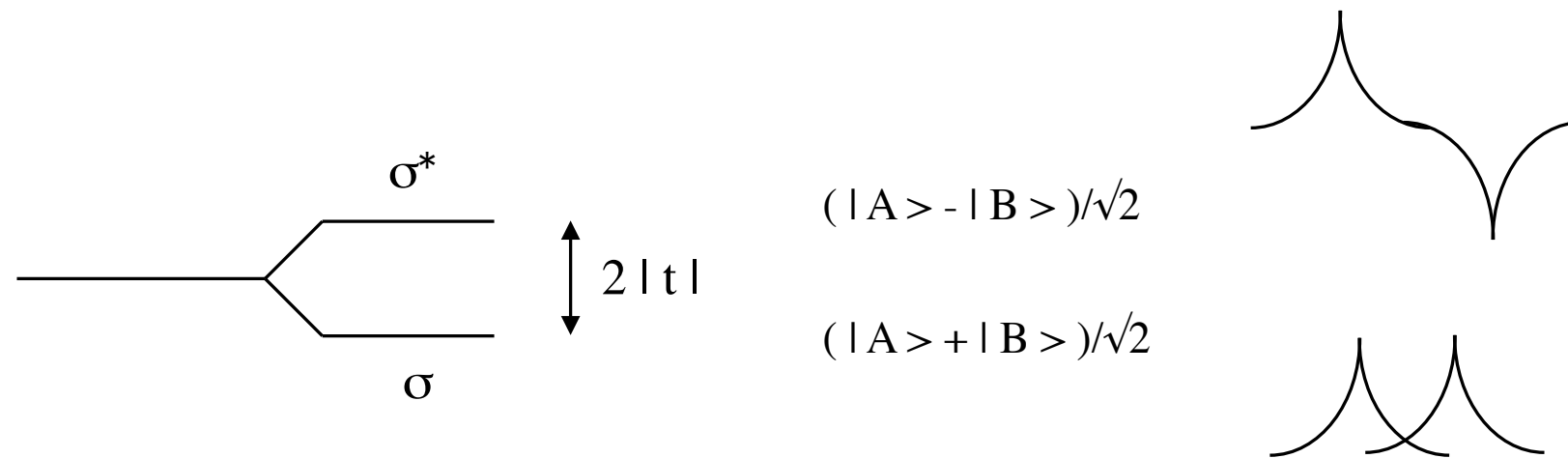
Champ cristallin



Intégrale de saut,
de transfert

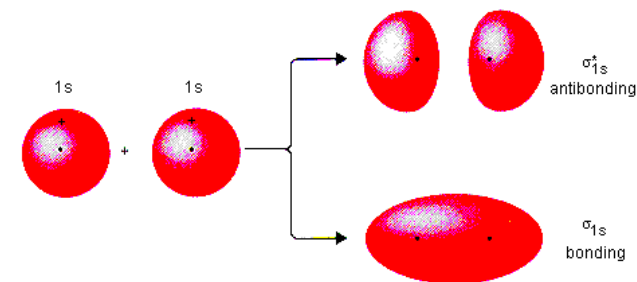
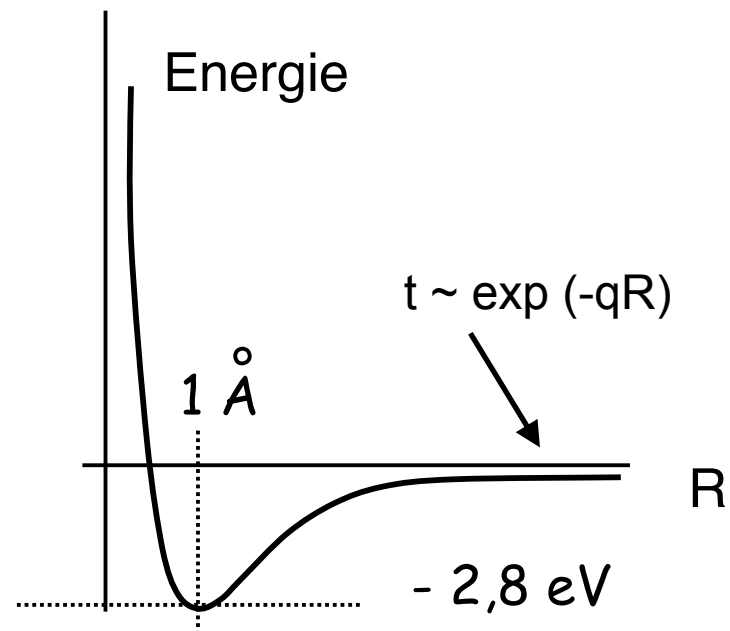


Liaison covalente

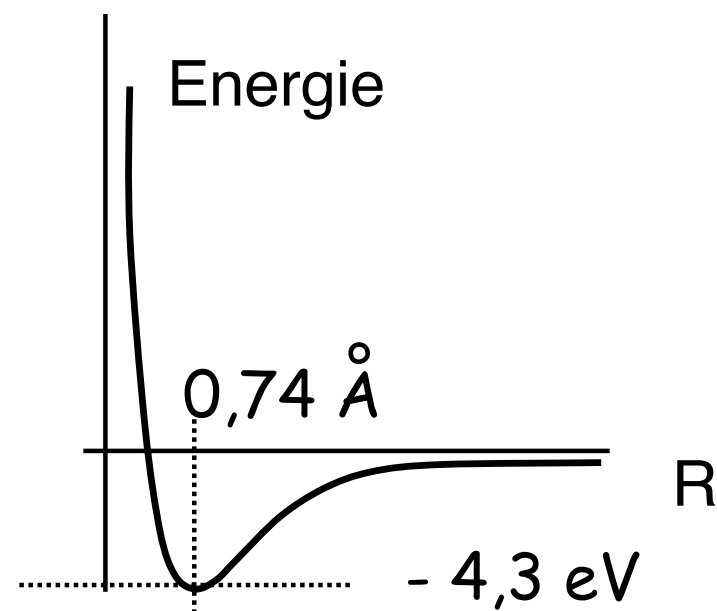
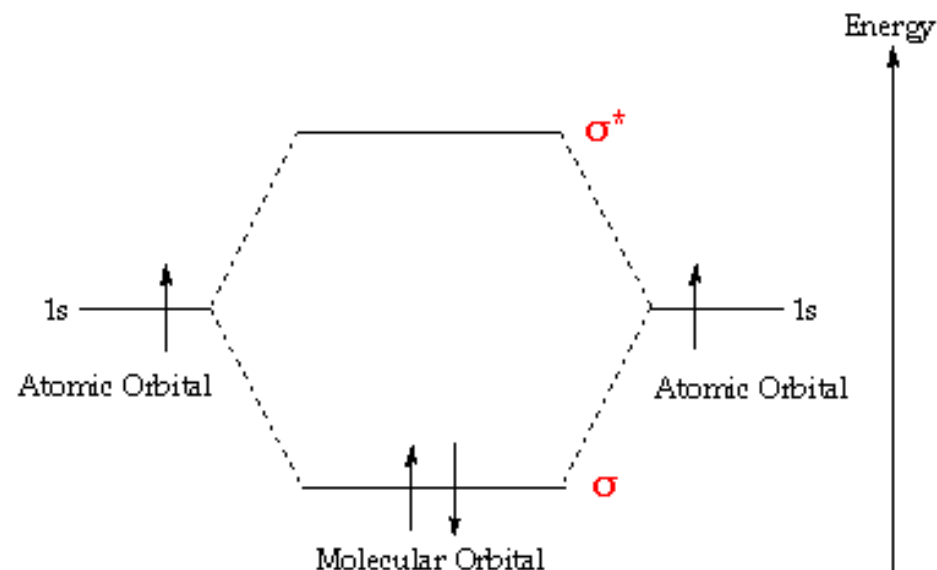


Etats liant et
antiliant

$$t < 0$$



Hydrogène

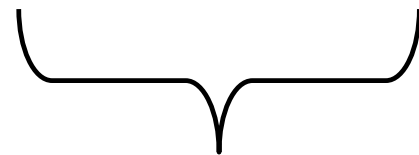


- Problème: Interactions électron-électron !
- V_A et V_B sont maintenant des potentiels à un électron effectifs
- Nécessite des méthodes de champ moyen, Hartree, Hartree-Fock ou des méthodes dites de fonctionnelle de la densité (électronique)

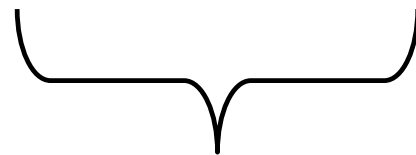
Corrélations



$$\begin{aligned}
 |\Psi\rangle &= |\Psi_L\rangle_1 |\Psi_L\rangle_2 \\
 &= \frac{1}{2} [|A1\rangle + |B1\rangle] [|A2\rangle + |B2\rangle] \\
 &= [|A1\rangle|B2\rangle + |A2\rangle|B1\rangle + |A1\rangle|A2\rangle + |B1\rangle|B2\rangle]
 \end{aligned}$$



H - H



H⁻ - H⁺

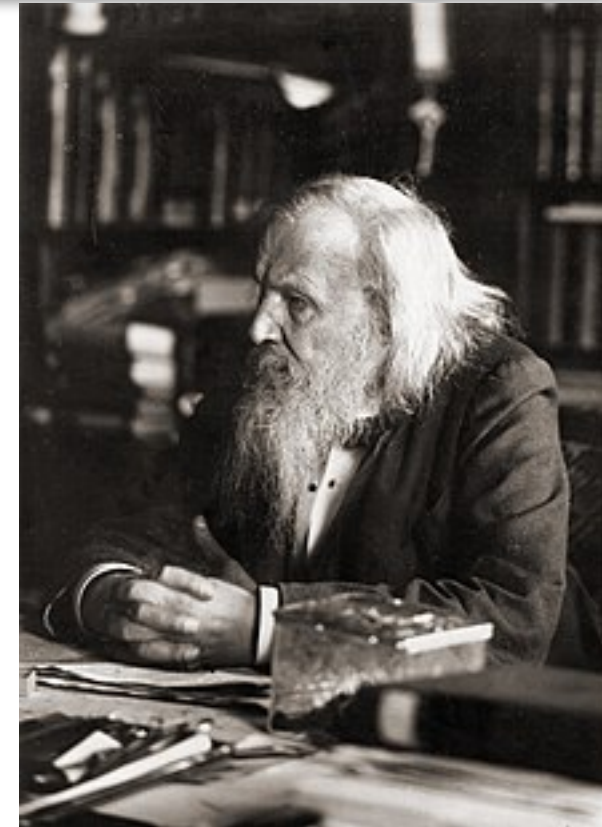
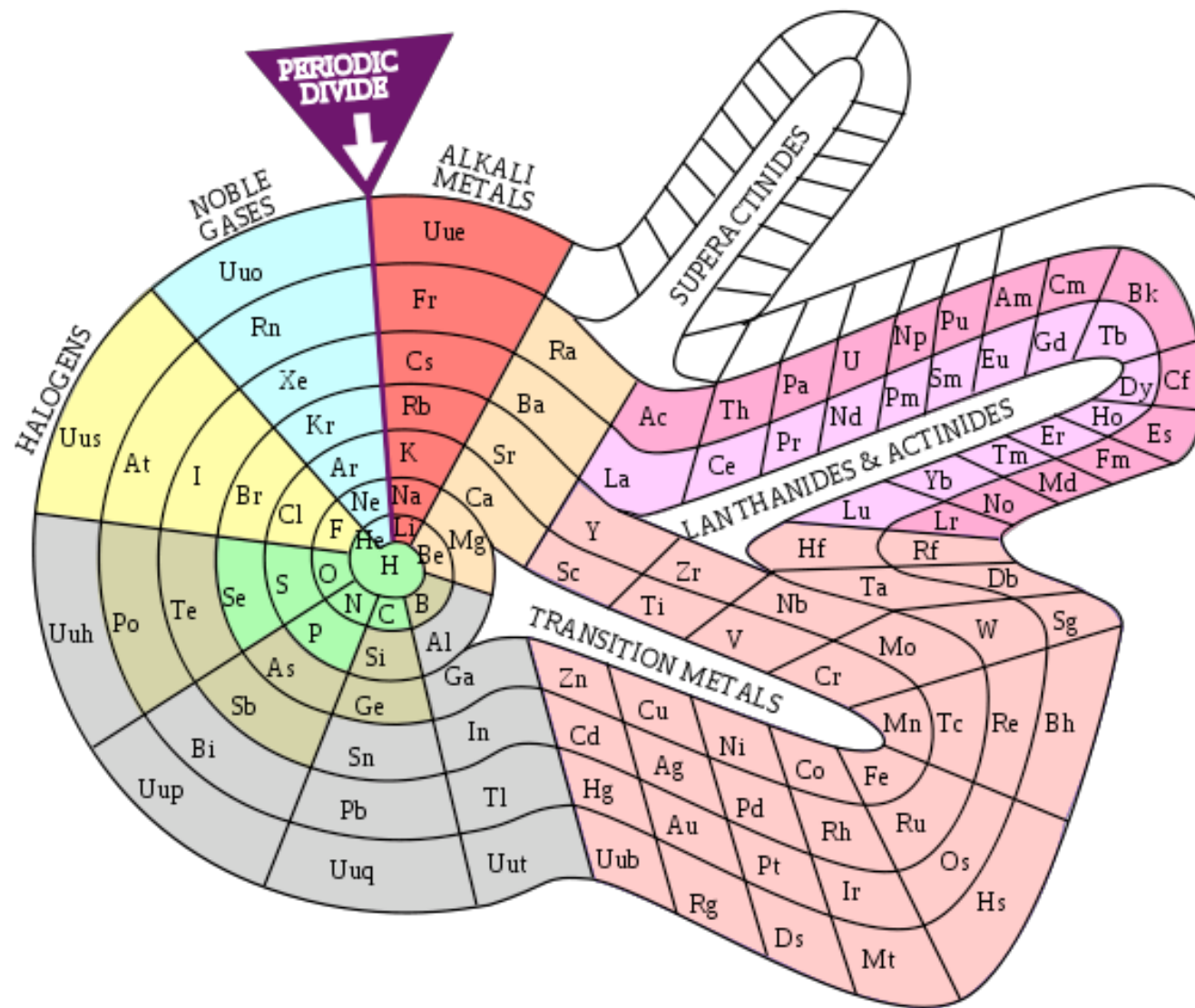
Orbitales atomiques:
Heitler-London



Orbitales moléculaires
Hund-Mulliken

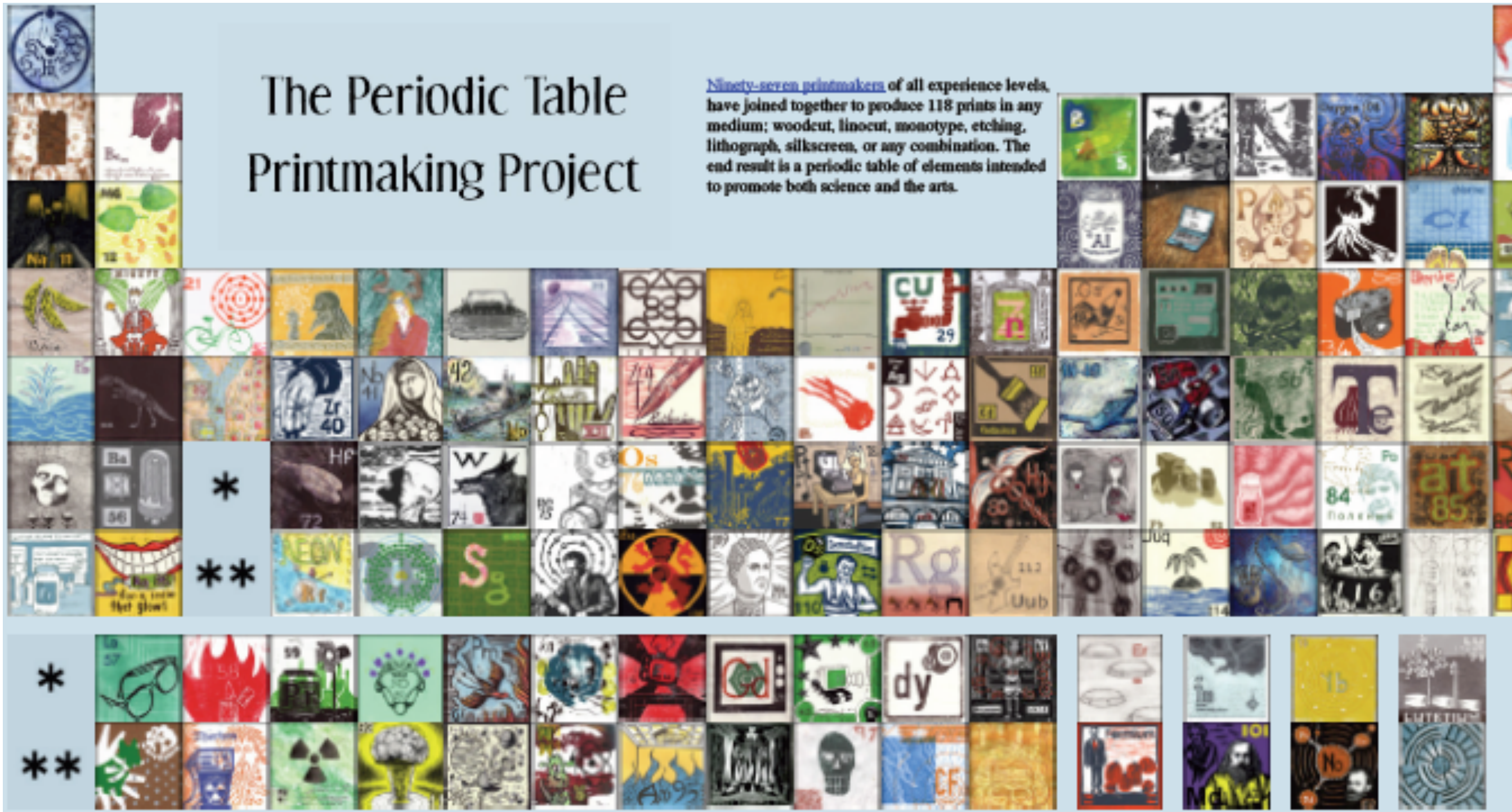
- La méthode des CLOA (combinaison linéaire d'orbitales atomiques) n'est pas très bonne à faible densité, R grand.
- En effet l'état à deux électrons peut s'écrire comme superposition linéaire d'atomes neutres et ionisés
- La configuration avec deux électrons coûte une énergie U, intégrale Coulombienne intra-atomique; ici U = 12,8 eV.
- On peut donner un poids différent à la configuration neutre et à la configuration « ionique »: interaction de configuration.
- En physique du solide, on parle de corrélations électroniques avec un « U de Hubbard ».

Mendeleiev



The Periodic Table Printmaking Project

Ninety-seven printmakers of all experience levels, have joined together to produce 118 prints in any medium; woodcut, linocut, monotype, etching, lithograph, silkscreen, or any combination. The end result is a periodic table of elements intended to promote both science and the arts.



元素周期表

王地正题



1		元素周期表																2					
氢																		氦					
3	4																	5	6	7	8	9	10
锂	铍																	硼	碳	氮	氧	氟	氖
11	12																	13	14	15	16	17	18
钠	镁																	铝	硅	磷	硫	氯	氩
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36						
钾	钙	钪	钛	钒	铬	锰	铁	钴	镍	铜	锌	镓	锗	砷	硒	溴	氪						
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54						
铷	锶	钇	锆	铌	钼	镉	铑	钨	锡	银	镉	铟	锡	铊	铋	碲	氙						
55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72						
铯	钡	镧	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈						
87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104						
钫	镭	锕	钍	镤	铀	镎	钚	镅	镆	锘	镧	铈	铈	铈	铈	铈	铈						
57	58	59	60	61	62	63	64	65	66	67	68	69	70										
镧	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈										
89	90	91	92	93	94	95	96	97	98	99	100	101	102										
铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈	铈										

1 IA 11A	Periodic Table of the Elements																18 VIIIA 8A
1 H Hydrogen 1.008	2 IIA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	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	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904	36 Kr Krypton 84.80
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide
Series

57 La Lanthanum 138.906	58 Ce Cerium 140.115	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.966	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.26	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
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Actinide
Series

89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]
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ici lien internet

Métaux simples, « normaux »

1
IA
11A

1
H
Hydrogen
1.008

2
IIA
2A

4
Be
Beryllium
9.012

3
Li
Lithium
6.941

11
Na
Sodium
22.990

19
K
Potassium
39.098

37
Rb
Rubidium
84.468

55
Cs
Cesium
132.905

87
Fr
Francium
223.020

12
Mg
Magnesium
24.305

20
Ca
Calcium
40.078

38
Sr
Strontium
87.62

56
Ba
Barium
137.327

88
Ra
Radium
226.025

3
IIIB
3B

4
IVB
4B

5
VB
5B

6
VIB
6B

7
VIIB
7B

8
VIII
8

9
VIII
8

10
VIII
8

11
IB
1B

12
IIB
2B

5
B
Boron
10.811

13
Al
Aluminum
26.982

31
Ga
Gallium
69.732

49
In
Indium
114.818

67
Ho
Holmium
164.930

85
At
Astatine
209.987

103
Lr
Lawrencium
[262]

6
C
Carbon
12.011

14
Si
Silicon
28.086

32
Ge
Germanium
72.61

50
Sn
Tin
118.71

68
Er
Erbium
167.26

100
Fm
Fermium
257.095

7
N
Nitrogen
14.007

15
P
Phosphorus
30.974

33
As
Arsenic
74.922

51
Sb
Antimony
121.760

69
Tm
Thulium
168.934

101
Md
Mendelevium
258.1

8
O
Oxygen
15.999

16
S
Sulfur
32.066

34
Se
Selenium
78.09

52
Te
Tellurium
127.6

84
Po
Polonium
[208.982]

116
Lv
Livermorium
[298]

9
F
Fluorine
18.998

17
Cl
Chlorine
35.453

35
Br
Bromine
79.904

53
I
Iodine
126.904

83
Bi
Bismuth
208.980

115
Uup
Ununpentium
unknown

10
Ne
Neon
20.180

18
Ar
Argon
39.948

36
Kr
Krypton
84.80

54
Xe
Xenon
131.29

86
Rn
Radon
222.018

118
Uuo
Ununoctium
unknown

18
VIII
8A

2
He
Helium
4.003

Lanthanide Series

57
La
Lanthanum
138.906

58
Ce
Cerium
140.115

59
Pr
Praseodymium
140.908

60
Nd
Neodymium
144.24

61
Pm
Promethium
144.913

62
Sm
Samarium
150.36

63
Eu
Europium
151.966

64
Gd
Gadolinium
157.25

65
Tb
Terbium
158.925

66
Dy
Dysprosium
162.50

67
Ho
Holmium
164.930

68
Er
Erbium
167.26

69
Tm
Thulium
168.934

70
Yb
Ytterbium
173.04

71
Lu
Lutetium
174.967

Actinide Series

89
Ac
Actinium
227.028

90
Th
Thorium
232.038

91
Pa
Protactinium
231.036

92
U
Uranium
238.029

93
Np
Neptunium
237.048

94
Pu
Plutonium
244.064

95
Am
Americium
243.061

96
Cm
Curium
247.070

97
Bk
Berkelium
247.070

98
Cf
Californium
251.080

99
Es
Einsteinium
[254]

100
Fm
Fermium
257.095

101
Md
Mendelevium
258.1

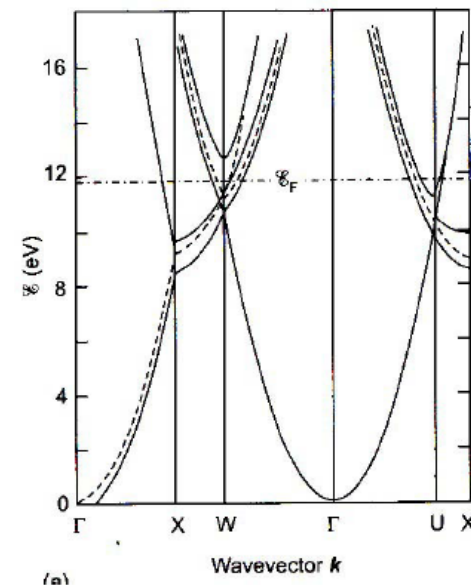
102
No
Nobelium
259.101

103
Lr
Lawrencium
[262]

Periodic Table of the Elements

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bcc	3 Li Lithium 6.941	4 Be Beryllium 9.012182	hcp
bcc	11 Na Sodium 22.989770	12 Mg Magnesium 24.3050	hcp
bcc	19 K Potassium 39.0983	20 Ca Calcium 40.078	fcc
bcc	37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	fcc
bcc	55 Cs Cesium 132.90545	56 Ba Barium 137.327	bcc
	87 Fr Francium (223)	88 Ra Radium (226)	



Al
Structure de bandes

Les métaux « normaux »
peuvent se décrire dans une
approximation d'électrons
presque libres, du moins la
structure de bande. Et la
cohésion ? (~1 eV)

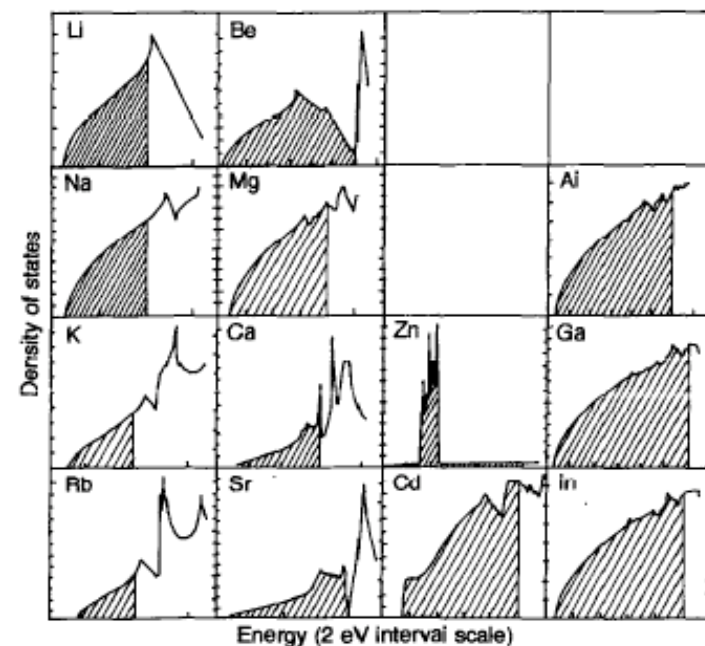
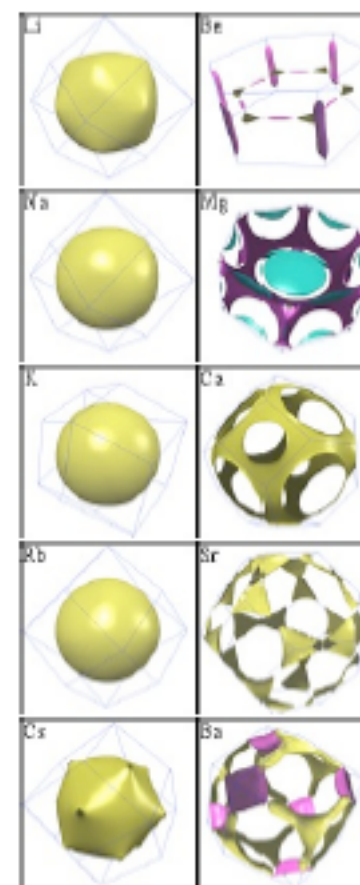


Fig. 5.13 The densities of states of sp-valent metals. (After Moruzzi *et al.* (1978).)

Densité d'états



Surface de Fermi

Métaux nobles

1
IA
11A

2
IIA
2A

13
IIIA
3A

14
IVA
4A

15
VA
5A

16
VIA
6A

17
VIIA
7A

18
VIIIA
8A

1
H
Hydrogen
1.008

3
Li
Lithium
6.941

11
Na
Sodium
22.990

19
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15.999

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S
Sulfur
32.066

34
Se
Selenium
78.09

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Te
Tellurium
127.6

80
Hg
Mercury
200.59

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F
Fluorine
18.998

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Cl
Chlorine
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Br
Bromine
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Iodine
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He
Helium
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10
Ne
Neon
20.180

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Ar
Argon
39.948

36
Kr
Krypton
84.80

54
Xe
Xenon
131.29

86
Rn
Radon
222.018

118
Uuo
Ununoctium
unknown

117
Uus
Ununseptium
unknown

116
Lv
Livermorium
[298]

115
Uup
Ununpentium
unknown

114
Fl
Flerovium
[289]

113
Uut
Ununtrium
unknown

112
Cn
Copernicium
[277]

111
Rg
Roentgenium
[272]

110
Ds
Darmstadtium
[269]

109
Mt
Meitnerium
[268]

108
Hs
Hassium
[269]

107
Bh
Bohrium
[264]

106
Sg
Seaborgium
[266]

105
Db
Dubnium
[262]

104
Rf
Rutherfordium
[261]

103
Lr
Lawrencium
[262]

102
No
Nobelium
259.101

101
Md
Mendelevium
258.1

100
Fm
Fermium
257.095

99
Es
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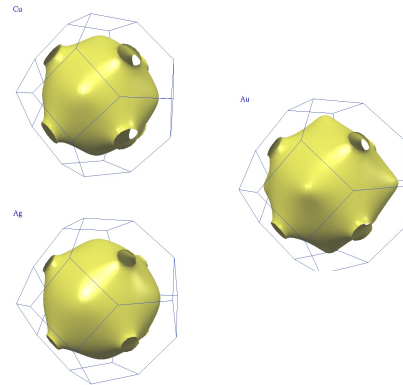
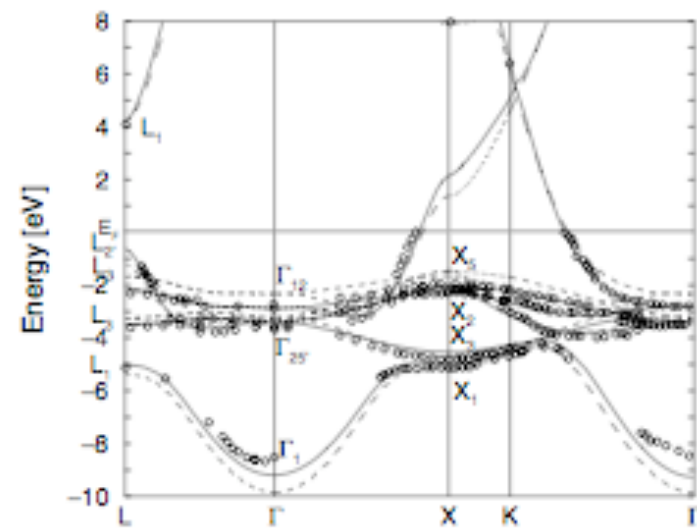
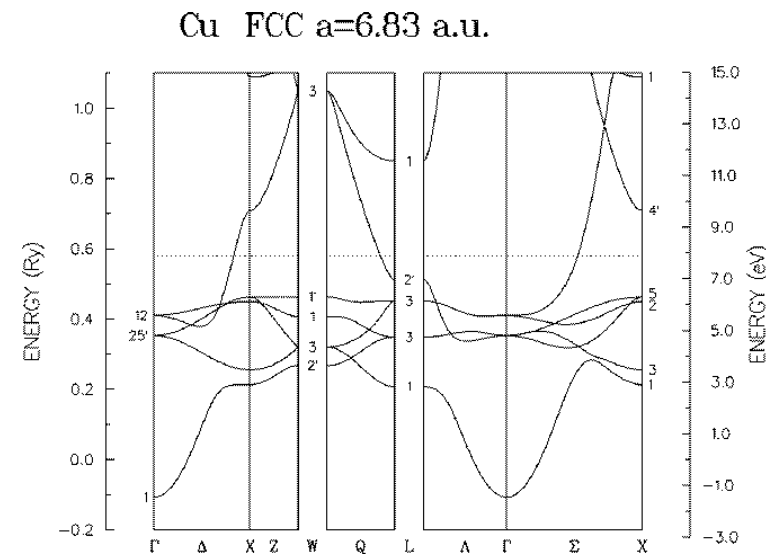
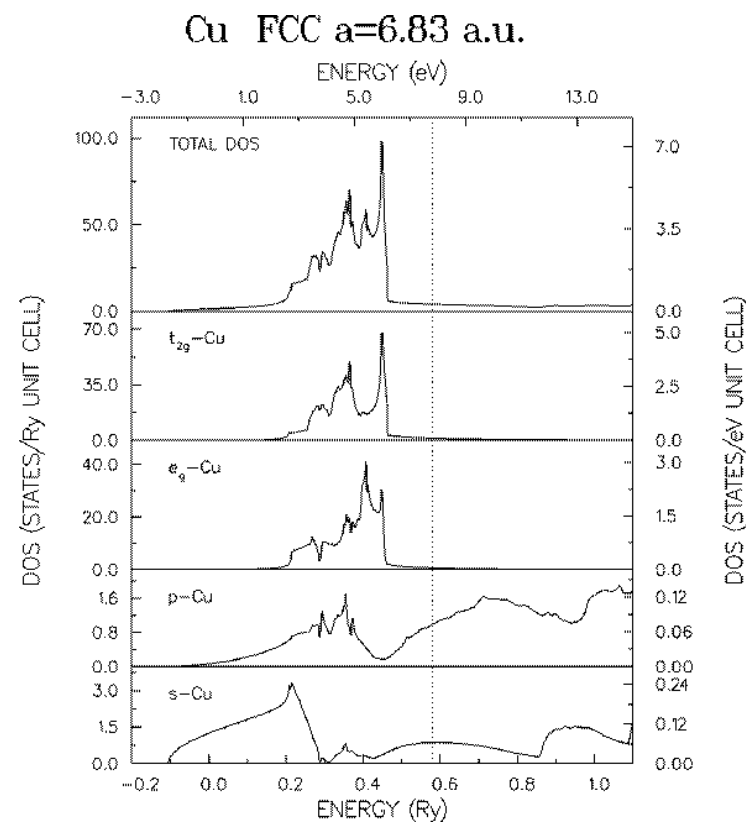


FIG. 2. Solid line: present GW results for the bulk copper band structure, compared with the DFT-LDA results (dashed line), and with the experimental data reported in Ref. [16] (circles).

- Electrons au niveau de Fermi presque libres + électrons d (bande pleine)
- Surface de Fermi quasi-sphérique
- $E_c \sim 3-4$ eV

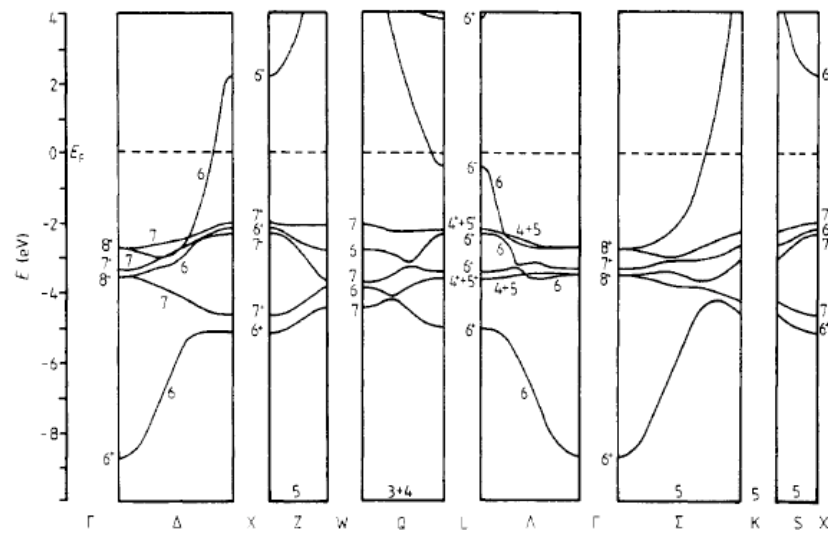


Figure 2. Relativistic band structure of Cu along high symmetry directions.

Cu

► Structures de bande

► Propriétés optiques

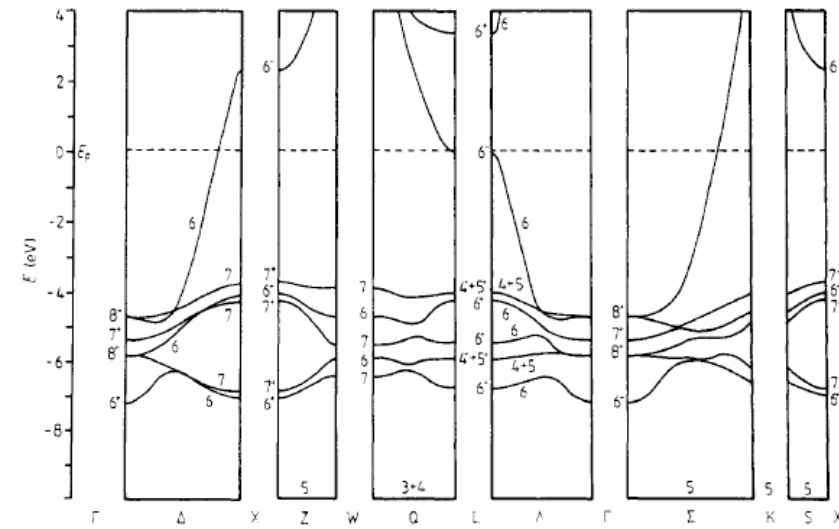


Figure 3. Relativistic band structure of Ag along high symmetry directions.

Ag

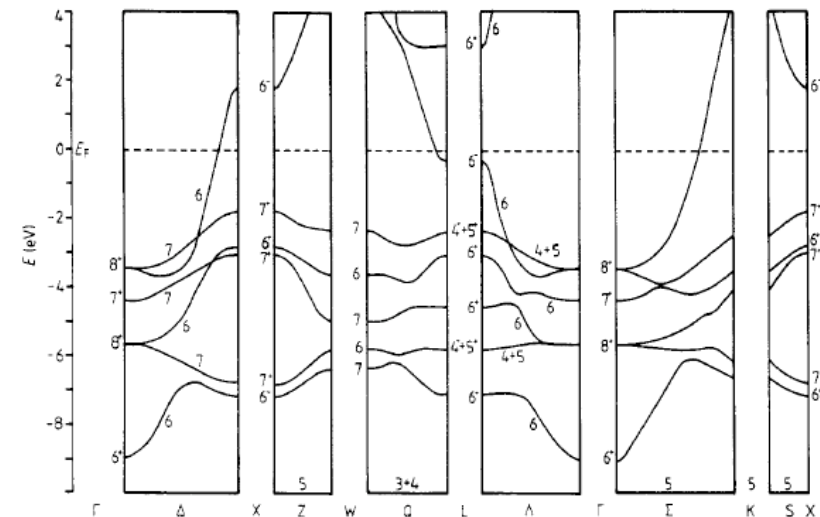
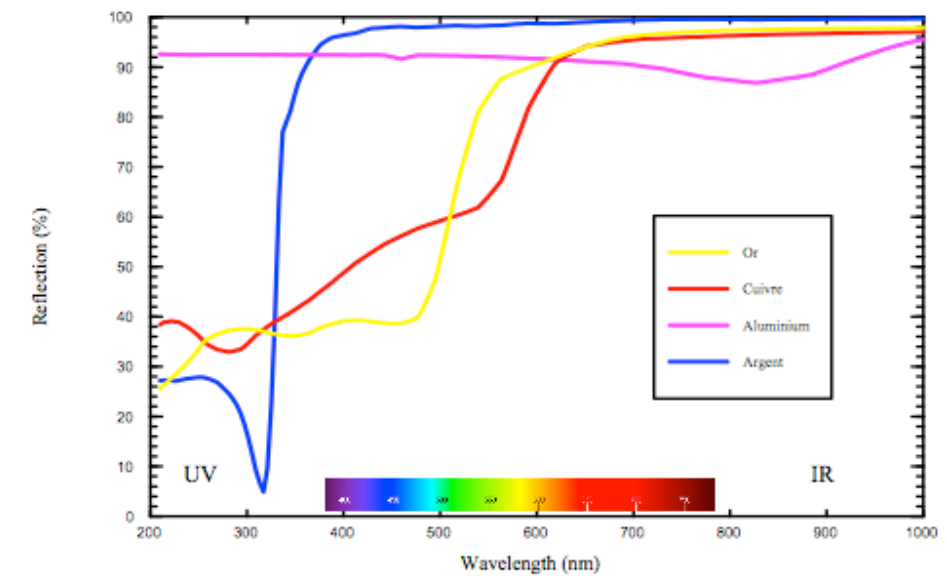


Figure 4. Relativistic band structure of Au along high symmetry directions.

Au



Métaux de transition

[illegible]

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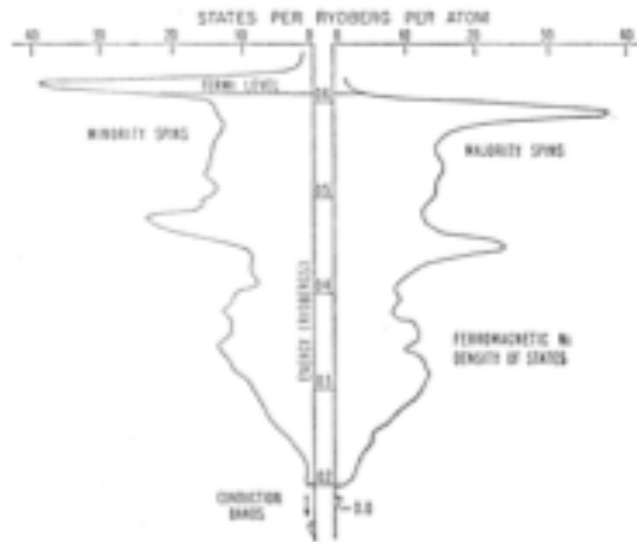


FIG. 12. Densities of states for minority- and majority-spin electrons in ferromagnetic Ni. The lower parts of the conduction bands are only shown schematically because the exact relative positions of the Γ_1 levels corresponding to majority and minority spins are uncertain.

- Densités d'états
- Structures de bande

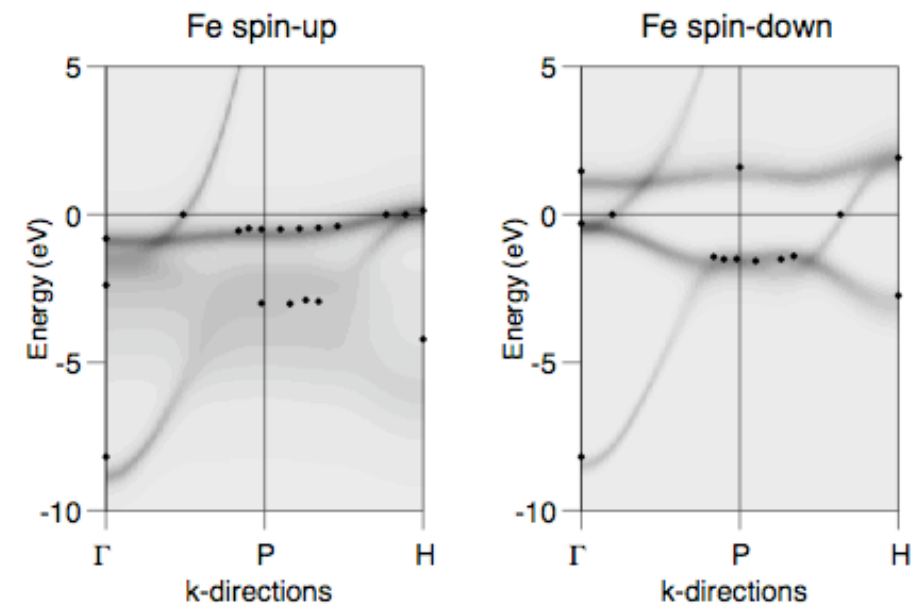
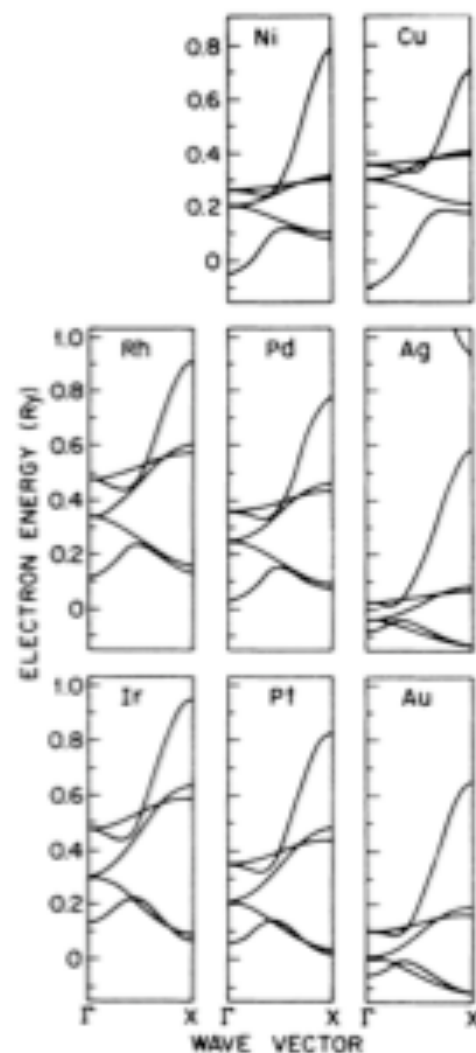


FIG. 3. Spectral function of ferromagnetic iron for spin-up (a) and spin-down (b) and the two k -directions in the Brillouin zone compare with the experimental angle resolved photoemission and de Haas - van Alphen (at the $E_F=0$) points (from Ref. 3).

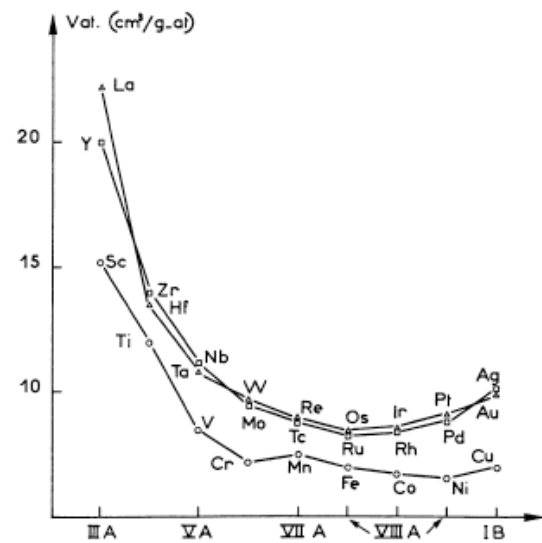


FIG. 1. — Volume atomique des métaux de transition, d'après Gschneidner [1].

(1) Cette approximation est introduite pour la commodité des calculs ; à condition d'utiliser pour $\beta(R)$ une fonction dont les dérivées premières et secondes ont des valeurs comparables autour de la position d'équilibre du réseau, tous les résultats

encore à voir le maximum de K décalé vers la droite, ce qu'on observe effectivement. Les figures 2 et 3 illustrent le comportement de E_c et K respectivement.

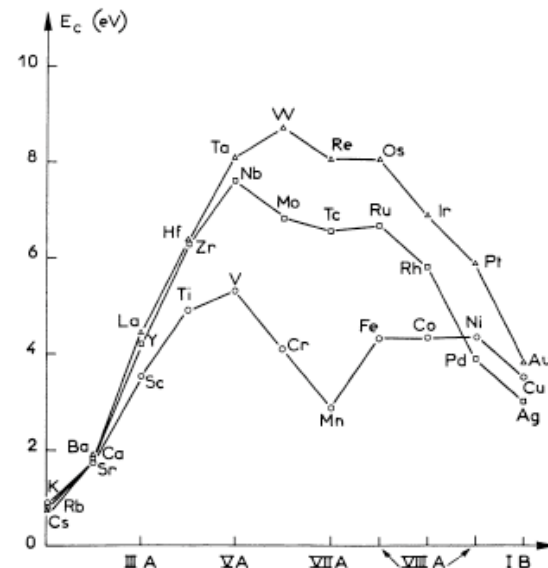


FIG. 2. — Energie de cohésion des métaux de transition, d'après Gschneidner [1].

- Energie de cohésion (5-10 eV)
- Constantes élastiques

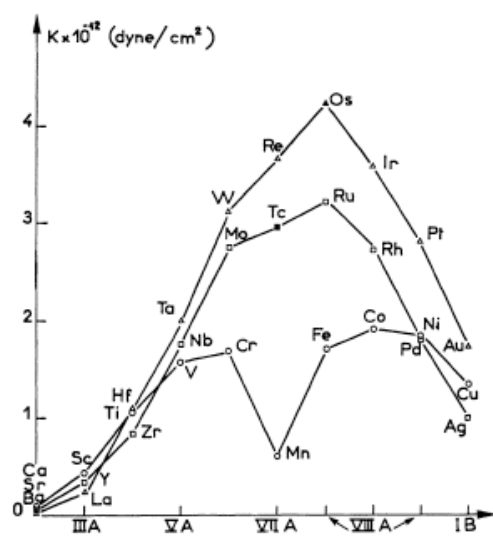


FIG. 3. — Module de compressibilité des métaux de transition ; les points noirs correspondent à des valeurs estimées (voir Gschneidner [1]).

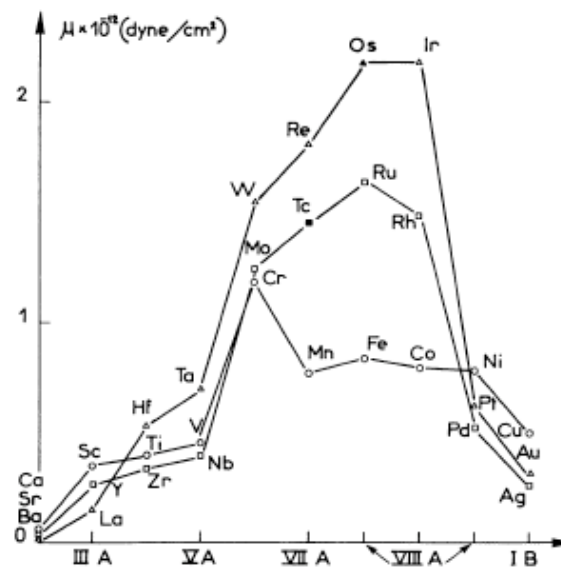
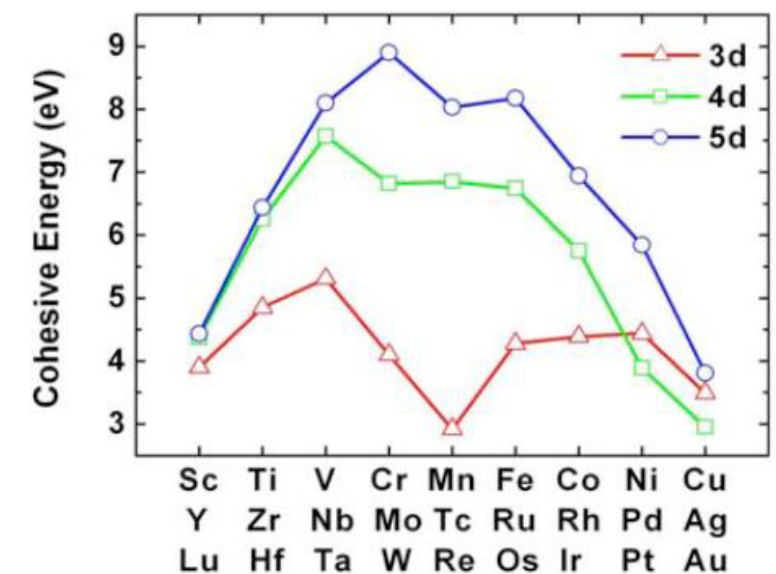


FIG. 4. — Module de cisaillement des métaux de transition ; les points noirs correspondent à des valeurs estimées (voir Gschneidner [1]).



Li hcp	Be hcp											
Na hcp	Mg hcp	1	2	3.5	5	6	7	8.5	9.5	10	n_d	
K bcc	Ca fcc	Sc hcp	Ti hcp	V bcc	Cr bcc	Mn (bcc)	Fe bcc	Co hcp	Ni fcc	Cu fcc	Zn hcp	
Rb bcc	Sr fcc	Y hcp	Zr hcp	Nb bcc	Mo bcc	Tc hcp	Ru hcp	Rh fcc	Pd fcc	Ag fcc	Cd hcp	
Cs bcc	Ba bcc	Lu hcp	Hf hcp	Ta bcc	W bcc	Re hcp	Os hcp	Ir fcc	Pt fcc	Au fcc	Hg (fcc)	
Fr	Ra bcc											

Les propriétés dépendent surtout du nombre d'électrons d qui contribuent fortement à la cohésion

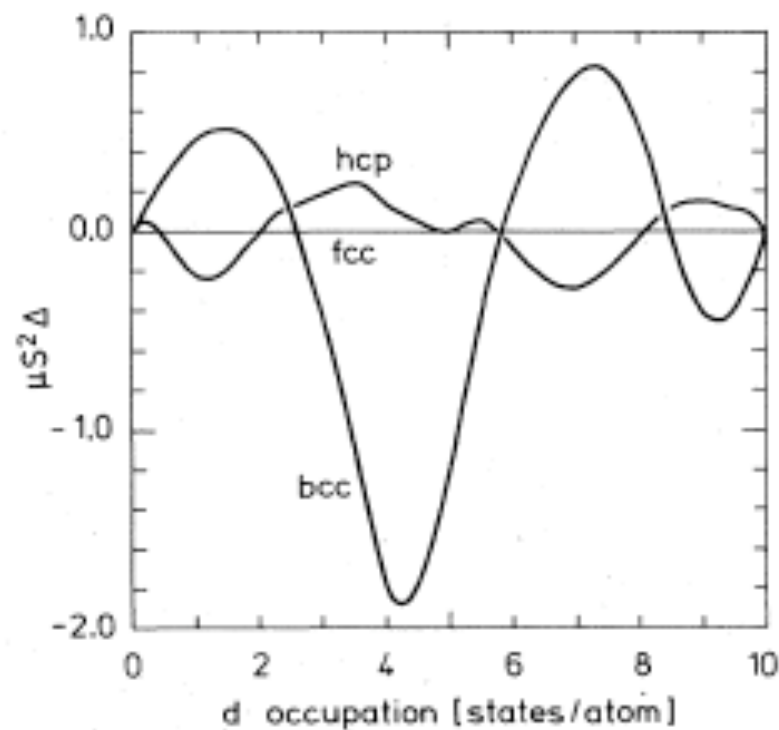


FIG. 2. Structural energy differences obtained from canonical d bands, by means of Eq. (4), as functions of the calculated canonical d occupation.

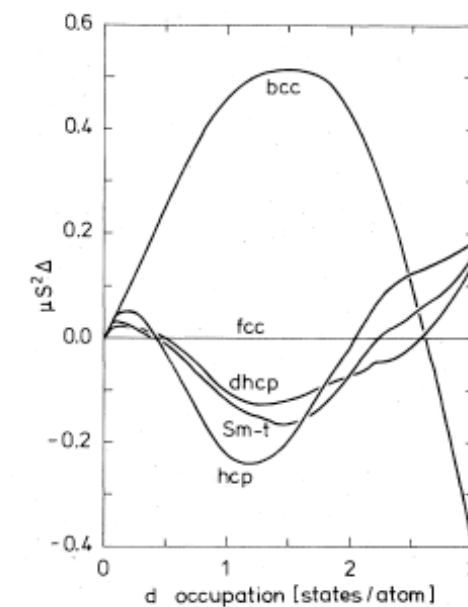


FIG. 3. Structural energy differences obtained from canonical d bands, by means of Eq. (4), in the d -occupation-number range appropriate to the lanthanide crystal-structure sequence.

Terres rares

Periodic Table of the Elements

Periodic Table of the Elements																	
1 IA 11A H Hydrogen 1.008																	18 VIIIA 8A He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012																
11 Na Sodium 22.990	12 Mg Magnesium 24.305																
		3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904	36 Kr Krypton 84.80
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown
Lanthanide Series		57 La Lanthanum 138.906	58 Ce Cerium 140.115	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.966	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.26	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967	
Actinide Series		89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]	

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
dhcp	fcc	dhcp	dhcp	dhcp	Sm-t	bcc	hcp	hcp	hcp	hcp	hcp	hcp	hcp

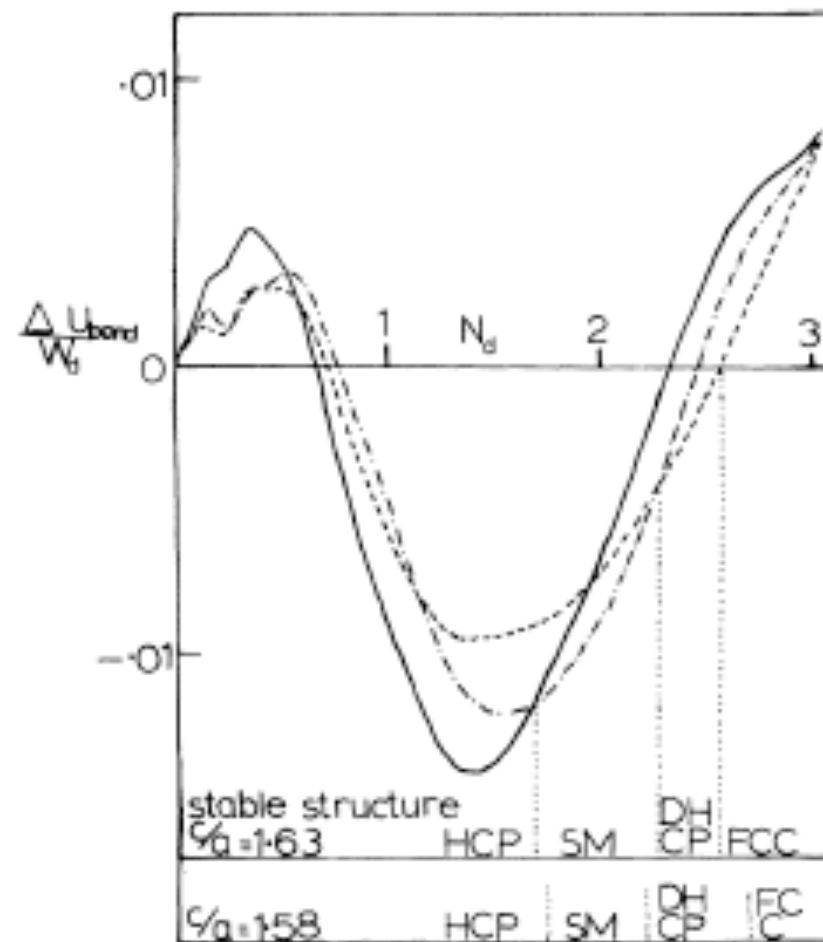


FIG. 2. The relative bonding energies of hcp- (—), dhcp- (---) and Sm-type (- · - ·) with respect to the fcc structure as a function of d -band occupancy N_d . The resulting stable structures for the ideal and a nonideal axial ratio are also shown.

Les propriétés de cohésion dépendent surtout du nombre d'états délocalisés s, p, d

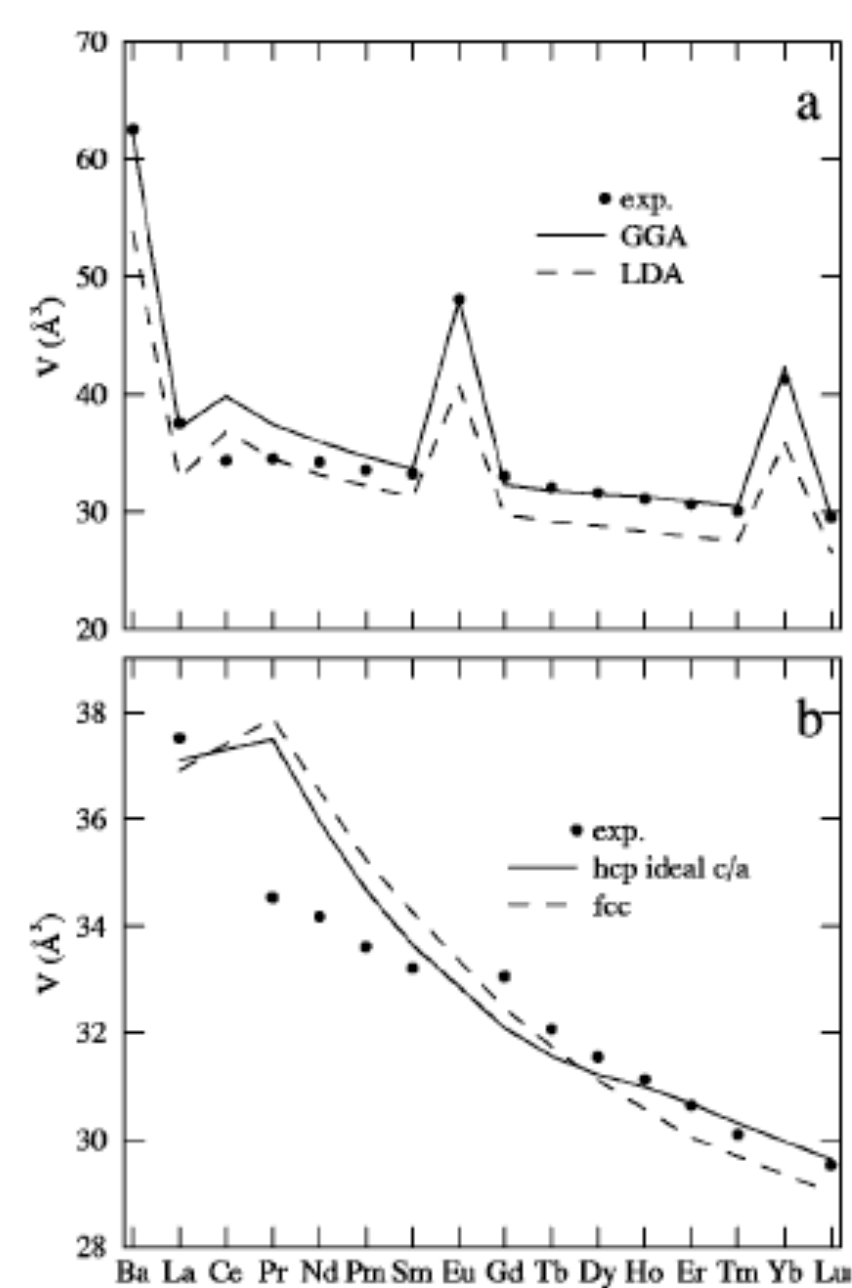


FIG. 1. (a) Experimental volumes at ambient temperature (taken from Ref. 14) and calculated volumes using LDA and GGA. Ba and Lu are calculated in the bcc structure, Ce and Yb in the fcc structure. All other elements are calculated in the hcp structure assuming the experimental c/a ratio. (b) Experimental volumes as above compared to calculated equilibrium volumes for two different crystal structures: hcp with ideal c/a ratio and fcc, for all trivalent lanthanides except Ce.

the equilibrium volume relative to LDA. The relative in-

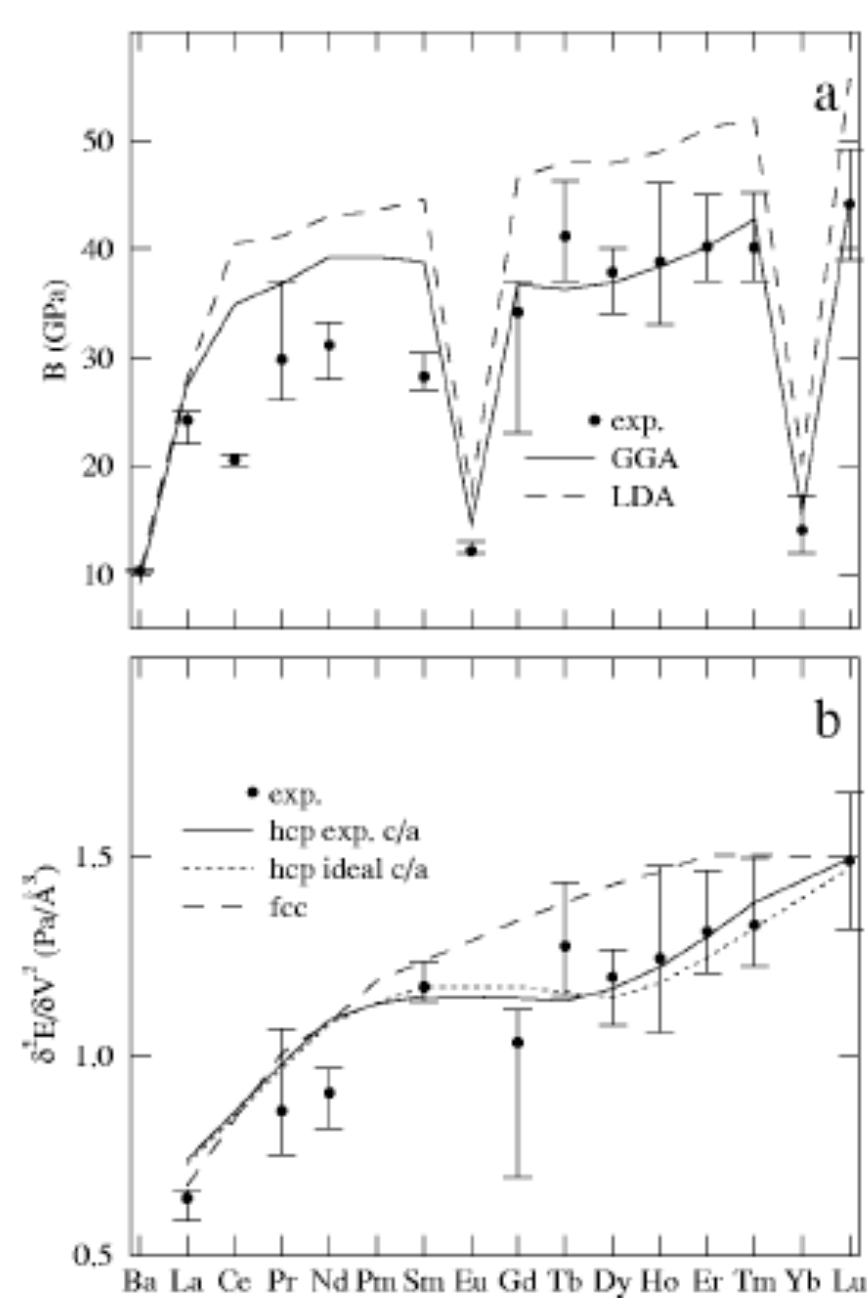


FIG. 2. (a) Experimental bulk moduli at ambient temperature (taken from Ref. 26) and calculated bulk moduli (evaluated at the theoretical equilibrium volume) for both LDA and GGA. Ba and Eu are calculated in the bcc structure, Ce and Yb in the fcc structure. All other elements are calculated in the hcp structure assuming a c/a ratio fixed at its experimental equilibrium value. (b) Calculated second energy derivative with respect to volume (evaluated at the theoretical equilibrium volume) for the trivalent lanthanides except Ce compared to experimental values calculated using the bulk moduli in Ref. 26 and volumes in Ref. 14.

- Les électrons f sont localisés et ne participent pas à la cohésion. Ils sont responsables du magnétisme.
- $U/t \gg 1$
D'où propriétés structurales semblables

Z ↕	Symbol ↕	Name ↕	Etymology	Selected applications
21	Sc	Scandium	from Latin <i>Scandia</i> (Scandinavia).	Light aluminium-scandium alloys for aerospace components, additive in metal-halide lamps and mercury-vapor lamps, ^[7] radioactive tracing agent in oil refineries
39	Y	Yttrium	after the village of Ytterby, Sweden, where the first rare earth ore was discovered.	Yttrium aluminium garnet (YAG) laser, yttrium vanadate (YVO ₄) as host for europium in television red phosphor, YBCO high-temperature superconductors, yttria-stabilized zirconia (YSZ), yttrium iron garnet (YIG) microwave filters, ^[7] energy-efficient light bulbs (part of triphosphor white phosphor coating in fluorescent tubes, CFLs and CCFLs, and yellow phosphor coating in white LEDs), ^[9] spark plugs, gas mantles, additive to steel, cancer treatments
57	La	Lanthanum	from the Greek "lanthanein", meaning <i>to be hidden</i> .	High refractive index and alkali-resistant glass, flint, hydrogen storage, battery-electrodes, camera lenses, fluid catalytic cracking catalyst for oil refineries
58	Ce	Cerium	after the dwarf planet Ceres, named after the Roman goddess of agriculture.	Chemical oxidizing agent, polishing powder, yellow colors in glass and ceramics, catalyst for self-cleaning ovens, fluid catalytic cracking catalyst for oil refineries, ferrocerium flints for lighters, robust intrinsically hydrophobic coatings for turbine blades.
59	Pr	Praseodymium	from the Greek "prasios", meaning <i>leek-green</i> , and "didymos", meaning <i>twin</i> .	Rare-earth magnets, lasers, core material for carbon arc lighting, colorant in glasses and enamels, additive in didymium glass used in welding goggles, ^[7] ferrocerium firesteel (flint) products.
60	Nd	Neodymium	from the Greek "neos", meaning <i>new</i> , and "didymos", meaning <i>twin</i> .	Rare-earth magnets, lasers, violet colors in glass and ceramics, didymium glass, ceramic capacitors, electric motors of electric automobiles
61	Pm	Promethium	after the Titan Prometheus, who brought fire to mortals.	Nuclear batteries, luminous paint
62	Sm	Samarium	after mine official, Vasili Samarsky-Bykhovets.	Rare-earth magnets, lasers, neutron capture, masers, control rods of nuclear reactors
63	Eu	Europium	after the continent of Europe.	Red and blue phosphors, lasers, mercury-vapor lamps, fluorescent lamps, NMR relaxation agent
64	Gd	Gadolinium	after Johan Gadolin (1760–1852), to honor his investigation of rare earths.	High refractive index glass or garnets, lasers, X-ray tubes, computer memories, neutron capture, MRI contrast agent, NMR relaxation agent, magnetostrictive alloys such as Galfenol, steel additive
65	Tb	Terbium	after the village of Ytterby, Sweden.	Additive in Neodymium based magnets, green phosphors, lasers, fluorescent lamps (as part of the white triband phosphor coating), magnetostrictive alloys such as terfenol-D, naval sonar systems, stabilizer of fuel cells
66	Dy	Dysprosium	from the Greek "dysprositos", meaning <i>hard to get</i> .	Additive in Neodymium based magnets, lasers, magnetostrictive alloys such as terfenol-D, hard disk drives
67	Ho	Holmium	after Stockholm (in Latin, "Holmia"), native city of one of its discoverers.	Lasers, wavelength calibration standards for optical spectrophotometers, magnets
68	Er	Erbium	after the village of Ytterby, Sweden.	Infrared lasers, vanadium steel, fiber-optic technology
69	Tm	Thulium	after the mythological northern land of Thule.	Portable X-ray machines, metal-halide lamps, lasers
70	Yb	Ytterbium	after the village of Ytterby, Sweden.	Infrared lasers, chemical reducing agent, decoy flares, stainless steel, stress gauges, nuclear medicine, monitoring earthquakes
71	Lu	Lutetium	after Lutetia, the city that later became Paris.	Positron emission tomography – PET scan detectors, high-refractive-index glass, lutetium tantalate hosts for phosphors, catalyst used in refineries, LED light bulb

Actinides

Periodic Table of the Elements																		1 IA 11A		18 VIIIA 8A															
1 H Hydrogen 1.008																		2 He Helium 4.003																	
3 Li Lithium 6.941		4 Be Beryllium 9.012														5 B Boron 10.811		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		3 IIIB 3B		4 IVB 4B		5 VB 5B		6 VIB 6B		7 VIIB 7B		8 VIII 8		9 VIII 8		10 VIII 8		11 IB 1B		12 IIB 2B		13 IIIA 3A		14 IVA 4A		15 VA 5A		16 VIA 6A		17 VIIA 7A		18 VIIIA 8A	
19 K Potassium 39.098		20 Ca Calcium 40.078		21 Sc Scandium 44.956		22 Ti Titanium 47.88		23 V Vanadium 50.942		24 Cr Chromium 51.996		25 Mn Manganese 54.938		26 Fe Iron 55.933		27 Co Cobalt 58.933		28 Ni Nickel 58.693		29 Cu Copper 63.546		30 Zn Zinc 65.39		31 Ga Gallium 69.732		32 Ge Germanium 72.61		33 As Arsenic 74.922		34 Se Selenium 78.09		35 Br Bromine 79.904		36 Kr Krypton 84.80	
37 Rb Rubidium 84.468		38 Sr Strontium 87.62		39 Y Yttrium 88.906		40 Zr Zirconium 91.224		41 Nb Niobium 92.906		42 Mo Molybdenum 95.94		43 Tc Technetium 98.907		44 Ru Ruthenium 101.07		45 Rh Rhodium 102.906		46 Pd Palladium 106.42		47 Ag Silver 107.868		48 Cd Cadmium 112.411		49 In Indium 114.818		50 Sn Tin 118.71		51 Sb Antimony 121.760		52 Te Tellurium 127.6		53 I Iodine 126.904		54 Xe Xenon 131.29	
55 Cs Cesium 132.905		56 Ba Barium 137.327		57-71		72 Hf Hafnium 178.49		73 Ta Tantalum 180.948		74 W Tungsten 183.85		75 Re Rhenium 186.207		76 Os Osmium 190.23		77 Ir Iridium 192.22		78 Pt Platinum 195.08		79 Au Gold 196.967		80 Hg Mercury 200.59		81 Tl Thallium 204.383		82 Pb Lead 207.2		83 Bi Bismuth 208.980		84 Po Polonium [208.982]		85 At Astatine 209.987		86 Rn Radon 222.018	
87 Fr Francium 223.020		88 Ra Radium 226.025		89-103		104 Rf Rutherfordium [261]		105 Db Dubnium [262]		106 Sg Seaborgium [266]		107 Bh Bohrium [264]		108 Hs Hassium [269]		109 Mt Meitnerium [268]		110 Ds Darmstadtium [269]		111 Rg Roentgenium [272]		112 Cn Copernicium [277]		113 Uut Ununtrium unknown		114 Fl Flerovium [289]		115 Uup Ununpentium unknown		116 Lv Livermorium [298]		117 Uus Ununseptium unknown		118 Uuo Ununoctium unknown	
Lanthanide Series				57 La Lanthanum 138.906		58 Ce Cerium 140.115		59 Pr Praseodymium 140.908		60 Nd Neodymium 144.24		61 Pm Promethium 144.913		62 Sm Samarium 150.36		63 Eu Europium 151.966		64 Gd Gadolinium 157.25		65 Tb Terbium 158.925		66 Dy Dysprosium 162.50		67 Ho Holmium 164.930		68 Er Erbium 167.26		69 Tm Thulium 168.934		70 Yb Ytterbium 173.04		71 Lu Lutetium 174.967			
Actinide Series				89 Ac Actinium 227.028		90 Th Thorium 232.038		91 Pa Protactinium 231.036		92 U Uranium 238.029		93 Np Neptunium 237.048		94 Pu Plutonium 244.064		95 Am Americium 243.061		96 Cm Curium 247.070		97 Bk Berkelium 247.070		98 Cf Californium 251.080		99 Es Einsteinium [254]		100 Fm Fermium 257.095		101 Md Mendelevium 258.1		102 No Nobelium 259.101		103 Lr Lawrencium [262]			

Nature of the 5f states in actinide metals

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(Published 6 February 2009)

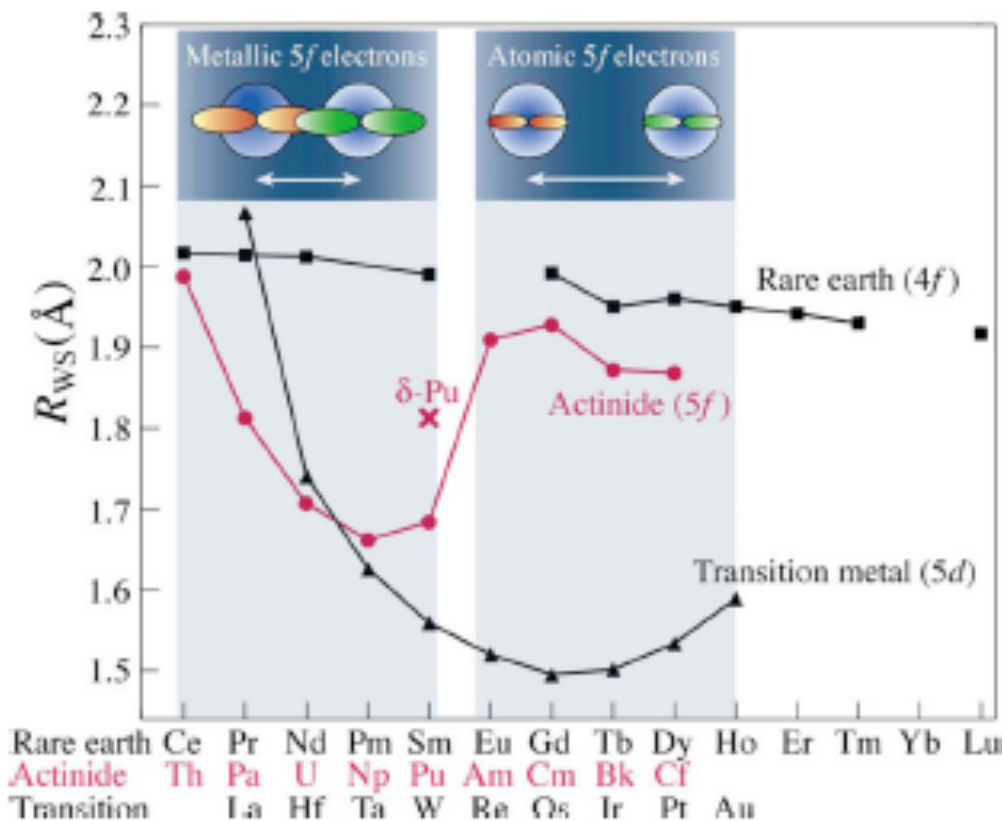


FIG. 1. (Color online) Wigner-Seitz radius of each metal as a function of atomic number Z for the 5d, 4f, and 5f metal series. From Boring and Smith, 2000. The upper-left insets schematically illustrate localized and delocalized 5f states between adjacent actinide atoms. From Albers, 2001.

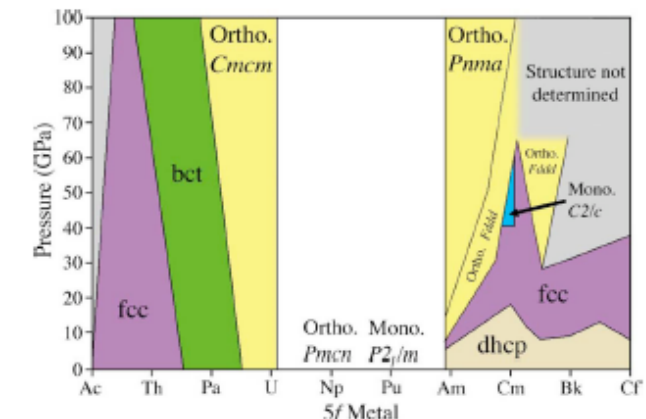
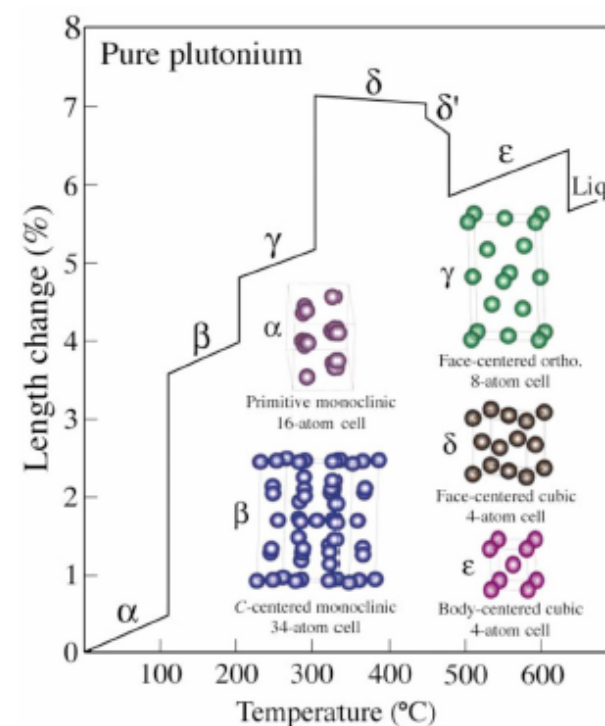


FIG. 4. (Color online) A “pseudobinary” phase diagram of the light to middle 5f actinide metals as a function of pressure (from Lindbaum *et al.*, 2003, with the phase boundaries for Cm updated using Heathman *et al.*, 2005, and Cm-Bk alloys from Heathman *et al.*, 2007). The pressure behaviors of Np and Pu are not shown, but the ground-state crystal structure of each metal is indicated.

cal guesses based on thermodynamic principles. Thus, while the pseudobinary phase diagram is not strictly correct, it does afford great insight into the general behav-

- Les électrons 5f sont moins localisés et participent à la cohésion jusqu'au plutonium
- Début de série comme métaux de transition (en plus compliqué); fin de série comme les terres rares
- $U/t \approx 1$ cas difficile
- (Friedel 1956 !)

Covalents

Periodic Table of the Elements																		18 VIIIA 8A																	
1 IA 11A		2 IIA 2A														13 IIIA 3A		14 IVA 4A		15 VA 5A		16 VIA 6A		17 VIIA 7A		18 VIIIA 8A									
1 H Hydrogen 1.008		2 He Helium 4.003																																	
3 Li Lithium 6.941		4 Be Beryllium 9.012																				5 B Boron 10.811		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 Aluminum 26.982		14 Si Silicon 28.086		15 P Phosphorus 30.974		16 S Sulfur 32.066		17 Cl Chlorine 35.453		18 Ar Argon 39.948			
19 K Potassium 39.098		20 Ca Calcium 40.078		21 Sc Scandium 44.956		22 Ti Titanium 47.88		23 V Vanadium 50.942		24 Cr Chromium 51.996		25 Mn Manganese 54.938		26 Fe Iron 55.933		27 Co Cobalt 58.933		28 Ni Nickel 58.693		29 Cu Copper 63.546		30 Zn Zinc 65.39		31 Ga Gallium 69.732		32 Ge Germanium 72.61		33 As Arsenic 74.922		34 Se Selenium 78.09		35 Br Bromine 79.904		36 Kr Krypton 84.80	
37 Rb Rubidium 84.468		38 Sr Strontium 87.62		39 Y Yttrium 88.906		40 Zr Zirconium 91.224		41 Nb Niobium 92.906		42 Mo Molybdenum 95.94		43 Tc Technetium 98.907		44 Ru Ruthenium 101.07		45 Rh Rhodium 102.906		46 Pd Palladium 106.42		47 Ag Silver 107.868		48 Cd Cadmium 112.411		49 In Indium 114.818		50 Sn Tin 118.71		51 Sb Antimony 121.760		52 Te Tellurium 127.6		53 I Iodine 126.904		54 Xe Xenon 131.29	
55 Cs Cesium 132.905		56 Ba Barium 137.327		57-71		72 Hf Hafnium 178.49		73 Ta Tantalum 180.948		74 W Tungsten 183.85		75 Re Rhenium 186.207		76 Os Osmium 190.23		77 Ir Iridium 192.22		78 Pt Platinum 195.08		79 Au Gold 196.967		80 Hg Mercury 200.59		81 Tl Thallium 204.383		82 Pb Lead 207.2		83 Bi Bismuth 208.980		84 Po Polonium [208.982]		85 At Astatine 209.987		86 Rn Radon 222.018	
87 Fr Francium 223.020		88 Ra Radium 226.025		89-103		104 Rf Rutherfordium [261]		105 Db Dubnium [262]		106 Sg Seaborgium [266]		107 Bh Bohrium [264]		108 Hs Hassium [269]		109 Mt Meitnerium [268]		110 Ds Darmstadtium [269]		111 Rg Roentgenium [272]		112 Cn Copernicium [277]		113 Uut Ununtrium unknown		114 Fl Flerovium [289]		115 Uup Ununpentium unknown		116 Lv Livermorium [298]		117 Uus Ununseptium unknown		118 Uuo Ununoctium unknown	
Lanthanide Series				57 La Lanthanum 138.906		58 Ce Cerium 140.115		59 Pr Praseodymium 140.908		60 Nd Neodymium 144.24		61 Pm Promethium 144.913		62 Sm Samarium 150.36		63 Eu Europium 151.966		64 Gd Gadolinium 157.25		65 Tb Terbium 158.925		66 Dy Dysprosium 162.50		67 Ho Holmium 164.930		68 Er Erbium 167.26		69 Tm Thulium 168.934		70 Yb Ytterbium 173.04		71 Lu Lutetium 174.967			
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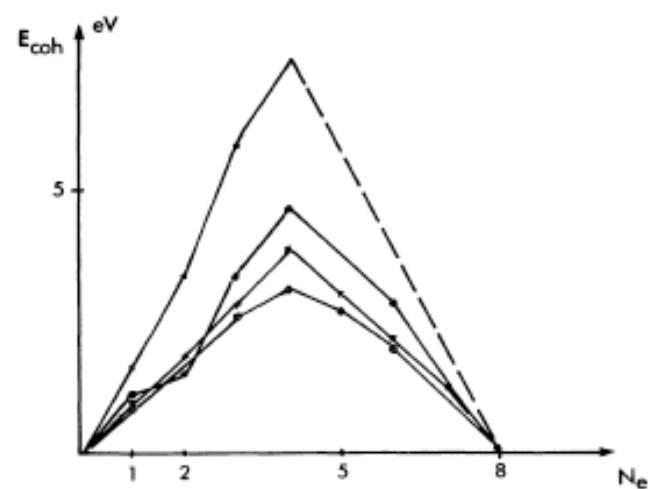
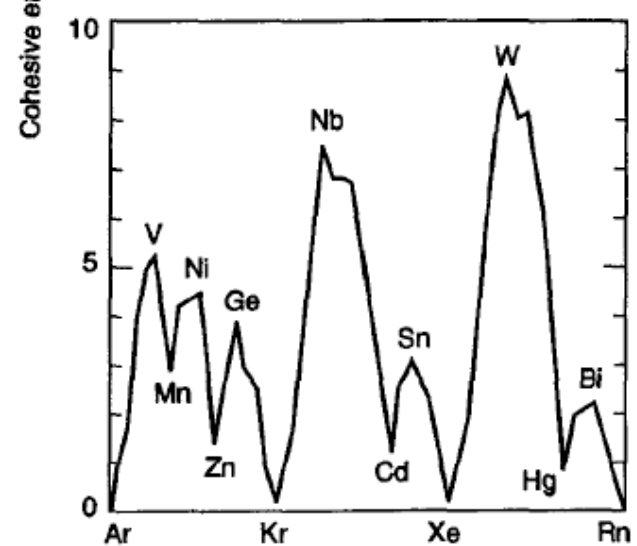
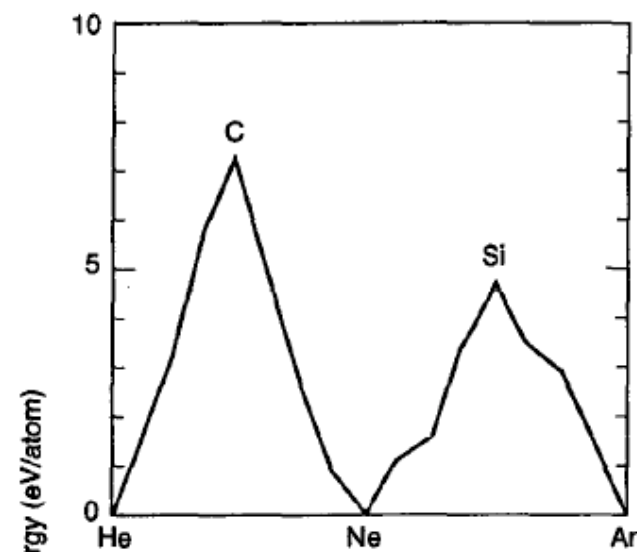


Fig. 1. — Experimental trends in the cohesive energy E_c versus the number of electrons N_e in the sp band, for the four first rows of the periodic table. Values are taken from [1].

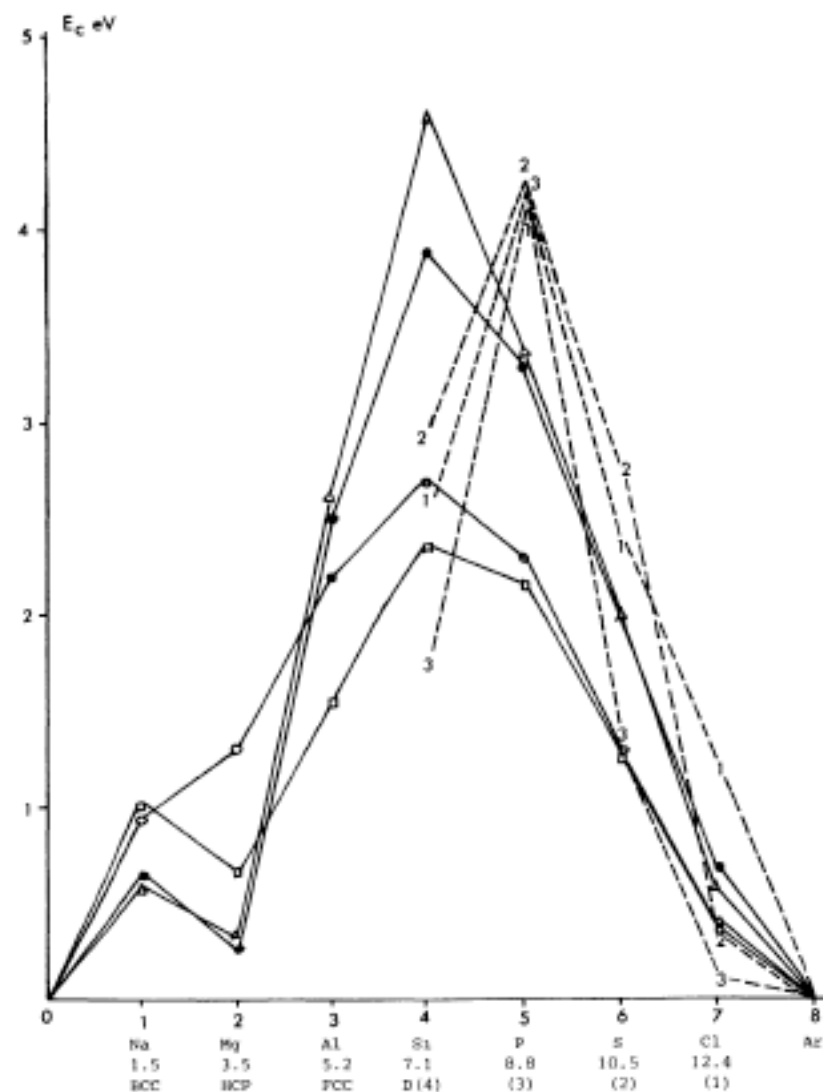


Fig. 7. — Calculated values of E_c for seven different structures : (●) simple cubic, (△) diamond, (○) f.c.c., (□) b.c.c., and finally in dashed lines, structures with $Z = 1, 2$ and 3 .

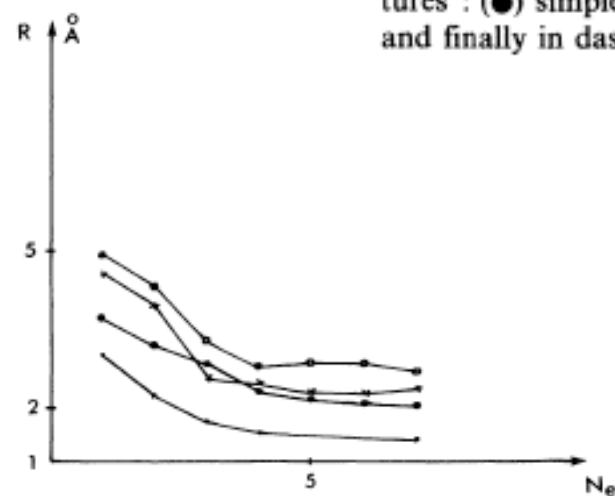
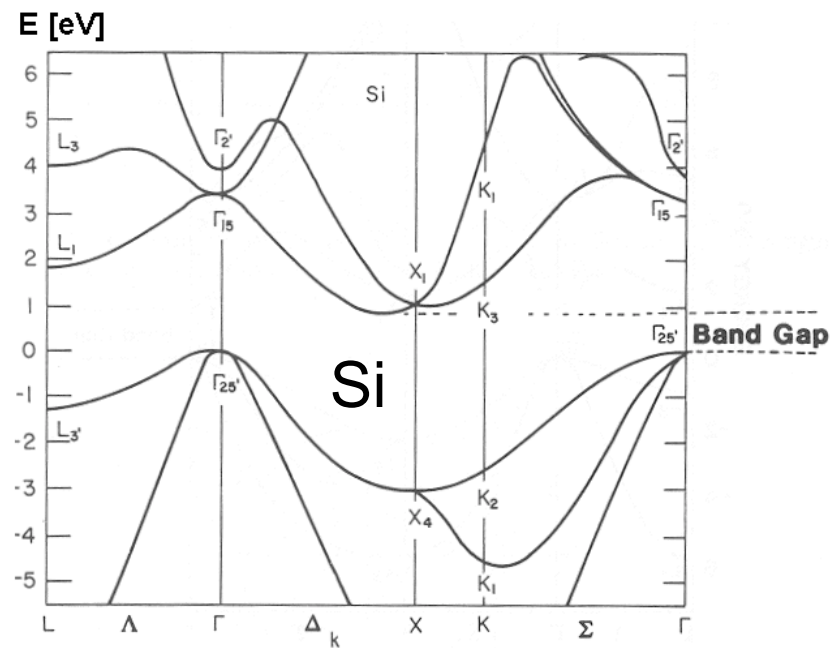


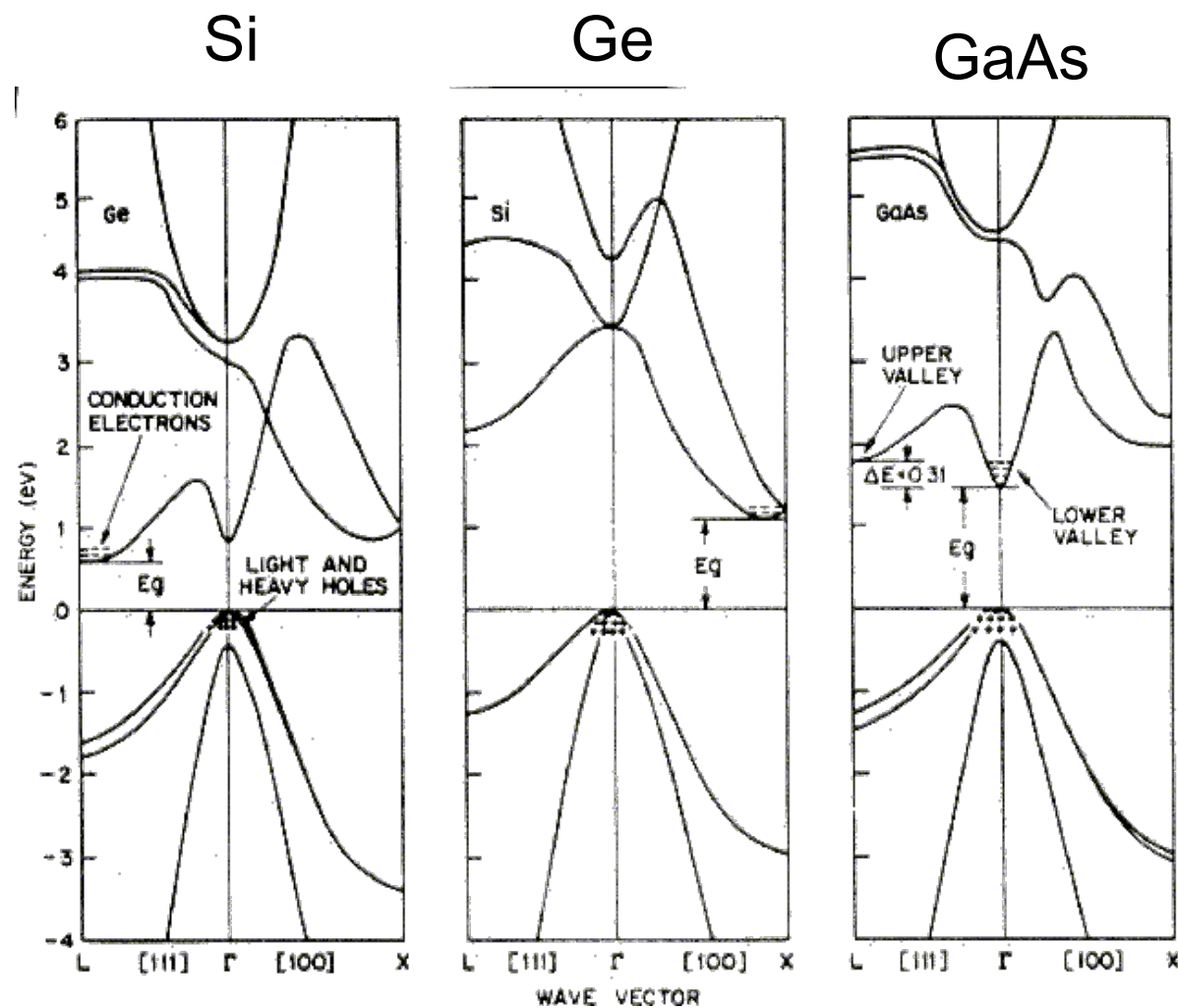
Fig. 2. — Experimental trends in the nearest neighbour distance R versus N_e . Values are taken from [2].

Allan Lannoo 1983



► Gap indirect pour C, Si, Ge

► Gap direct pour GaAs



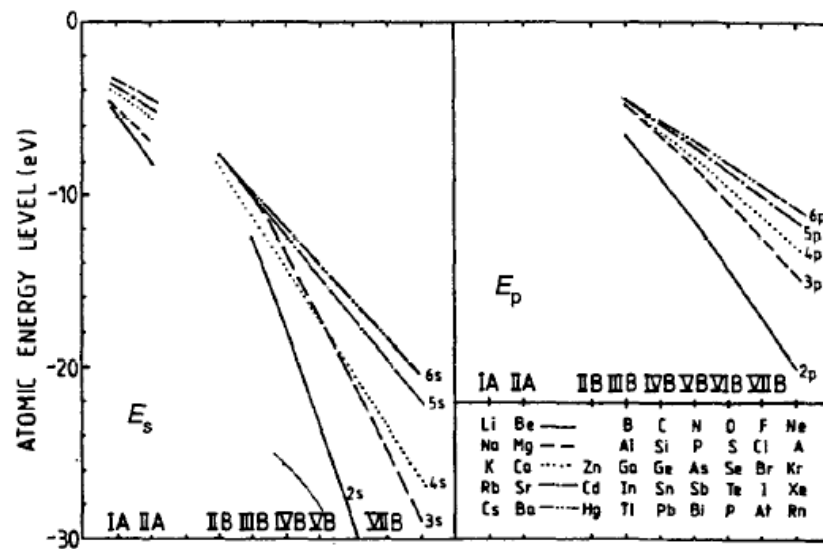
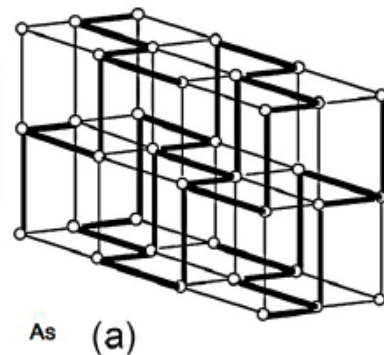


Fig. 2.16 The valences and p energy levels (after Herman and Skillman (1963)).

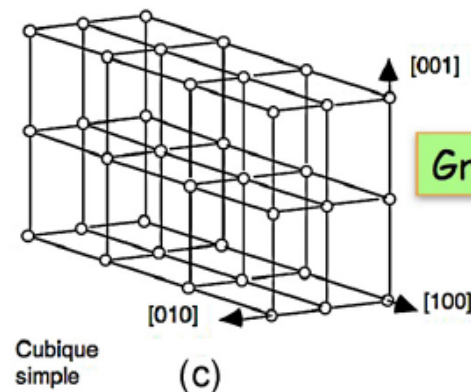
- Hybridation sp dans la colonne du carbone
- Caractère p de plus en plus marqué pour les colonnes suivantes

Group V: Arsenic
...S-L-S-L...



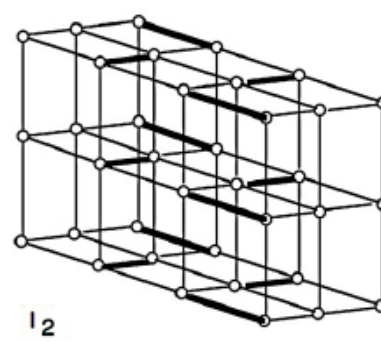
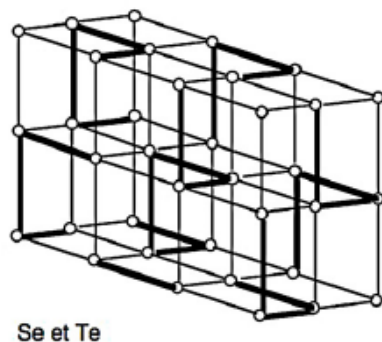
Gaspard
Cras 2015

Simple cubic



Group VI: Po

Group VI: Se, Te
...S-L-L-S-L-L...



Group VII: Br₂, I₂
mix SLL and LLL

- Structures cristallines colonne V: cubique simple + Peierls distortion (J.-P. Gaspard, Ch Bichara)
Cf: phase change compounds Ge Te, ...

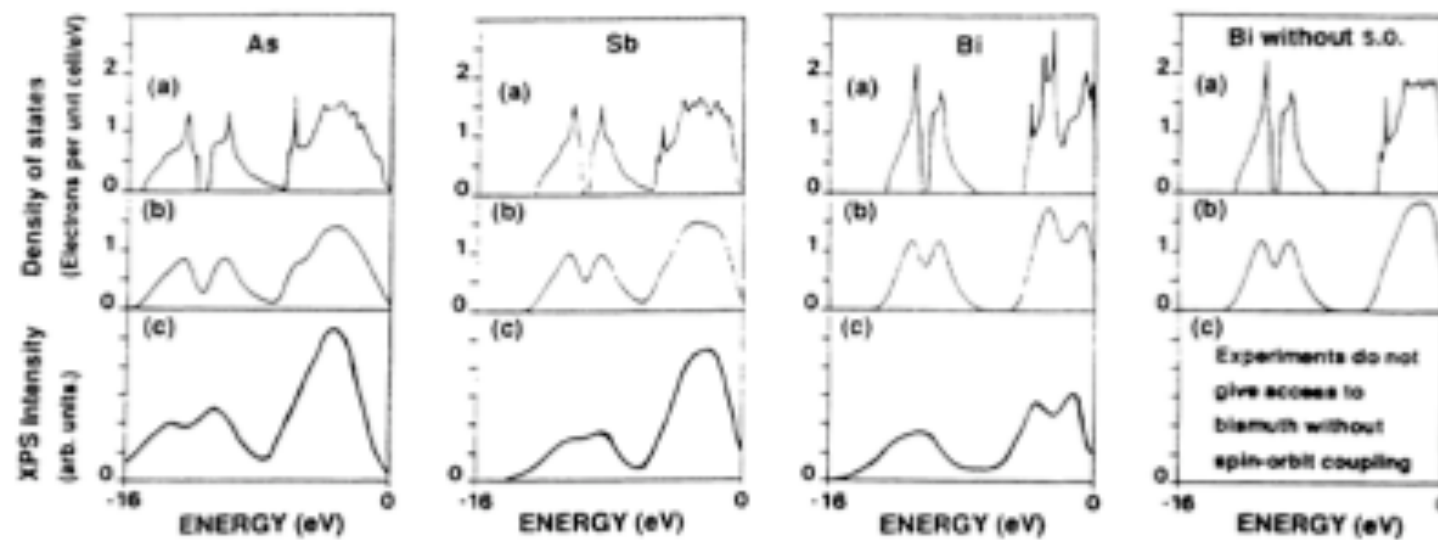


FIG. 9. For the four “elements” As, Sb, Bi, and Bi without s.o. coupling, comparison of (a) theoretical (DOS), (b) theoretical smoothed DOS (0.6 eV Gaussian smoothing), and (c) experimental XPS from Ref. 29. The experimental XPS spectra for Bi without spin-orbit coupling is, of course, missing.

- Les états de valence sont bien décrits en « liaisons fortes » sp
- Les électrons de conduction sont plus souvent proches d'électrons libres

Gaz rares, pour mémoire

Periodic Table of the Elements																		18 VIII A 8A	
1 IA 11A		2 IIA 2A										13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 VIII A 8A		
1 H Hydrogen 1.008		4 Be Beryllium 9.012										5 B Boron 10.811	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		3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904	36 Kr Krypton 84.80		
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sciencenotes.org

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Structure électronique

Que veut on calculer ?

Propriétés de l'état fondamental (à 0 K)

stabilité des structures cristallines, propriétés de cohésion ,
élastiques, énergie de défauts

Propriétés reliées à des excitations à une particule
(électron, trou)

potentiel d'ionisation, photoémission, effet tunnel

Propriétés reliées à des excitation à deux particules
(électron + trou)

propriétés optiques: absorption, luminescence
(exciton, plasmon) propriétés de transport

Température finie

phonons, couplage électron-phonon

Avec quelles méthodes ?

Méthodes empiriques

interactions de paires, constantes de force

Méthodes semi-empiriques

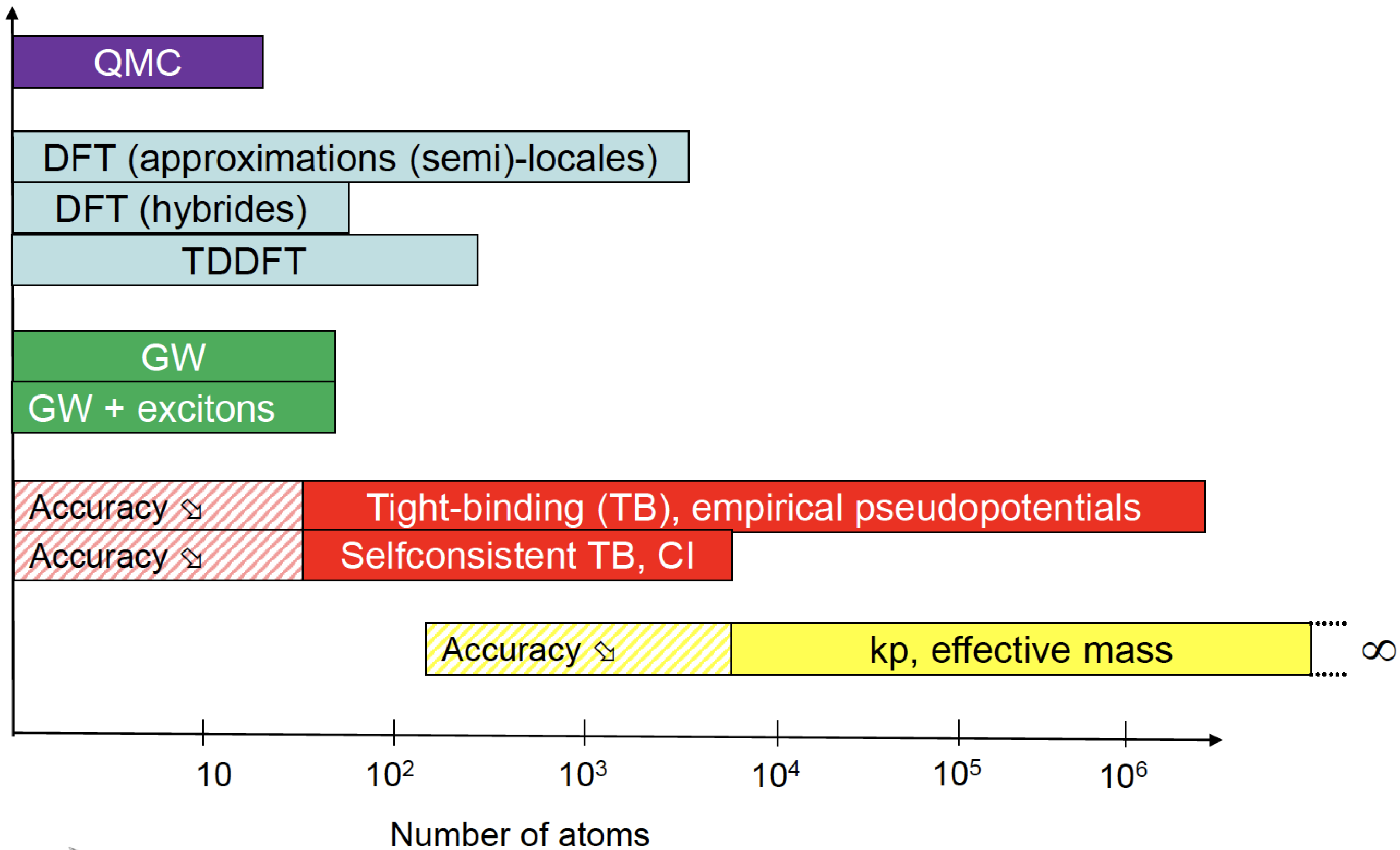
électrons presque libres, liaisons fortes

Méthodes « ab initio »

DFT (état fondamental), Monte Carlo quantique

excitations: quasiparticules, GW, Bethe-Salpeter

fortes corrélations: DFT+U, DFMT



Méthodes ab initio

Approximation adiabatique



Born-Oppenheimer approximation

(Adiabatic approximation)

$$\hat{H} = \hat{T}_N(\mathbf{R}) + \hat{T}_e(\mathbf{r}) + \hat{V}_{eN}(\mathbf{r}, \mathbf{R}) + \hat{V}_{NN}(\mathbf{R}) + \hat{V}_{ee}(\mathbf{r})$$

The Hamiltonian acts on the **many-particle** wave function of the systems, which depends on both ions and electrons:



Max Born
1882-1970



J. Robert
Oppenheimer
1904-1967

$$\Psi = \Psi(\underbrace{r_1, r_2, \dots, r_K}_{\text{electrons}}, \underbrace{R_1, R_2, \dots, R_N}_{\text{nuclei}})$$

Approximations:

Assume that $\hat{T}_N(\mathbf{R}) = -\hbar^2 \sum_I \frac{\nabla_I^2}{2M_I}$ is small
(makes sense, ion mass $M_I \gg$ electron mass)

Assume further that

depends on the nuclear
positions as **parameters**

$$\Psi(\{\mathbf{R}_I\}, \{\mathbf{r}_i\}) \approx \underbrace{\chi(\{\mathbf{R}_I\})}_{\text{nuclei}} \cdot \underbrace{\psi(\{\mathbf{R}_I\}; \{\mathbf{r}_i\})}_{\text{electrons}}$$

Le problème général

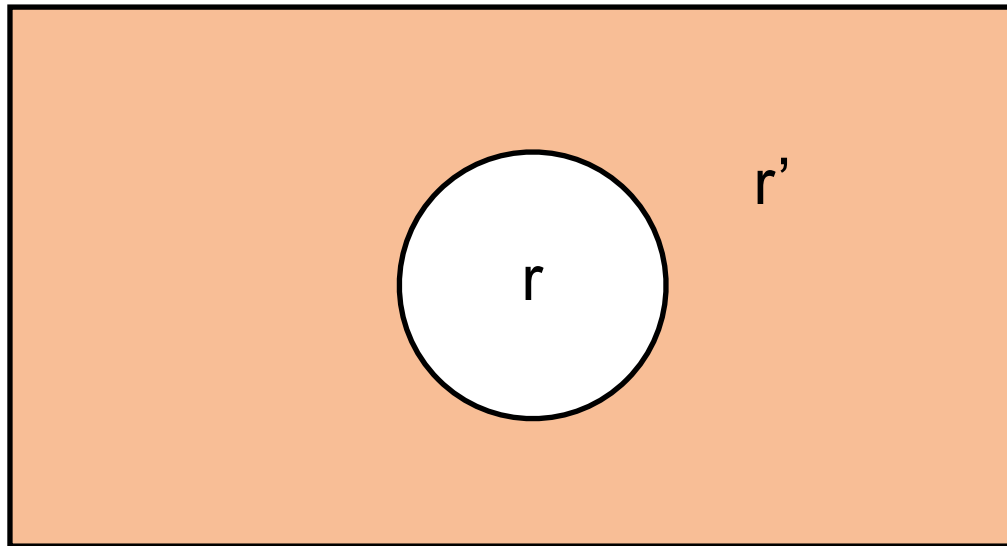
$$H = \sum_{i=1}^N \left(\frac{p_i^2}{2m} + V_{el-ion}(\vec{r}_i) \right) + \frac{1}{2} \sum_{i,j=1}^N \frac{e^2}{r_{ij}}$$
$$H \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = E \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

Energie totale: ajouter l'énergie ion-ion

- ▶ Equation de Schrödinger à 3N variables (+spin)
- ▶ Les ions occupent des positions fixes
- ▶ Les mouvements des électrons sont corrélés à cause du terme d'interaction e-e
- ▶ La fonction d'onde doit être antisymétrique: deux électrons ne peuvent pas être dans le même état au même endroit
- ▶ Principe de Pauli

Approximation de Hartree

Approximation de champ moyen



The Hartree method
1928
D.R. Hartree
(1897-1958)
Cambridge, UK



$$H = \frac{p^2}{2m} + V_{el-ion}(\vec{r}) + V_h(\vec{r})$$
$$H\phi_\alpha(\vec{r}) = \varepsilon_\alpha\phi_\alpha(\vec{r})$$
$$V_h(\vec{r}) = \int d\vec{r}' \sum_{\beta occ} \frac{e^2 |\phi_\beta(\vec{r}')|^2}{|\vec{r}' - \vec{r}|} = e^2 \int d\vec{r}' \frac{n(\vec{r}')}{|\vec{r}' - \vec{r}|}$$

- L'électron en r interagit avec le potentiel moyen dû aux autres électrons
- On en déduit des énergies et fonctions d'onde à un électron (états a) qui permettent de recalculer le potentiel « autocohérent (self-consistent) »
- Problème: le potentiel dépend en principe de a ! Sinon « self-interaction »

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \simeq \phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\dots\phi_N(\vec{r}_N)$$

- ▶ Les électrons se meuvent de façon indépendante (contradiction ?)
- ▶ Les équations de Hartree sont les meilleures pour de telles fonctions d'onde (théorème variationnel)
- ▶ Grave défaut: elles ne respectent pas le principe de Pauli
- ▶ Il faut antisymétriser la fonction d'onde
- ▶ (déterminant de Slater). En appliquant le principe variationnel on obtient alors de nouvelles équations dites de Hartree-Fock.

Hartree Fock

The Hartree-Fock method
1930
V.A. Fock
(1898–1974)
Leningrad, Russia



$$H_{hf}\phi_{\alpha}(\vec{r}) = H_h\phi_{\alpha}(\vec{r}) + \int d\vec{r}' \Sigma_x(\vec{r}, \vec{r}')\phi_{\alpha}(\vec{r}) = \varepsilon_{\alpha}\phi_{\alpha}(\vec{r})$$

$$\Sigma_x(\vec{r}, \vec{r}') = -e^2 \sum_{\beta \text{ occ}} \frac{\phi_{\beta}(\vec{r})\phi_{\beta}^*(\vec{r}')}{|\vec{r}' - \vec{r}|}$$

$$V_{Slater}(\vec{r}) = -\frac{0.916}{R_s[n(\vec{r})]} = -\frac{3}{2} \left[\frac{3}{\pi} n(\vec{r}) \right]^{1/3}$$



J. Slater

- Le nouveau potentiel non local dit potentiel (ou self-énergie) d'échange est compliqué.
- Il a cependant le mérite de compenser exactement le terme d'auto-interaction de l'approximation de Hartree
- Si on fait la moyenne locale, on obtient la méthode X_{α} de Slater
- Historiquement très important

Density Functional Theory (DFT)

Hohenberg-Kohn-Sham

L'énergie de l'état fondamental ne dépend que de la densité électronique

Comme fonctionnelle de la densité l'énergie est minimum pour la densité d'équilibre

On peut construire un hamiltonien à une particule qui donnera cette densité (Kohn-Sham) pourvu qu'on connaisse le potentiel V_{xc} qui ne dépend que de la densité

1. BASIC LEMMA OF HK

Statement:

If a potential $v(r)$ leads to the ground state density $n(r)$, and $v'(r)$ also leads to $n(r)$, then

$$v'(r) = v(r) + C, \quad (3)$$

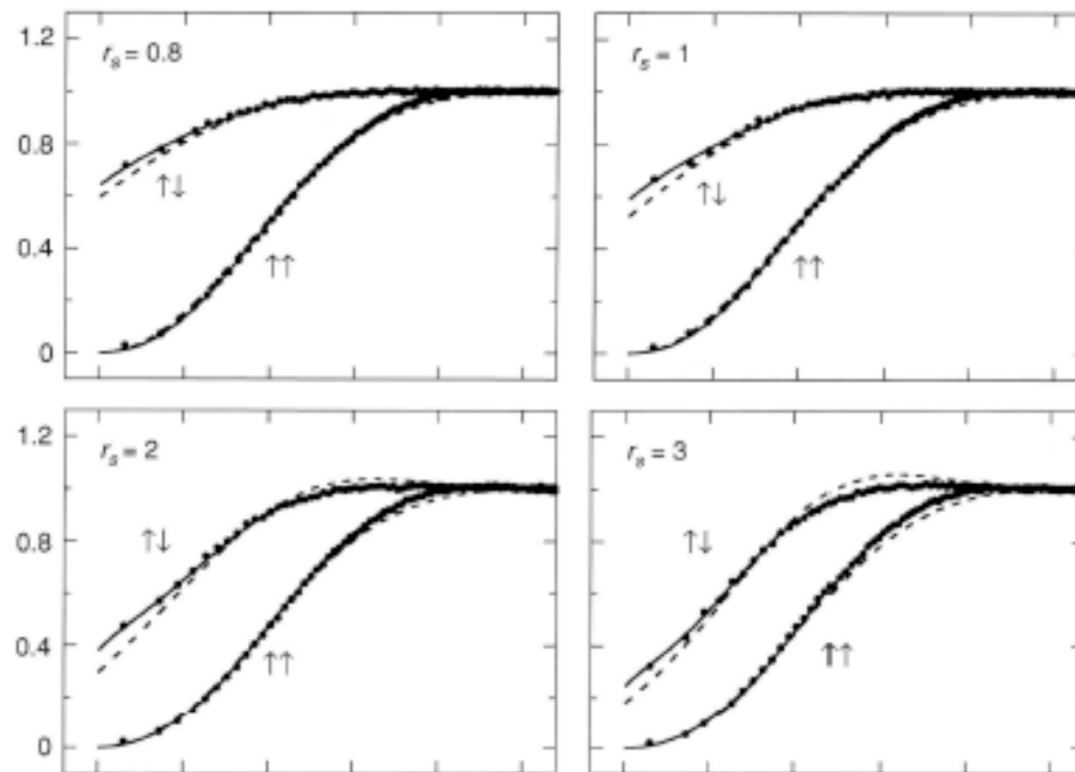
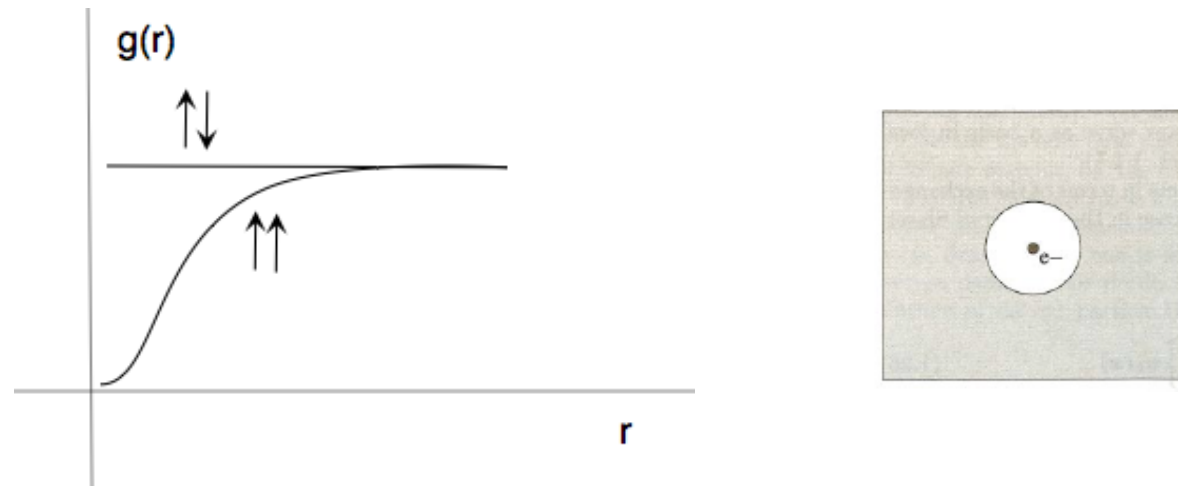
i.e. $n(r) \rightarrow v(r)$ "uniquely" (to within an uninteresting additive constant)



W. Kohn

- Intérêt d'avoir un potentiel effectif local qui décrit aussi les corrélations (par définition: ce qui n'est pas dans Hartree ou échange)
- La DFT fournit un cadre théorique qui permet de justifier une telle construction, du moins pour l'état de base

Trou d'échange et de corrélation



Monte Carlo Q

- ▶ Hartree: néglige toute corrélation dans le mouvement des électrons
- ▶ Hartree-Fock: introduit des corrélations pour des spins parallèles (échange)
- ▶ Très bien pour décrire les effets de magnétisme
- ▶ Pas très bien pour les énergies: trop disymétrique

Equations Kohn Sham et LDA

$$H_{ks}\phi_{\alpha}(\vec{r}) = H_h\phi_{\alpha}(\vec{r}) + V_{xc}(\vec{r})\phi_{\alpha}(\vec{r})$$

$$V_{xc}(\vec{r}) = \frac{\partial E_{xc}[n(\vec{r})]}{\partial n(\vec{r})}$$

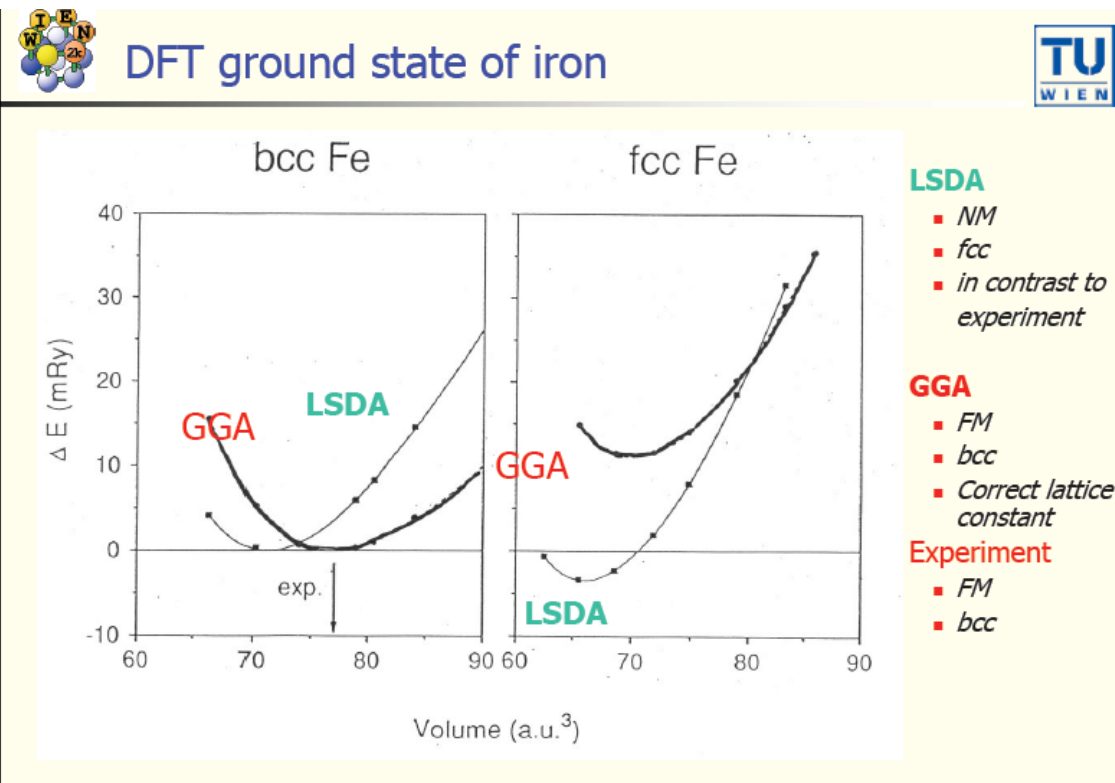
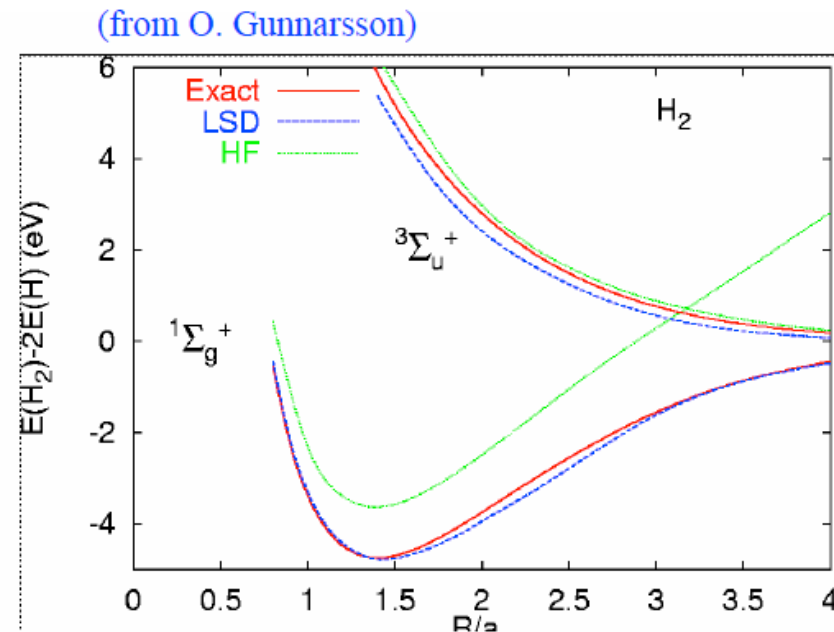
LDA

$$E_{xc}[n(\vec{r})] = \int d\vec{r} n(\vec{r}) \varepsilon_{xc}(n(\vec{r}))$$

- Le potentiel V_{xc} d'échange et de corrélation est défini comme la dérivée de la fonctionnelle (inconnue !) E_{xc} . On n'est donc pas très avancé, mais on sait qu'on peut construire un hamiltonien effectif avec un potentiel local pour décrire l'état fondamental.
- La méthode est une généralisation de l'ancienne méthode Thomas-Fermi
- Si on utilise le potentiel d'un gaz d'électrons en interaction, on retrouve Slater à un facteur 2/3 près !!

Les fonctionnelles

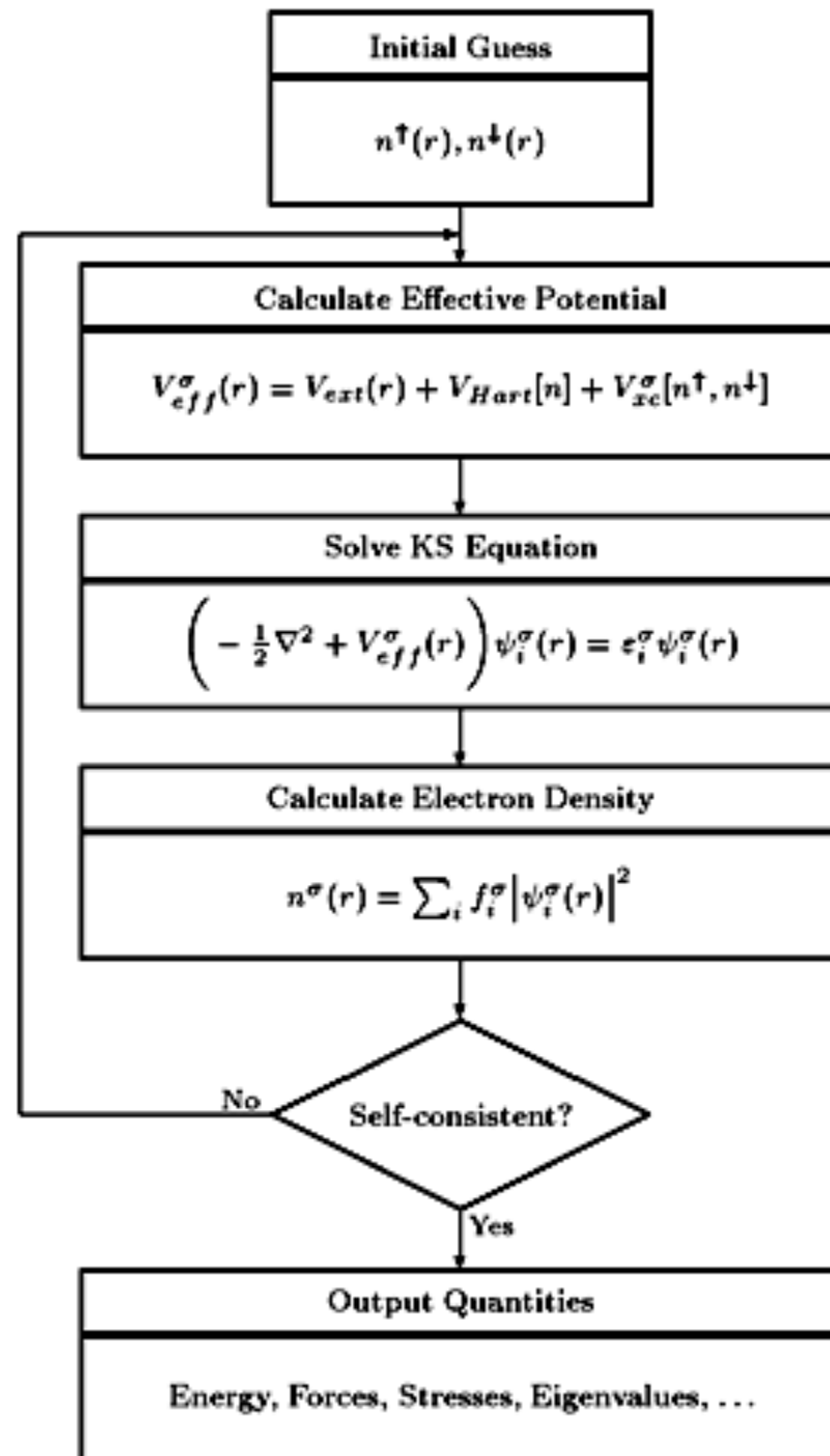
- Hydrogen molecules - using the LSDA



- Possibilité de polarisation de spin (Cf unrestricted HF).
- Plutôt très bon, mais pas toujours suffisant, si la densité varie beaucoup.
- Puis *GGA*, mais beaucoup de variantes
- Autres fonctionnelles: orbital dependent functionals
- Fonctionnelles hybrides: mélange avec échange exact
- PBE0, HSE03, B3LYP, ...

DFT En pratique

Self-Consistent Kohn-Sham Equations



Structure, type of atoms

Guess for input

Solve KS Eqs

New density and potential

Self-consistency

Output

Total enegy, forces,...

Eigenvalues

► Choix de fonctionnelle

► Pseudopotentiels

► Bases

- localisées
- ondes planes

► Dynamique: méthode à la Car-Parinello

Logiciels implémentant la DFT [\[modifier | modifier le code \]](#)

 Article détaillé : [List of quantum chemistry and solid state physics software](#).

- **ABINIT** Site officiel [\[archive \]](#)
- **ADF** Site officiel [\[archive \]](#)
- **AIMPRO** Site officiel [\[archive \]](#)
- **Augmented Spherical Wave** Site officiel [\[archive \]](#)
- **Atomistix Toolkit** Site officiel [\[archive \]](#)
- **CADPAC** Site officiel [\[archive \]](#)
- **CASTEP** Site officiel [\[archive \]](#)
- **CP2K** Site officiel [\[archive \]](#)
- **CPMD** Site officiel [\[archive \]](#)
- **CRYSTAL** Site officiel [\[archive \]](#)
- **DACAPO** Site officiel [\[archive \]](#)
- **DALTON** Site officiel [\[archive \]](#)
- **deMon2K** Site officiel [\[archive \]](#)
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- **DMol3** Site officiel [\[archive \]](#)
- **EXCITING** Site officiel [\[archive \]](#)
- **Fireball** Site officiel [\[archive \]](#)
- **Firefly** Site officiel [\[archive \]](#)
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- **SPR-KKR** Site officiel [\[archive \]](#)
- **TURBOMOLE** Site officiel [\[archive \]](#)
- **VASP** Site officiel [\[archive \]](#)
- **WIEN2k** Site officiel [\[archive \]](#)

DFT : Good

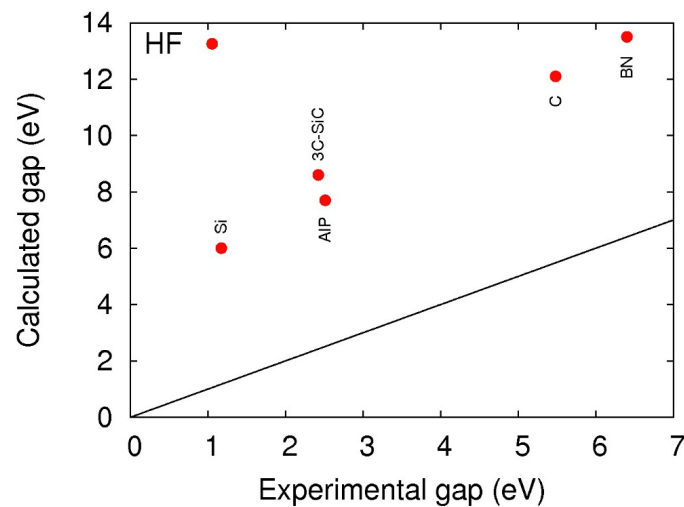
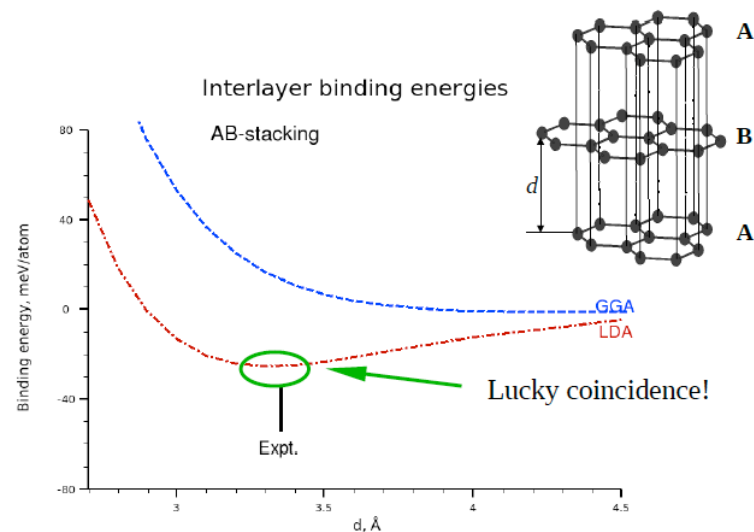
H	Cohesive energy of elemental crystals (GGA/PBE)																He
	ΔE_{coh}																
Li	Be											B	C	N	O	F	Ne
4%	8%											6%	5%	6%	17%	40%	31%
Na	Mg											Al	Si	P	S	Cl	Ar
4%	2%											0%	3%	1%	6%	3%	7%
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
8%	3%	5%	12%	11%	3%	30%	12%	16%	8%	1%	20%	7%	4%	1%	6%	10%	80%
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
10%	7%	5%	0%	9%	9%	1%	2%	2%	6%	16%	37%	9%	0%	2%	10%	15%	84%
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
11%	1%	8%	3%	2%	1%	2%	3%	0%	9%	19%	69%	20%	4%	5%	8%		81%

K. Lejaeghere et al, Critical Reviews in Solid State and Materials Sciences 39, 1 (2014)

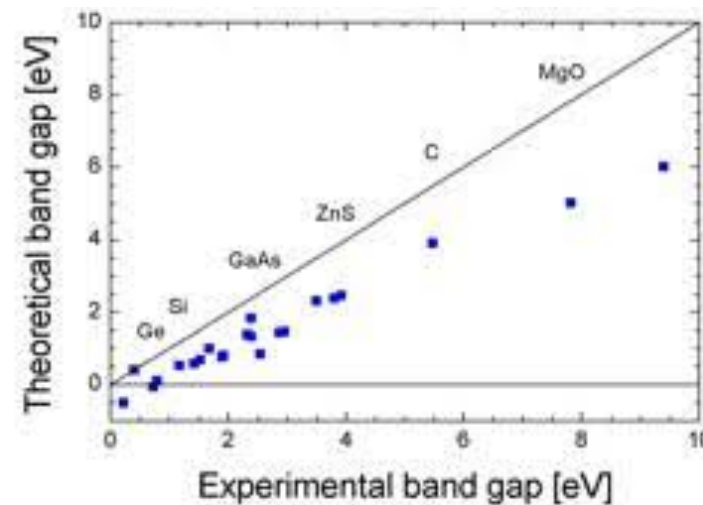
- Beaucoup de codes disponibles efficaces
- Bonnes propriétés
- structurales, élastiques, ...
- Bonne description semi-qualitative de la structure de bande

DFT : Bad

Graphite with GGA and LDA



HF



LDA

► Insuffisant pour les systèmes très corrélés (oxydes de métaux de transition, actinides, ...)

► van der Waals

► Le problème du gap et des excitations électroniques:

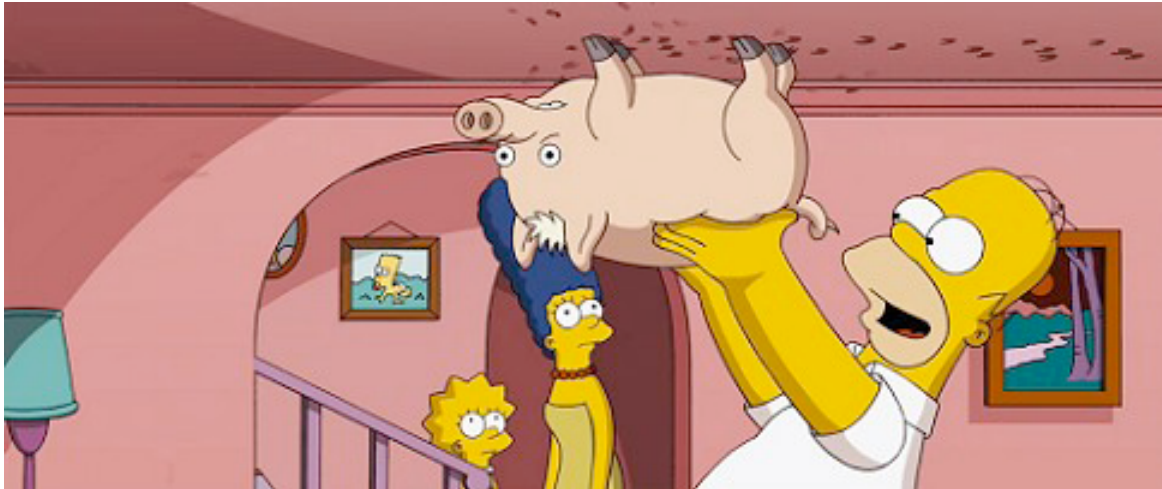
- problème de self interaction en LDA

Une méthode *ab initio* ou semi-empirique ?

Les méthodes basées sur la théorie de la fonctionnelle de la densité sont considérées à l'heure comme une théorie *ab initio* par la plupart des scientifiques. En effet, les théorèmes de Hohenberg et Kohn ainsi que le développement amenant aux équations monoélectroniques de Kohn et Sham sont parfaitement rigoureux et sont obtenus sans avoir recours à d'éventuelles approximations. Cependant, la fonctionnelle d'échange-corrélation apparaissant dans les équations rend toutes résolutions exactes impossibles, sa forme analytique étant inconnue. Comme décrit plus haut, il est donc nécessaire d'approximer cette fonctionnelle soit en formulant une forme mathématique approchée de la fonctionnelle ou bien en *fittant* un certain nombre de données expérimentales. Cette approche est typique des *méthodes semi-empiriques* et la méthode DFT pourrait donc tout aussi bien être classée dans cette catégorie. L'énergie totale en DFT est exprimée en termes dépendant de la densité électronique plutôt qu'en termes de fonctions d'onde. Il est sans doute plus pertinent de considérer la méthode DFT comme une classe à part dans les méthodes numériques de *chimie quantique*.

Wikipedia

van der Waals

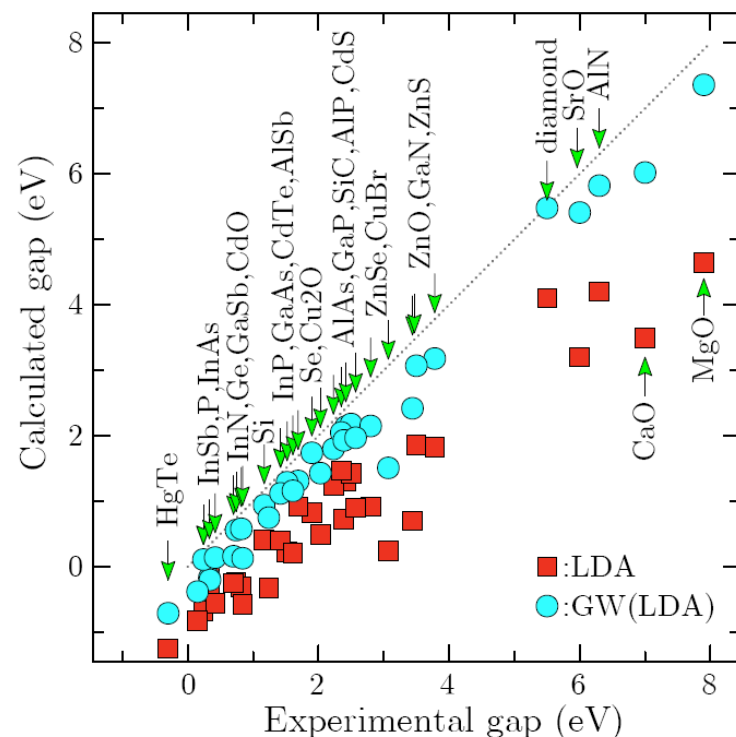
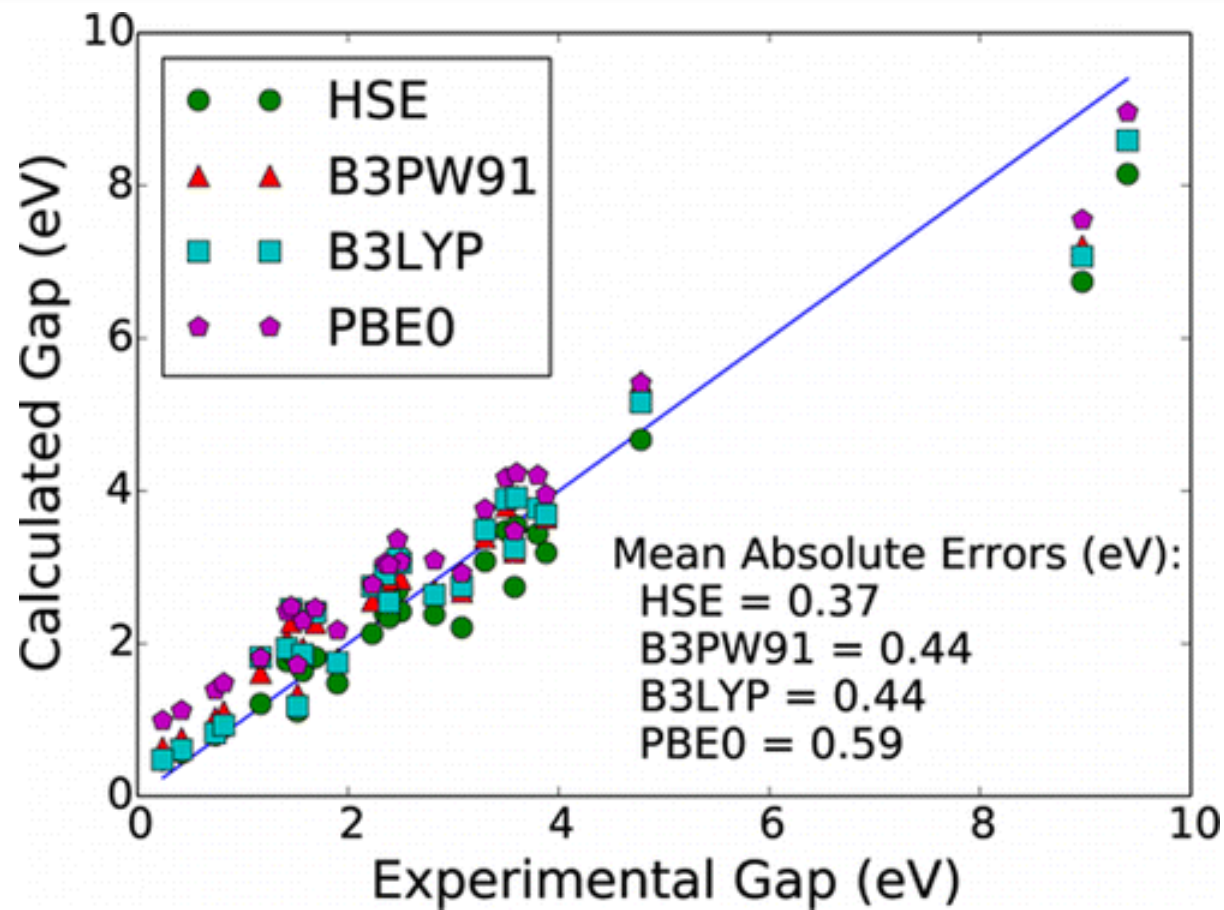


- ▶ Très important en général
- ▶ Pour les solides, systèmes lamellaires, empilements 2D
- ▶ Nécessité de modifier les fonctionnelles ou d'ajouter des interactions effectives

Van der Waals functionals

This page gives hints on how to use Van der Waals functionals with the ABINIT package.

Gap



GW

- Pour améliorer le gap
- orbitales hybrides
- Many Body Perturbation Theory: GW auto-cohérent ou non. Plus compliqué mais plus général

Au-delà de la DFT

MBPT Many Body Perturbation Theory **post HF**
Interactions de configuration

Monte Carlo Quantique

Corrélations fortes:

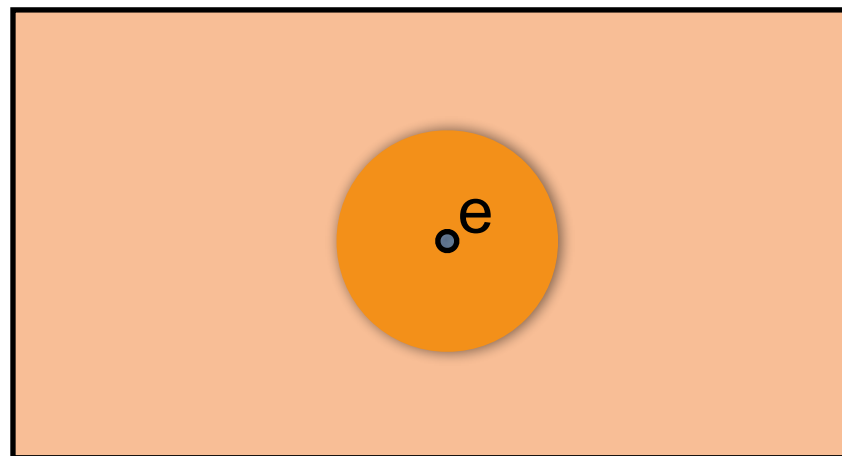
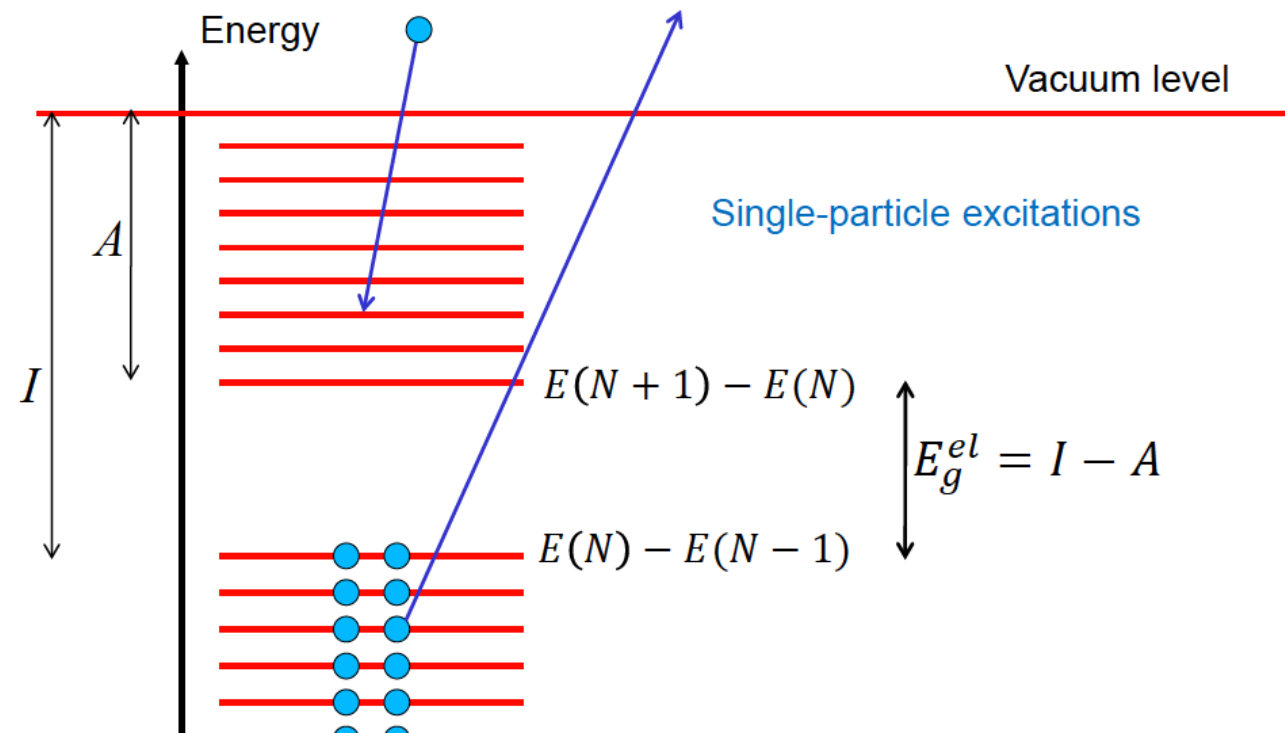
LDA + U

DMFT Dynamic Mean Field Theory

Propriétés optiques

TDDFT Time Dependent Density Functional Theory

BSE Bethe Salpeter Equation



- Excitation à une particule: en Hartree-Fock, les excitations sont fournies par la structure de bande. Dans la DFT ce n'est en principe qu'un intermédiaire de calcul pour l'état de base.
- On ajoute un électron (trou) et on calcule la charge induite et le potentiel induit (self-énergie) par une méthode de perturbation à partir de la DFT = Quasiparticule: électron plus nuage de polarisation. Méthode de fonction de Green (G) et de potentiel écranté (W).
- Inclut des aspects dynamiques (temps de vie). Σ a une partie imaginaire

$$H\phi_{\alpha}(\vec{r}) = H_h\phi_{\alpha}(\vec{r}) + \int d\vec{r}' \Sigma(\vec{r}, \vec{r}', \varepsilon_{\alpha})\phi_{\alpha}(\vec{r}) = \varepsilon_{\alpha}\phi_{\alpha}(\vec{r})$$

Structure électronique et cohésion des solides

Modèles

Wigner-Seitz



In both lithium and sodium, it was found possible to construct a radial potential field $v_c(r)$ having the property that the eigenvalues of the equation

$$-\frac{\hbar^2}{2m}\Delta\psi + v_c(r)\psi = E\psi \quad (1)$$

b. Application of the Cellular Approximation.—All the alkali metals form body-centered cubic lattices for which the polyhedron that should be used in the cellular approximation is the truncated octahedron shown in Fig. 2, Chap. IX. It may be assumed, for simplicity, that these polyhedra can be replaced by spheres of equal volume. The error that is made in doing so can be shown to be negligible and will be discussed below. Since each of the spheres is electrostatically neutral, the coulomb potential in a given cell that arises from any other cell is zero. Hence, all that is necessary is to consider the coulomb field arising from the charge in a given cell in the sphere approximation. For this reason, we shall restrict the following discussion to a single sphere.

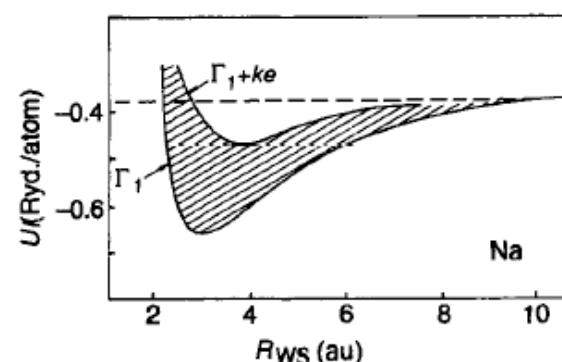


Fig. 5.14 The binding energy U as a function of the Wigner-Seitz radius R_{ws} for sodium. The bottom of the conduction band, Γ_1 , is given by the lower curve to which is added the average kinetic energy per electron (the shaded region). (After Wigner and Seitz (1933).)

- L'idée est que la structure de bandes est semblable à celle d'électrons libres. Il suffit donc de connaître l'énergie en Γ en bas de la parabole.
- La fonction d'onde est périodique: si on garde **le même potentiel** on a juste à changer les conditions aux limites par rapport à l'atome.
- On gagne de l'énergie, même si on doit ajouter de l'énergie cinétique
- Très bons résultats pour les métaux normaux

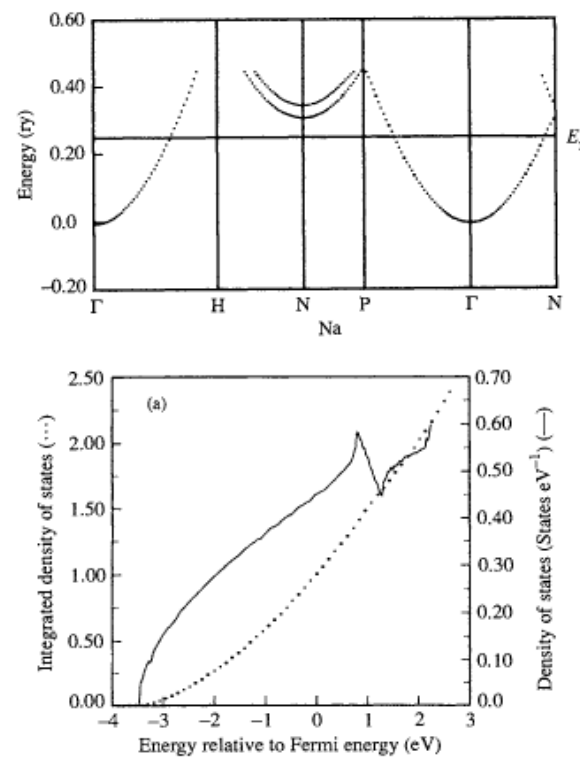
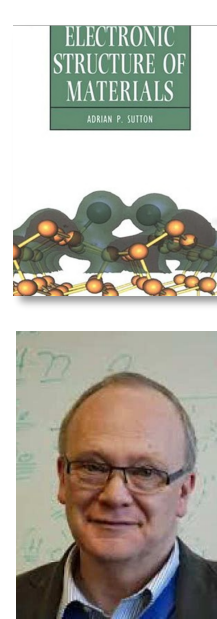


Fig. 7.7 Computed energy bands and densities of states for (a) Na. From Moruzzi *et al.* (1978). *Continued.*

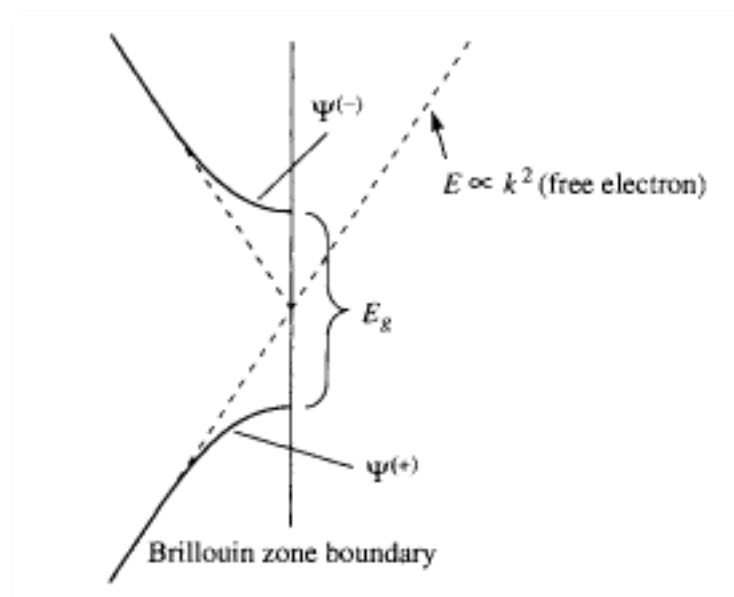


A. Sutton

In a simple metal the pseudopotential of the ion cores is weak. We may apply perturbation theory by regarding the uniform electron gas of the appropriate density as the unperturbed system and the ionic pseudopotentials as the perturbing potential. In the previous section we carried this out to first order in the pseudopotential. To distinguish between the energies of different atomic arrangements of the metal at constant density we must extend the analysis to second order in the pseudopotential. When this is done the cohesive energy per atom may be written in the following physically transparent form

$$E_{\text{coh}} = E_1(r_s) + \frac{1}{2} \sum_{\mathbf{R} \neq 0} \phi(\mathbf{R}, r_s). \quad (8.38)$$

The first term, $E_1(r_s)$, is density dependent and structure independent and accounts for more than 90 per cent of the cohesive energy of the metal. The second term is a sum of pair potentials, and it is this term that distinguishes between the energies of different crystal structures at the same density. The pair potentials are also dependent on the density. In the section on screening



- Calcul en perturbation par rapport au pseudopotentiel: band gaps
- Interactions de paires

Liaisons fortes (Hückel)

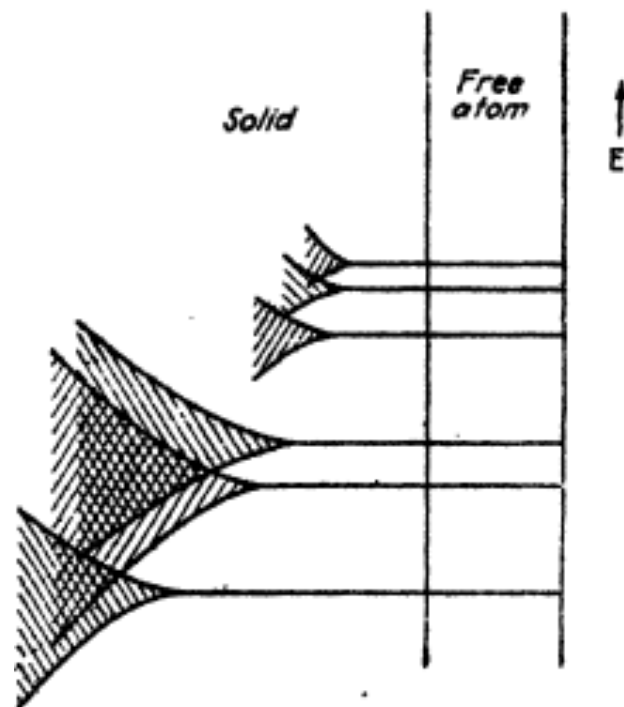


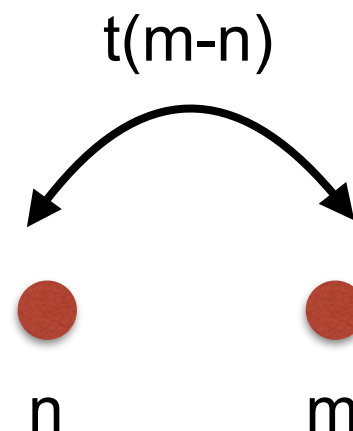
FIG. 19.—The one-electron levels of the free atom split into bands when the atom enters the solid.

- ▶ Bande s pour commencer
- ▶ Base orthonormale
- ▶ On ne garde que les intégrales de saut entre proches voisins
- ▶ Intégrales de dérive, champ cristallin négligées

$$\langle r | n \rangle = \phi(r - n)$$

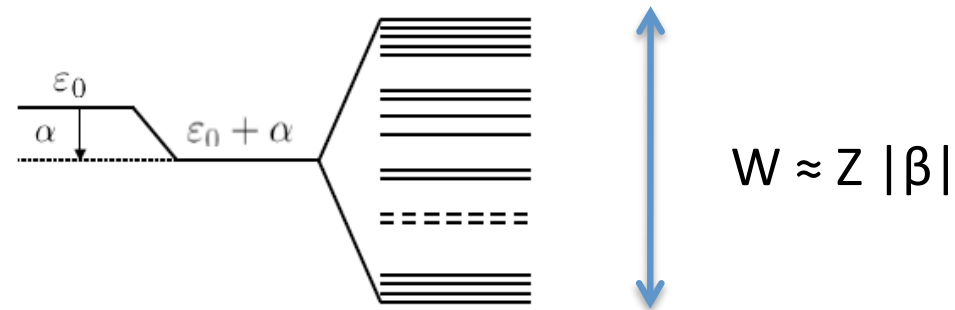
$$\langle n | m \rangle \simeq \delta_{nm}$$

$$\begin{aligned} \langle m | H | n \rangle &= \sum_{p \neq n} \langle m | V_p | n \rangle \simeq \langle m | V_p | n \rangle = t(m - n) \\ &= \int d\vec{r} \phi(\vec{r} - \vec{n}) V(\vec{r} - \vec{n}) \phi(\vec{r} - \vec{m}) < 0 \end{aligned}$$



Structure de bande

C. Barreteau



Let us consider the simple-cubic s band lattice with hopping into only between first neighbours (we will omit λ index).

$$H = \sum_n |n\rangle \varepsilon^0 \langle n| + \sum_{n,m}' |n\rangle \beta \langle m|$$

a) Volume

Bloch States :

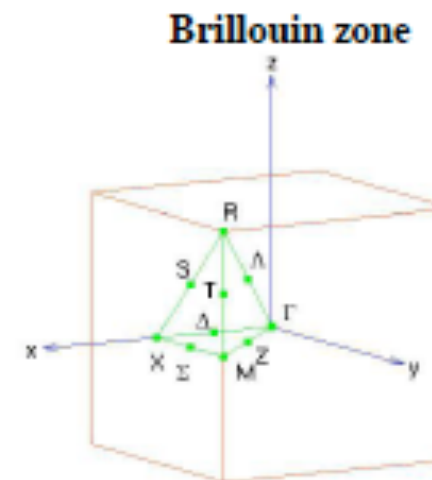
$$|k\rangle = \frac{1}{\sqrt{N_{at}}} \sum_n e^{i\mathbf{k}\cdot\mathbf{n}} |n\rangle$$

A standard calculation then yields :

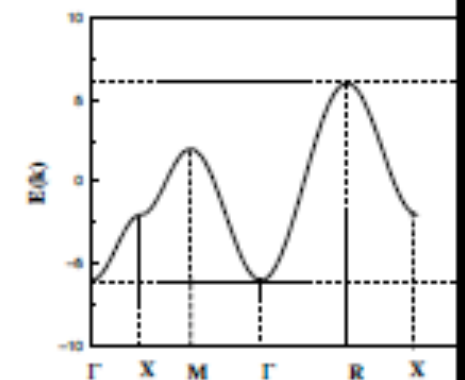
$$H|k\rangle = \varepsilon(\mathbf{k})|k\rangle \quad \text{with} \quad \varepsilon(\mathbf{k}) = E^0 + \beta \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}$$

$\mathbf{R}$: 1st neighbours vector. ($\mathbf{R} = \pm a(1,0,0), \pm a(0,1,0), \pm a(0,0,1)$)

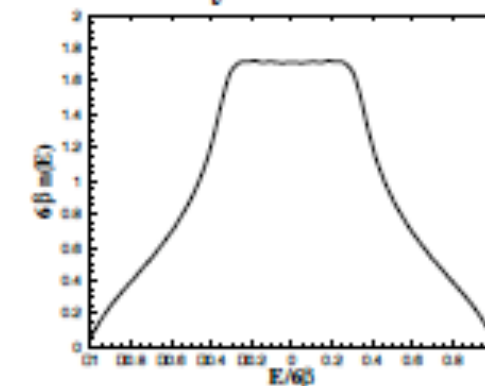
$$\varepsilon(\mathbf{k}) = \varepsilon^0 + 2\beta(\cos k_x a + \cos k_y a + \cos k_z a)$$



band structure

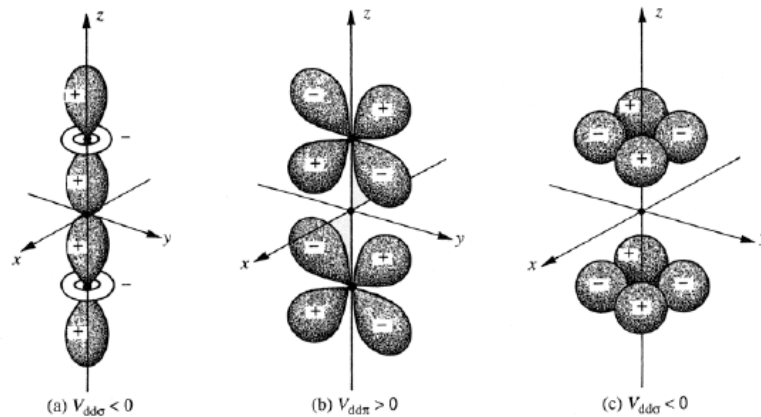
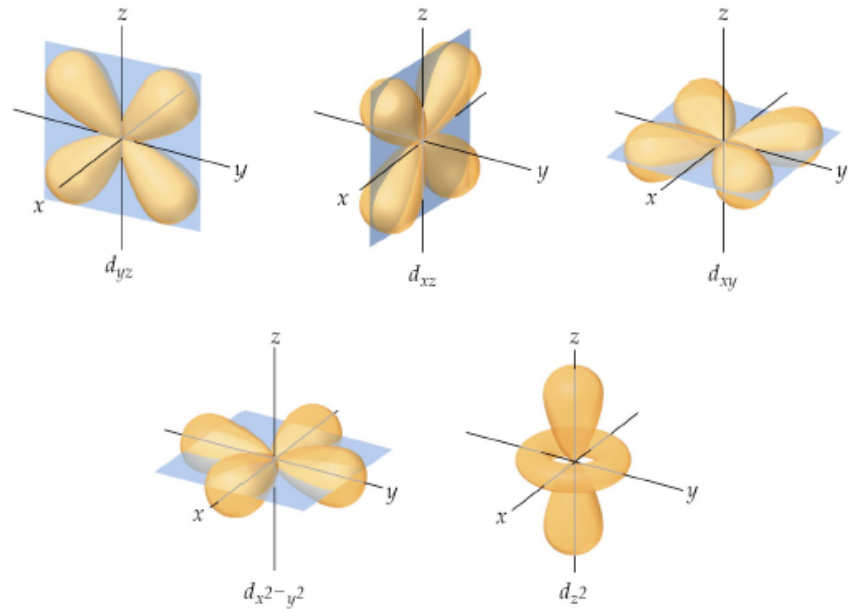


density of states



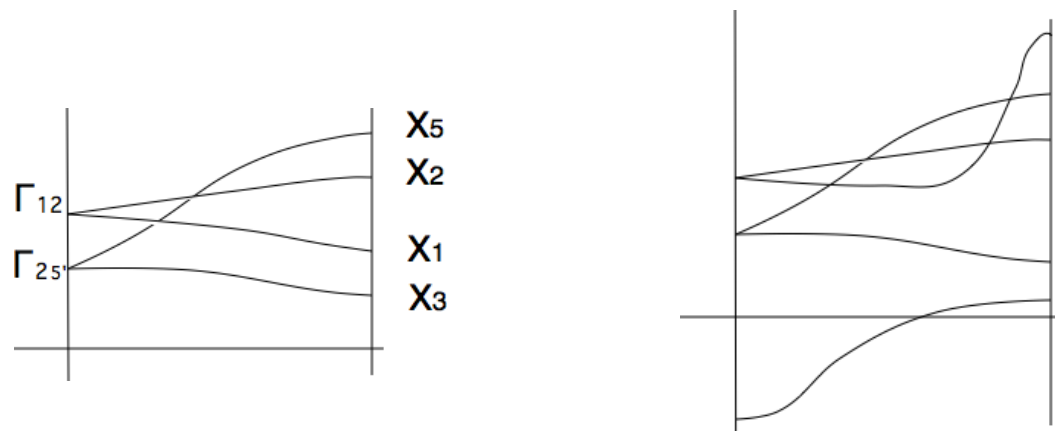
Etats d (métaux de transition)

« d » orbitals

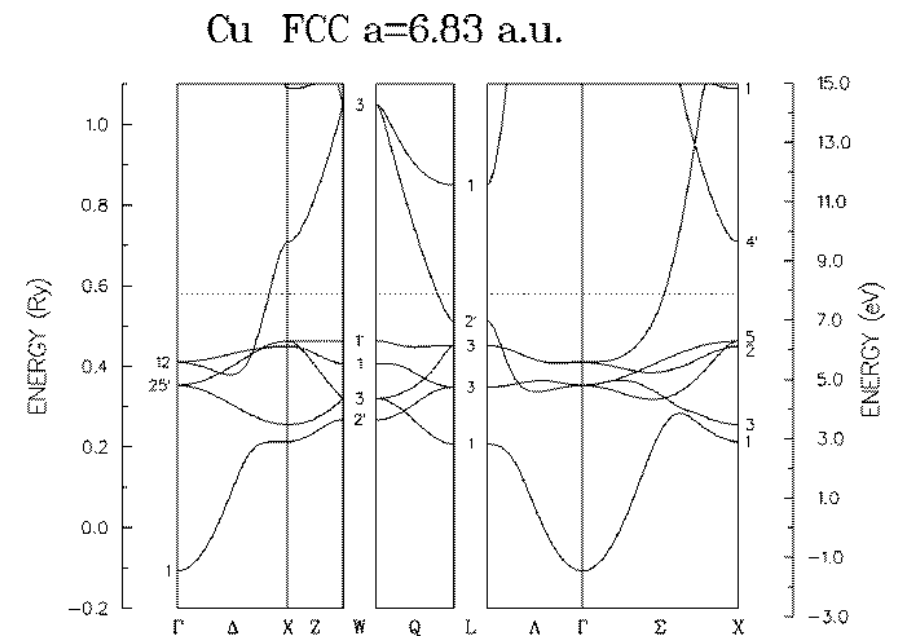
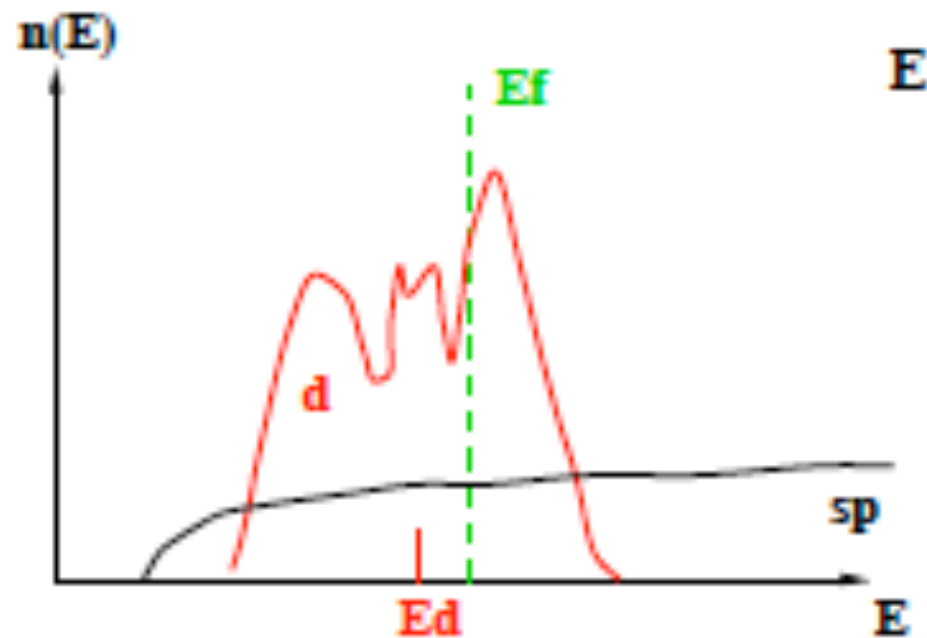


- ▶ Avec potentiel sphérique, trois intégrales de saut indépendantes $dd\sigma$, $dd\pi$, $dd\delta$
- ▶ Valeurs standard (-2,1,0) ou (-6,4,-1)
- ▶ Dépendance angulaire: Tables de Slater-Koster

Structure électronique des métaux de transition



- Bande d étroite avec 10 états sur quelques eV
- Bande sp large avec quelques états



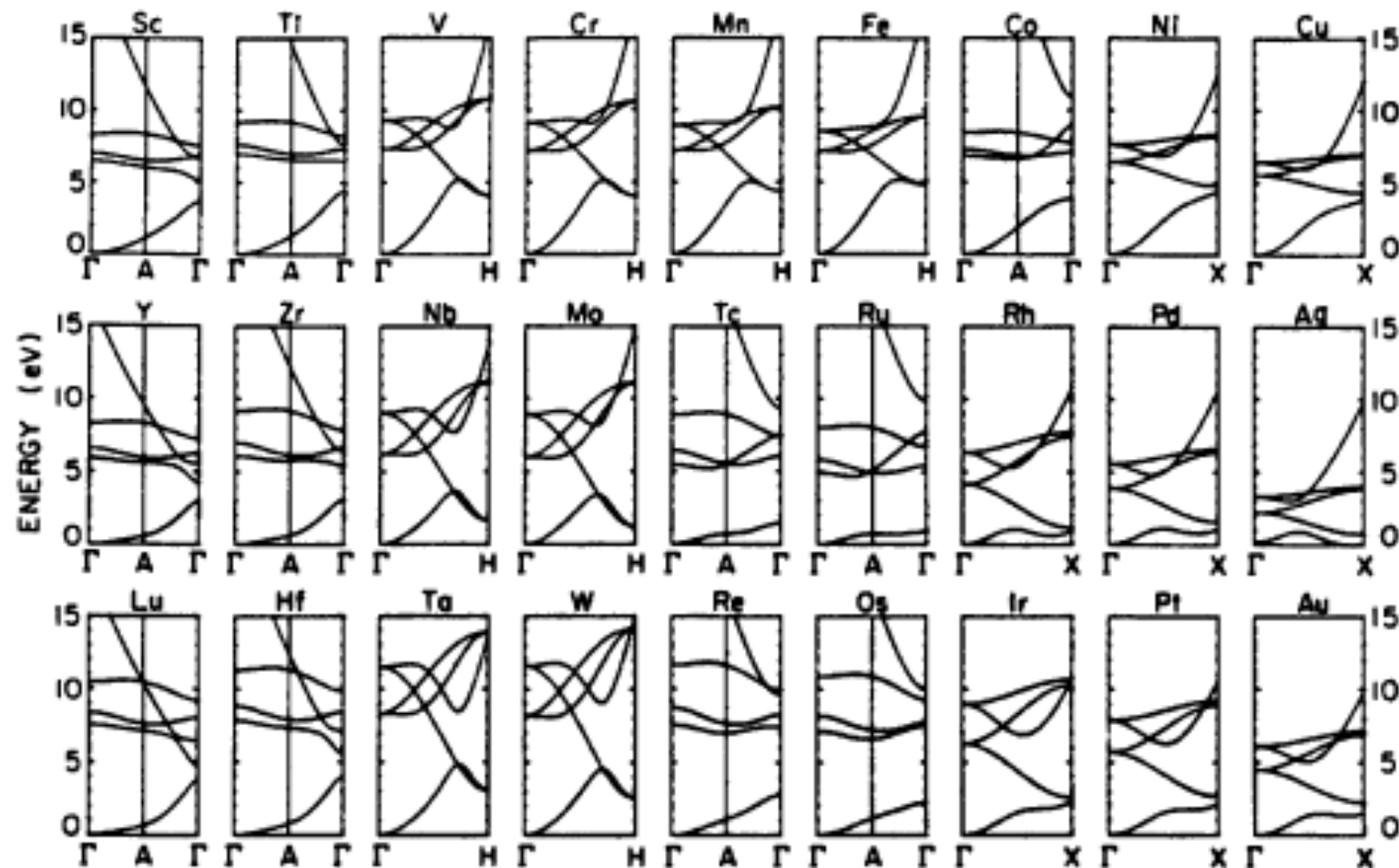


Fig. 15-4. Energy bands for the transition elements, obtained by Froyen, using the approximations described in the text, from Harrison and Froyen (1980). Bands for fcc structures extend from Γ to X, indicated below the figure. For bcc structures they extend from Γ to H. For hcp structures they extend from Γ to A to Γ in a double Brillouin Zone.



W. Harrison

Elementary Electronic Structure

Walter A. Harrison
Department of Applied Physics
Stanford University

World Scientific
Singapore • New Jersey • London • Hong Kong

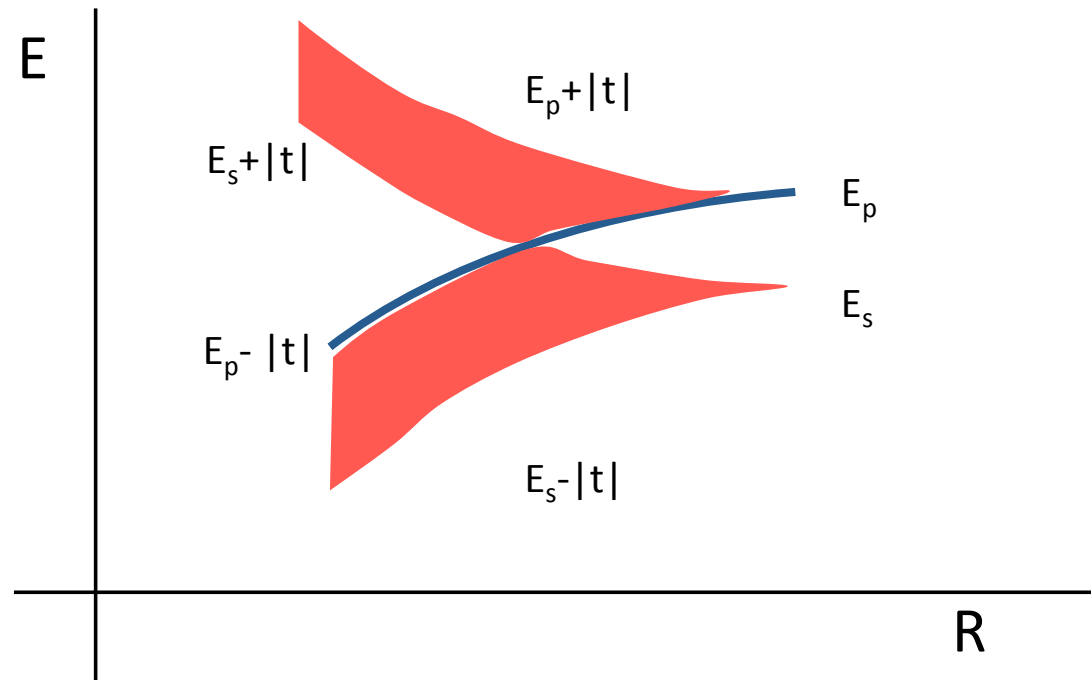
Electronic Structure and the Properties of Solids

THE PHYSICS OF THE CHEMICAL BOND

Walter A. Harrison
STANFORD UNIVERSITY

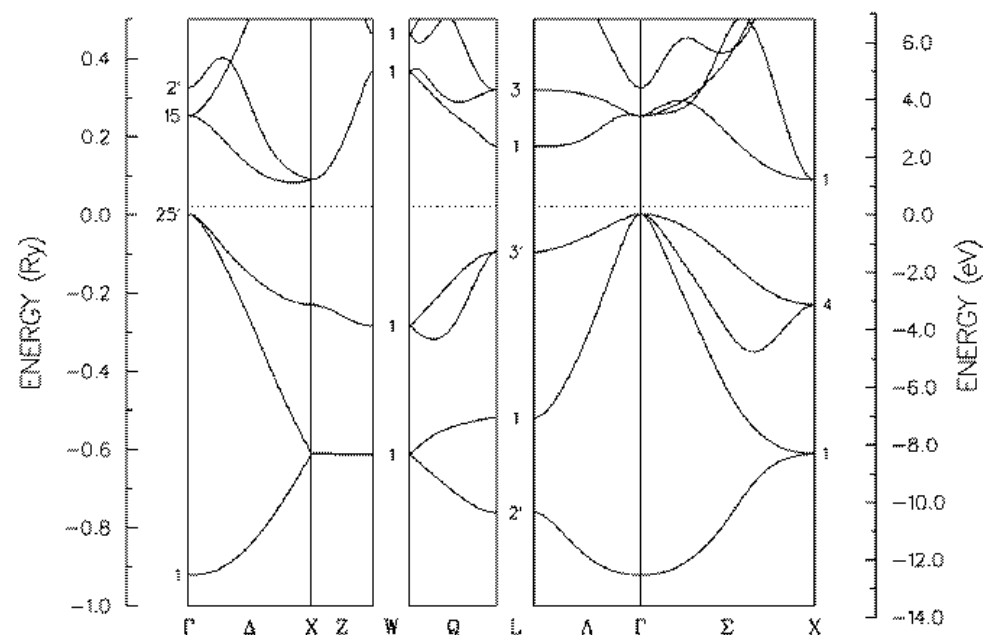
DOVER PUBLICATIONS, INC., New York

Semiconducteurs sp

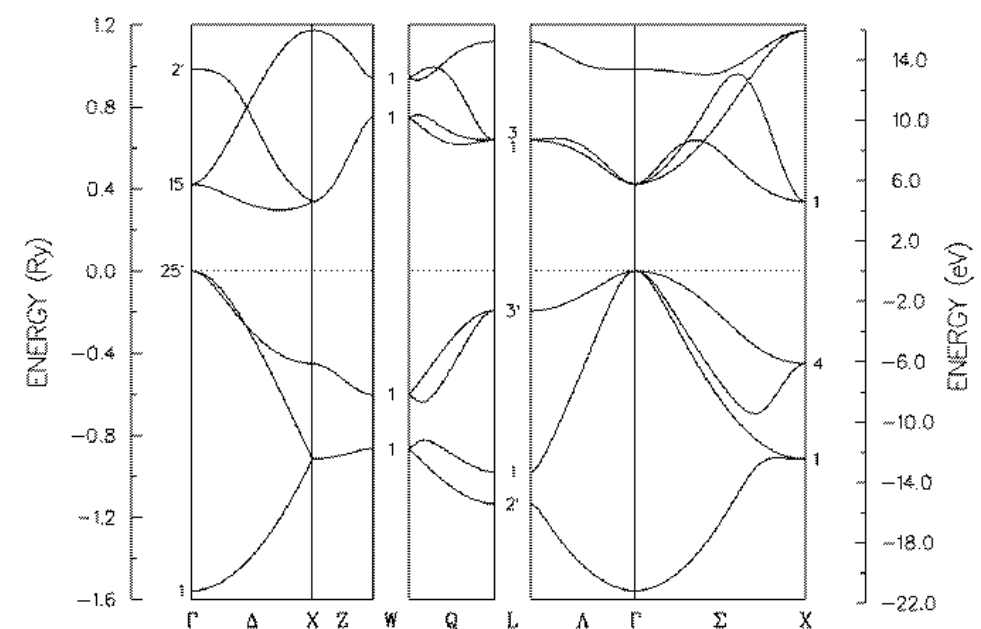


- Analyse similaire avec orbitales s et p
- Orbitales hybrides sp^n
- Le résultat est surprenant et dû à la nature antisymétrique des orbitales p et à la topologie des structures

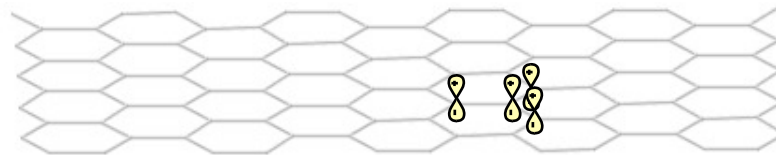
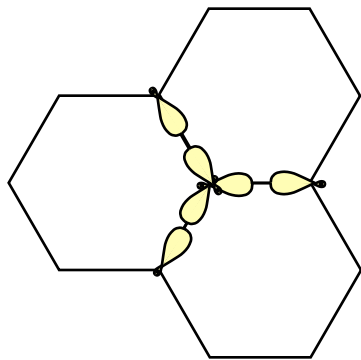
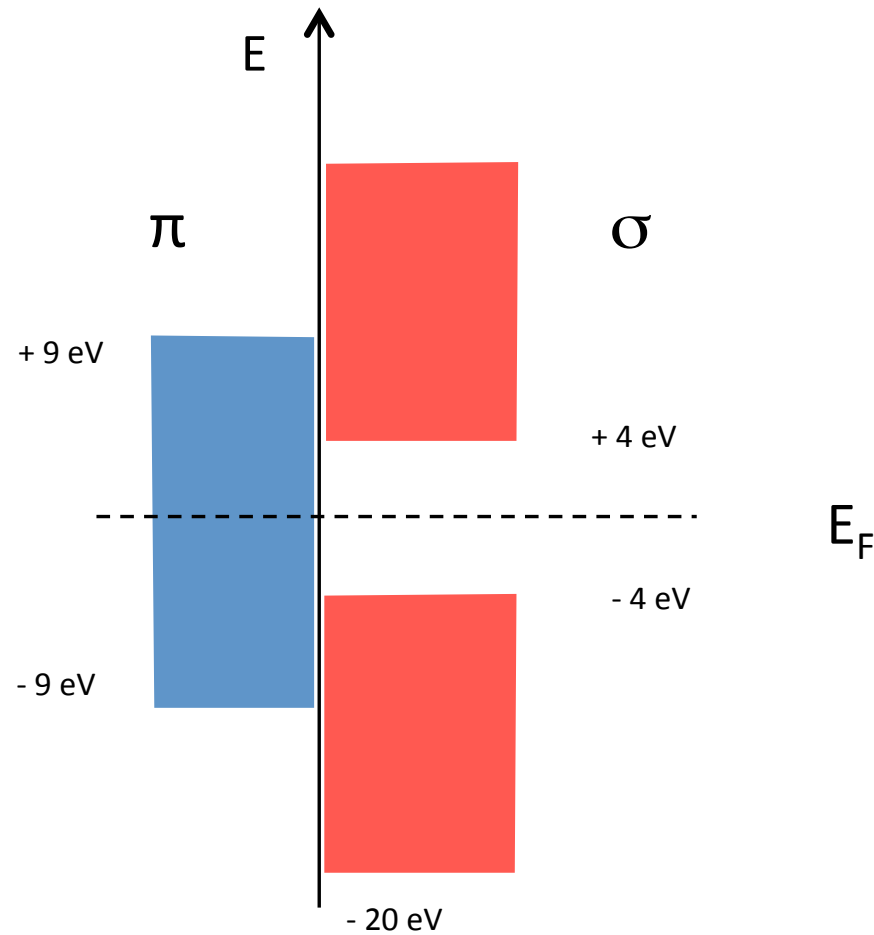
Si Diamond $a=10.26$ a.u.



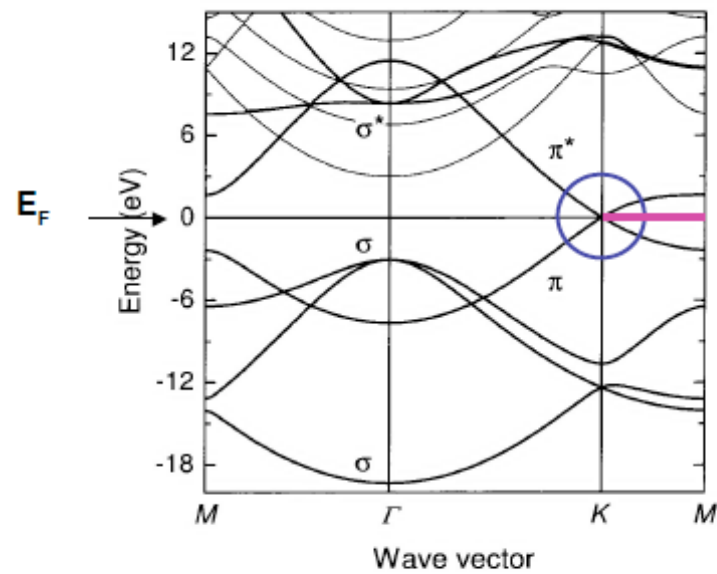
C Diamond $a=6.74$ a.u.



Graphène

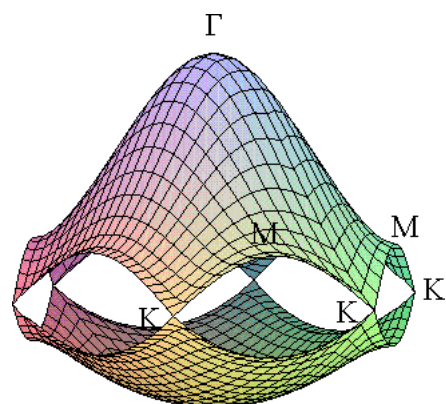
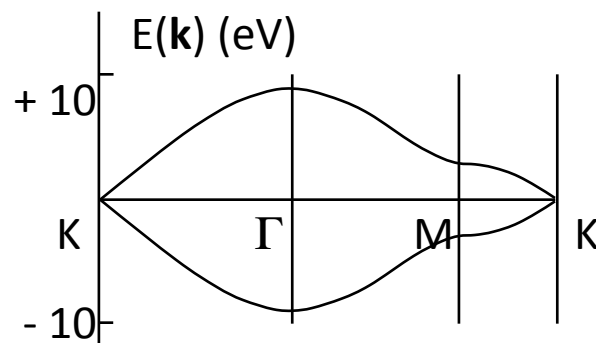


- On se place dans le cas $sp^2 + p_z$, les deux familles d'états étant orthogonales et donnant lieu à des liaisons de type σ et π
- Les liaisons σ fortes et contribuent à la cohésion, au module d'élasticité. Elles produisent un gap d'environ 8 eV à peu près centré sur le niveau de Fermi.
- Les liaisons π sont moins fortes mais fournissent les états au voisinage du niveau de Fermi

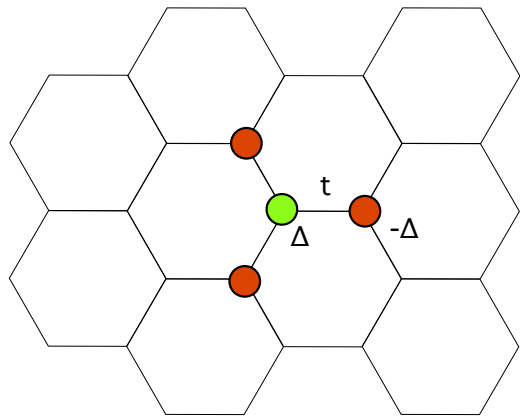


Carbon: atom = $1s^2 2s^2 2p^2$; graphene = $1s^2 (2s 2p^2)_\sigma 2p_\pi$

- Excellent modèle pour les états π
- Pour les états s de la bande de valence également



hBN monofeuillet

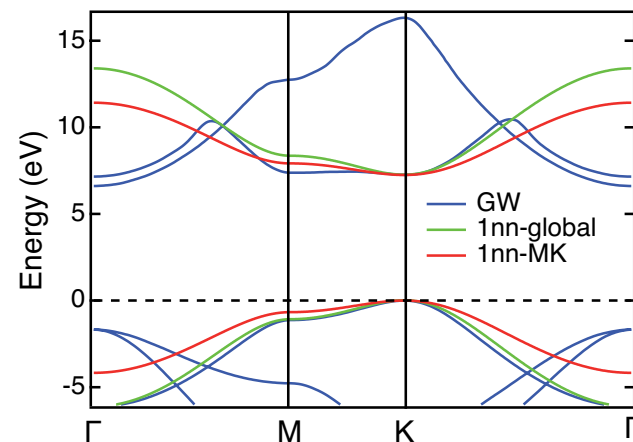


Bore

$$H = \begin{pmatrix} \Delta & -t \gamma(\mathbf{k}) \\ -t \gamma^*(\mathbf{k}) & -\Delta \end{pmatrix}$$

Azote

hBN

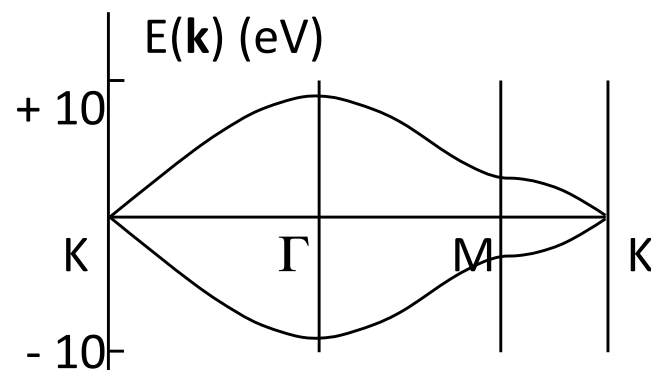


► Comme pour le graphène avec deux niveaux atomiques $\pm \Delta$

► $\text{Gap} = 2\Delta$

► Fit: $pp\pi = 2.3 \text{ eV}$, $\Delta = 3.6 \text{ eV}$

C



Densités d'états, fonction de Green, ...

$$\begin{aligned}n(E) &= \sum_{\alpha} \delta(E - \varepsilon_{\alpha}) \\&= \sum_{\alpha} \langle \alpha | \delta(E - H) | \alpha \rangle = \text{Tr} \delta(E - H)\end{aligned}$$

$$\begin{aligned}n(r, E) &= \langle r | \delta(E - H) | r \rangle \\&= \sum_{\alpha} |\langle \alpha | r \rangle|^2 \delta(E - \varepsilon_{\alpha})\end{aligned}$$

$$\begin{aligned}n(E) &= \int dr n(r, E) \\n(r) &= \int dE f(E) n(r, E)\end{aligned}$$

$$\begin{aligned}\delta(E - \varepsilon_{\alpha}) &= -\frac{\text{Im}}{\pi} \frac{1}{z - \varepsilon_{\alpha}} \quad ; \quad z = E + i0 \\ \delta(E - H) &= -\frac{\text{Im}}{\pi} G(z) \quad ; \quad G(z) = \frac{1}{z - H}\end{aligned}$$

► Densité d'états totale

► Densité d'états partielle

► Résolvante ou fonction de Green

Moments

$$\mu_n = \int dE E^n n(E)$$

pth moment

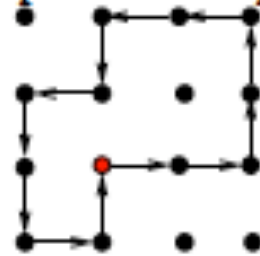
Let $\mu_n^{(p)}$ be the p th moment of the local density of states n_n (let's forget about the orbitals for the sake of simplicity) :

$$\mu_n^{(p)} = \int E^p n_n(E) dE = \int E^p \langle n | \delta(E - H) | n \rangle$$

It comes that :

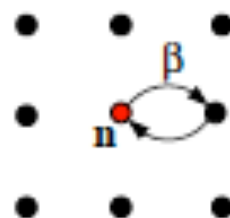
$$\mu_n^{(p)} = \langle n | H^p | n \rangle = \sum_{n_1, n_2, \dots, n_{p-1}} \langle n | H | n_1 \rangle \langle n_1 | H | n_2 \rangle \cdots \langle n_{p-1} | H | n \rangle$$

closed path in real space



Second Moment

$$\mu_n^{(2)} = \langle n | H^2 | n \rangle = \sum_m \beta^2(\mathbf{m}) = Z_n \beta^2$$



rectangular lattice

$$\mu_n^{(2)} = 4 \beta^2$$

Width of the density of states :

$$W_n = \sqrt{\mu_n^{(2)}} = \sqrt{Z_n} |\beta|$$

The width of the local density of states depends on the hopping integrals and on the square root of the number of neighbours.

- Les moments de la densité d'états se calculent en comptant le nombre de chemins fermés (bandes)
- Ceci est vrai pour toute structure (non périodique) !

$$\mu_2 = \sum_R \beta^2(R)$$

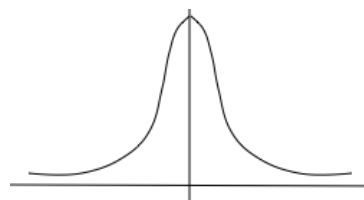
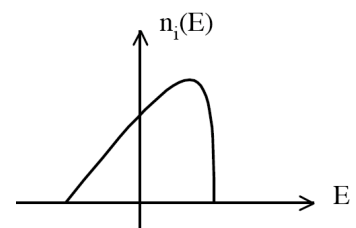
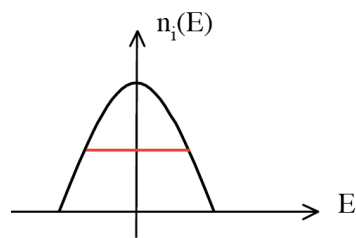
Etats d

$$\mu_2 = \sum_{n,\lambda} \langle n, \lambda | H^2 | n, \lambda \rangle = N(dd\sigma^2 + 2dd\pi^2 + 2dd\delta^2)$$

- ▶ Bande d: base $|n, \lambda \rangle$, $\lambda = 1, \dots, 5$
- ▶ De façon générale, il faut calculer des traces de produits de matrice

Moments

- ▶ μ_0 donne le nombre total d'états
- ▶ μ_1/μ_0 donne le centre de gravité de la distribution
- ▶ μ_2/μ_0 donne la largeur moyenne
- ▶ μ_3/μ_0 reflète l'asymétrie
- ▶ μ_4/μ_0 est sensible à l'importance des ailes



$$\mu_4/\mu_2^2 = 3$$



$$\mu_4/\mu_2^2 = 9/5$$



$$\mu_4/\mu_2^2 = 1$$

Densité d'états à partir des moments

$$\langle n | G | n \rangle = \frac{1}{z - a_1^n - \frac{b_1^n}{z - a_2^n - \frac{b_2^n}{\ddots \frac{b_N^n}{z - a_N^n - b_N^n \Sigma(z)}}}}$$



Thomas Joannes Stieltjes

Born 29 December 1856(1856-12-29)
 Zwolle, Netherlands
 Died 31 December 1894 (aged 38)
 Toulouse, France
 Fields Mathematician

- Problème des moments (Stielges 1894)
- Fraction continue à n étages:
 « meilleure » approximation de $G(z)$,
 connaissant ses $2n$ premiers moments
 (problème des moments)
- Algorithme de récursion très efficace
- Les coefficients sont reliés aux moments, mais ne ne sont pas des fonctionnelles linéaires de la densité d'états

Energie

$$\Delta U = U - U^{at} \simeq \Delta U^{band} + \frac{1}{2} \sum_{n \neq m} \int dr dr' \frac{Q_n(r) Q_m(r')}{|r - r'|}$$

$$E_{band} = \int dE f(E) (E - \varepsilon_0) n(E)$$

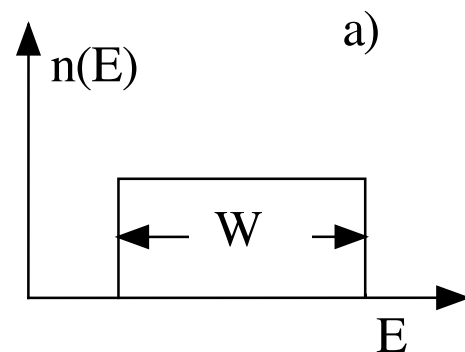
- ▶ En principe l'énergie n'est pas la somme des énergies de bande
- ▶ En pratique dans l'approximation des liaisons fortes, on montre que c'est à peu près vrai à condition d'ajouter un terme répulsif interatomique. Qn est la charge de l'atome neutre en n
- ▶ Il faut ajouter des contributions d'échange et de corrélation
- ▶ En pratique ce terme répulsif sera ajusté de façon empirique

$$U = E_{rep} + E_{band}$$

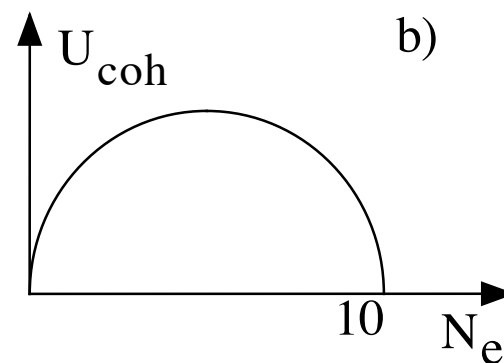
$$E_b \sim \sqrt{\mu_2} g(E_F / \sqrt{\mu_2})$$

$$N_e \sim h(E_F / \sqrt{\mu_2})$$

$$E_b \sim \sqrt{\mu_2} f(N_e)$$



modèle de Friedel



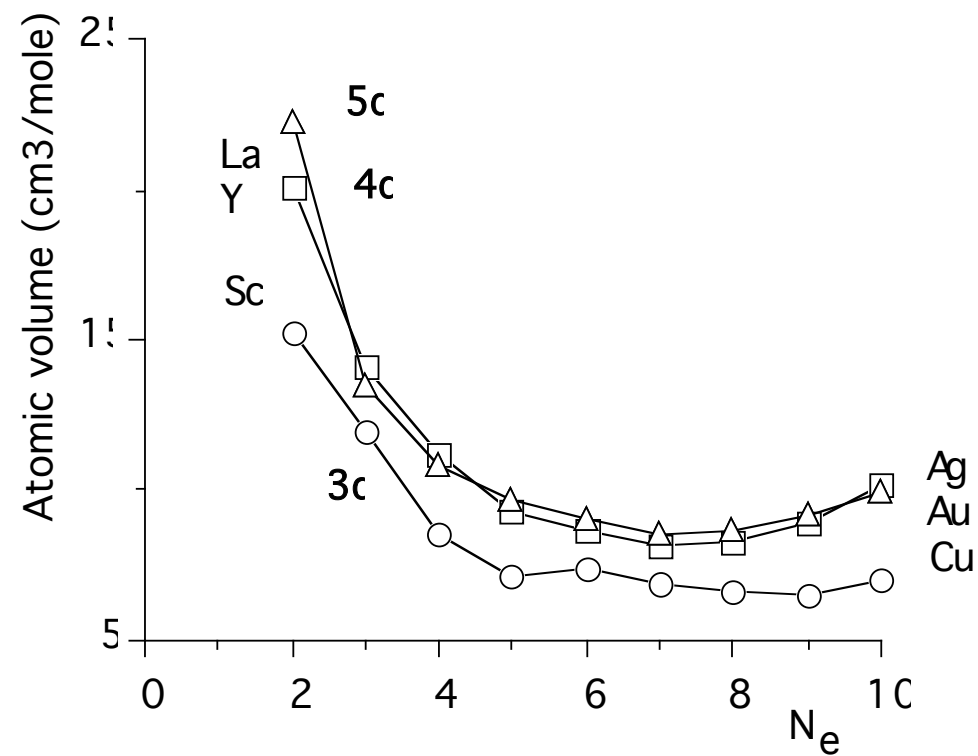
$$E_b = -N_e(1 - N_e)\sqrt{\mu_2}$$

- ▶ On ajoute un terme répulsif phénoménologique et on remplace $n(E)$ par une courbe normalisée, centrée, de second moment fixé
- ▶ L'échelle d'énergie est fixée par la racine carrée de μ_2 .
- ▶ Loi en $\sqrt{Z}$!
- ▶ L'énergie de bande par liaison varie en $1/\sqrt{Z}$ et se renforce donc quand on coupe des liaisons
- ▶ Typique d'un solide avec spectre continu
- ▶ Simple, mais explique beaucoup de chose

Energie de cohésion

$$U = E_r + E_b = - \sqrt{\sum_R dd\beta^2(R) f(N_e)} + \sum_R \Phi_{rep}(R)$$

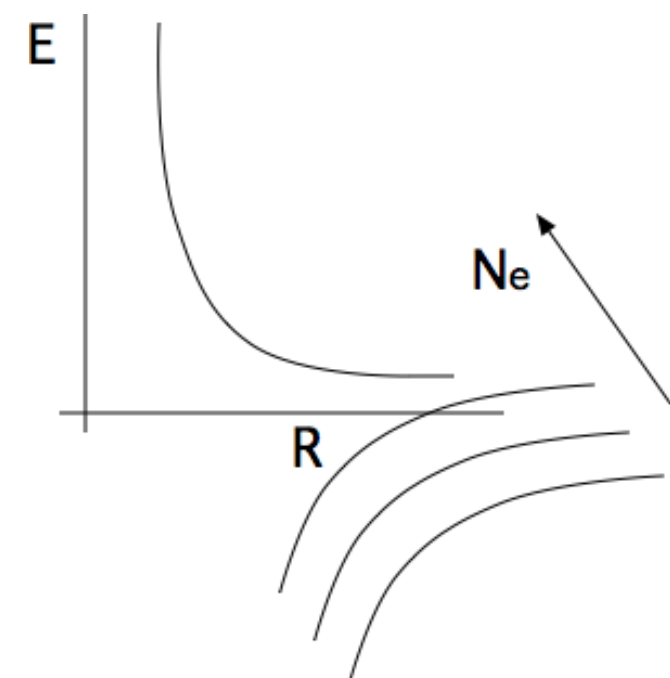
$$dd\beta(R) \sim e^{-qR} \quad ; \quad \phi(R) \sim e^{-pR}$$

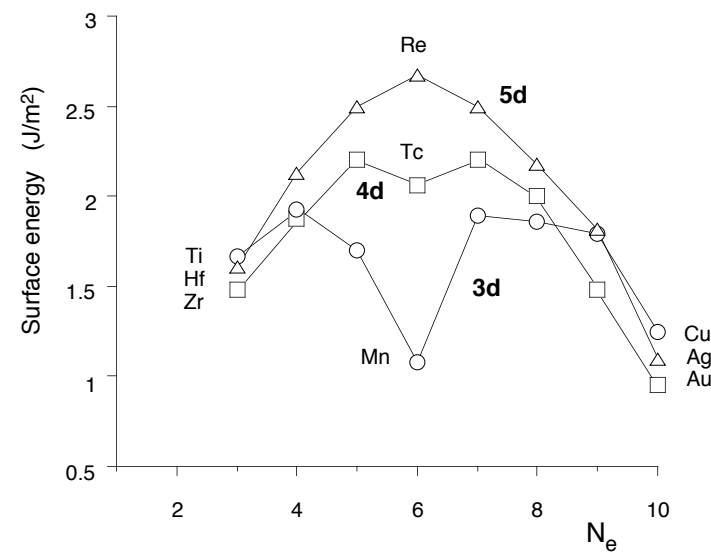
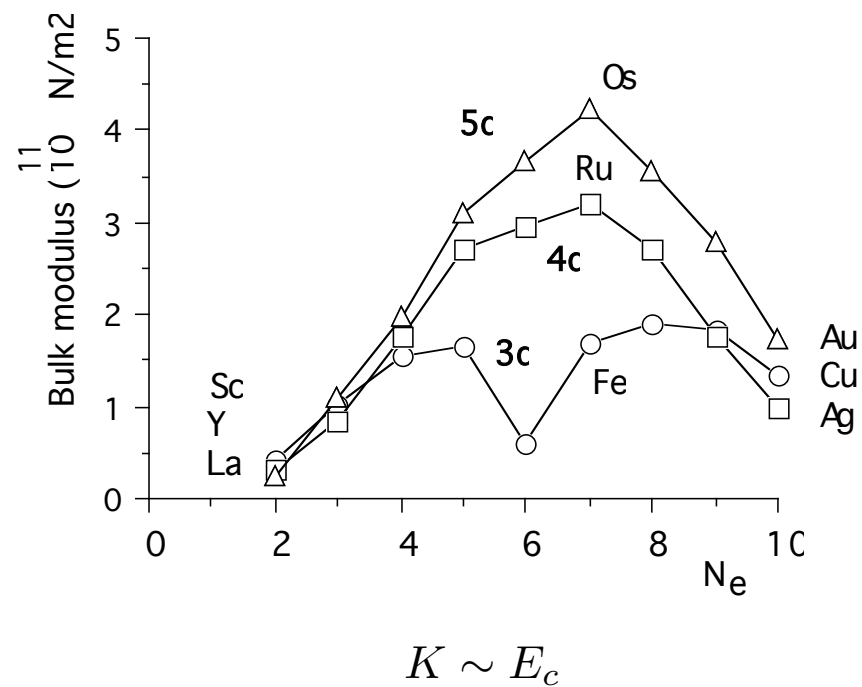
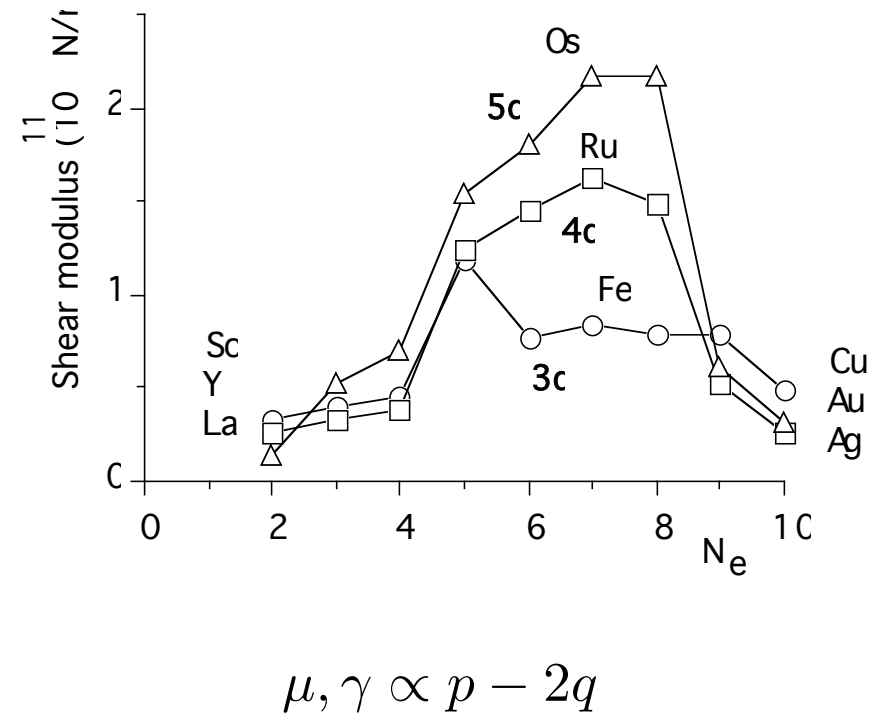
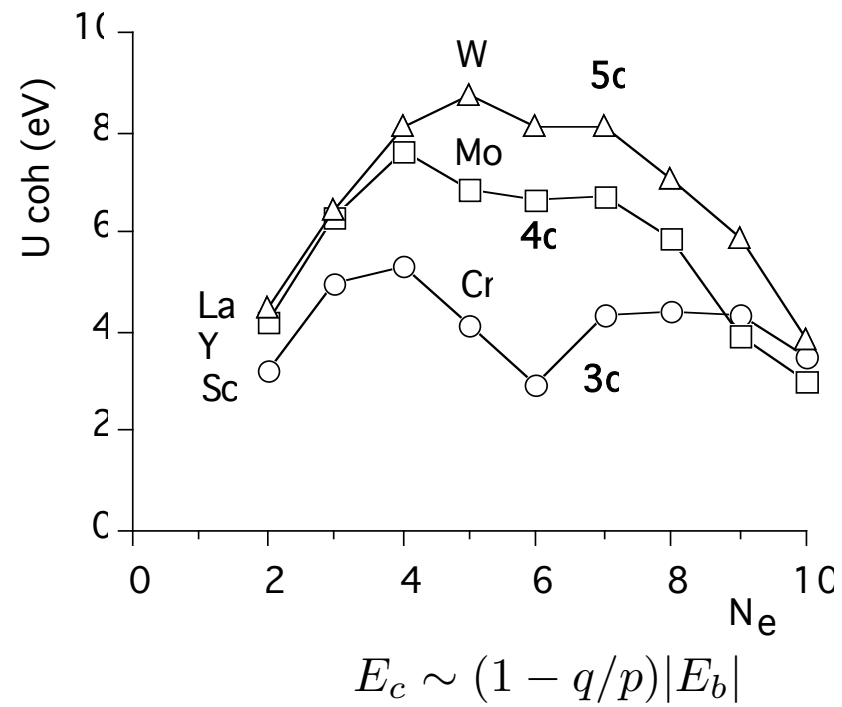


► Dépendance en R ?

► p/q de l'ordre de 3 à 5 pour les métaux de transition

► Moins pour sp





- Influences variées du terme attractif et du terme répulsif
- Constantes de cisaillement particulières

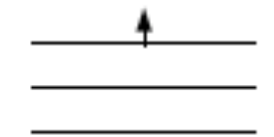
Lacune, relaxation de surface

$$U_{lac} \simeq \frac{1}{2} \frac{p - 2q}{p - q} |U/N|$$

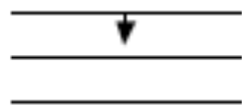
Table 2.
Vacancy formation
energies; after
Rosato et
al.(1989).

Energies (eV)	Ni	Pd	Pt
U/N	4.4	3.9	5.9
U _{vac} (theor.)	1.5	1.0	1.3
U _{vac} (exp.)	1.5 - 1.7		1.2 - 1.5

- Et donc $U_{lac} \approx \frac{1}{4} (U/N)$ au lieu de 1 pour un modèle de liaisons coupées
- Remarque: calculs ab initio difficiles !



Pair interactions



Second moment and
experiment

Fig.12. Relaxation of simple
surfaces of transition
metals.

Dépendance en Z

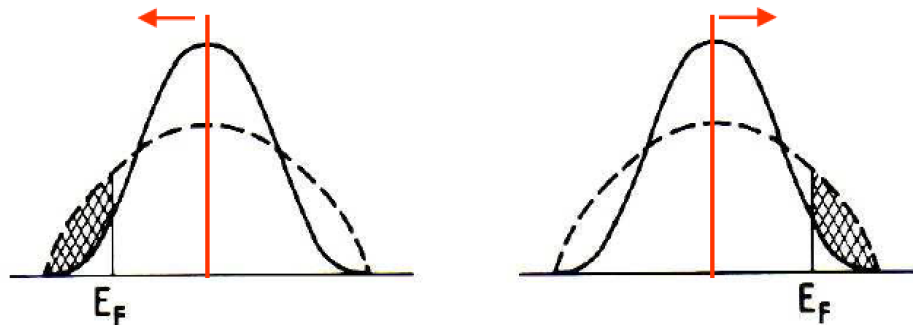
$$E_c \sim Z^{\frac{1}{2} \frac{p-2q}{p-q}}$$

Argument de J.-P. Gaspard

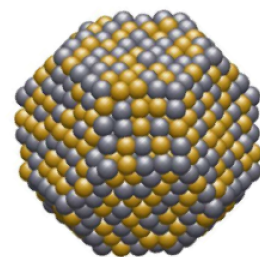
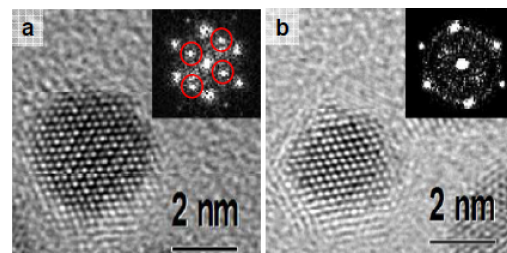


- ▶ En tenant compte du terme répulsif
- ▶ Très sensible à la valeur de p/q
- ▶ Le cas $p/q=2$ est spécial et ... dangereux
- ▶ p/q est plus petit dans le cas des covalents et peut favoriser des faibles coordinences

Autres applications



G. Tréglia et al. Ecole Fréjus 2010



Ch. Mottet Ecole Istres 2015

- Propriétés de surface (reconstruction)
- Densité d'état locale, transferts de charge
- Autocohérence: pour les métaux modification des niveaux atomiques pour assurer la neutralité locale
- Hybridation sd (Ch Goyhenex et al.)
- Magnétisme
- Agrégats (Ch Mottet et al.)
- Alliages
- Etc.

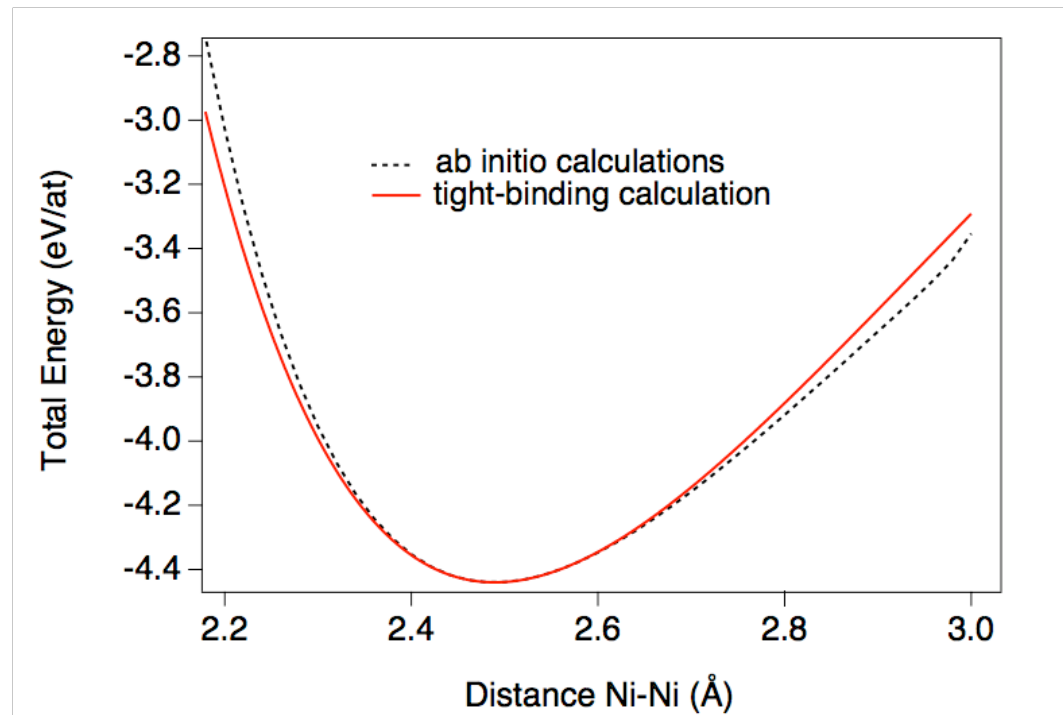
Relaxation des structures

$$U = E_r + E_b = - \sqrt{\sum_R dd\beta^2(R) f(N_e)} + \sum_R \Phi_{rep}(R)$$

- ▶ Pour un système non homogène, on peut écrire une telle formule en chaque site
- ▶ Mais il y a le problème des transferts de charges et le problème de les traiter de façon autocohérente
- ▶ Une bonne règle dans les métaux est de « forcer » la neutralité locale
- ▶ Se généralise aux covalents (plusieurs niveaux atomiques) et aux alliages

Comment fait-on ?

Nickel



	Structure	Lattice parameter (Å)	Cohesive energy (eV/atom)	B (GPa)	C' (GPa)	C_{44} (GPa)	Surface energy (mJ/m ²)
Ni	fcc	$a/\sqrt{2}=2.489$	-4.44	187.6	55.2	131.7	1840 (solid) 2385 (liquid)
This work	fcc	$a/\sqrt{2}=2.489$	-4.44	182.1	68.8	96.9	1660 (100) 1560 (111)

- Structure électronique ajustée (niveaux atomiques, intégrales de saut)
- + terme répulsif
- Ajustement sur volume atomique, cohésion, constantes élastiques, grandeurs pertinentes (lacune, surface, ...)
- Cas du nickel: bon accord avec 6 paramètres

Relaxation des structures

$$U = E_r + E_b = - \sqrt{\sum_R dd\beta^2(R) f(N_e)} + \sum_R \Phi_{rep}(R)$$

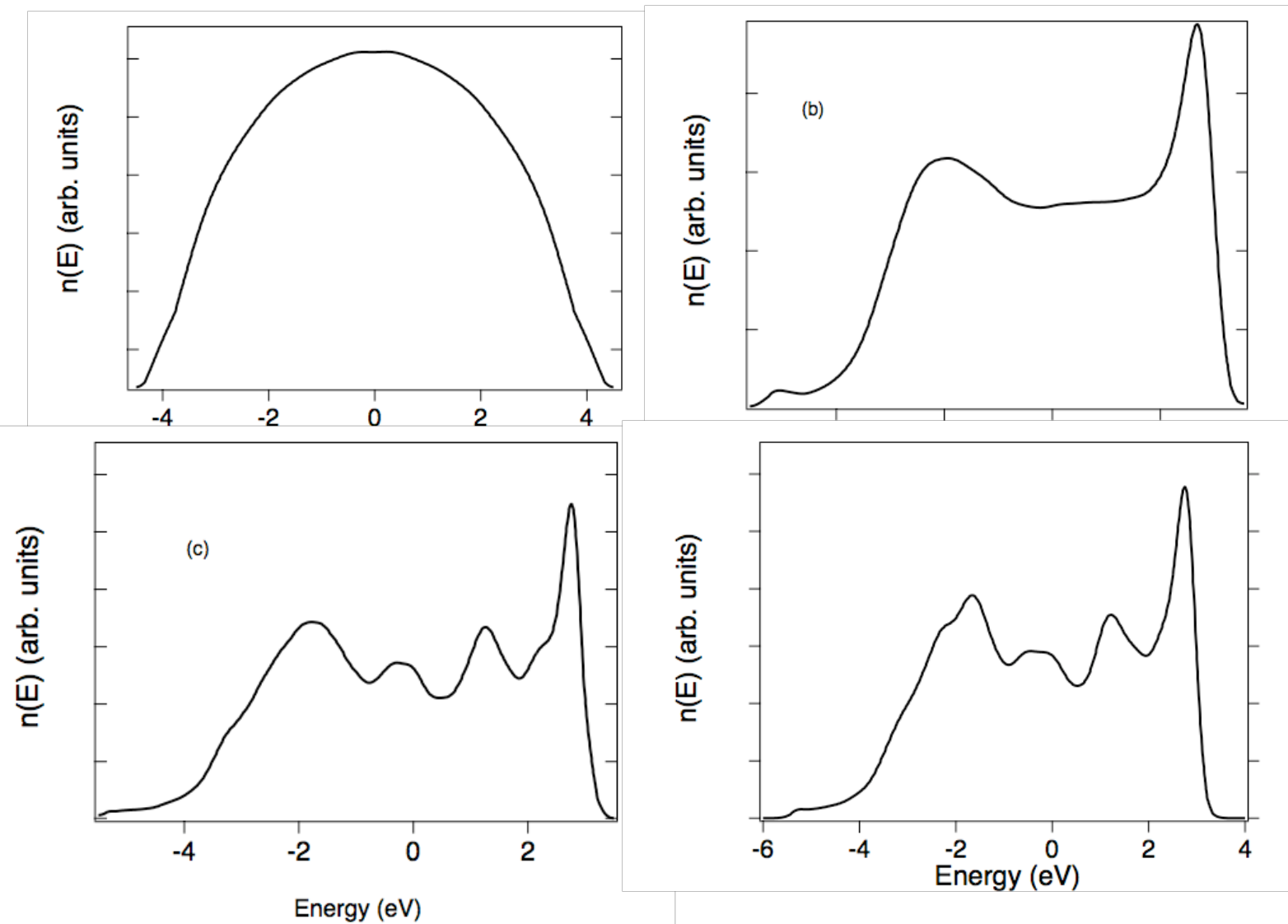
- ▶ Ne s'applique (en principe ...) que quand l'approximation des liaisons fortes est légitime
- ▶ Portée limitée en principe, mais modèle de Finnis-Sinclair ...
- ▶ Ne s'applique pas aux alliages et aux effets de structure fins: plus de moments sont nécessaires !
- ▶ L'EAM est une méthode complètement phénoménologique qui remplace le terme de second moment par un terme de même type (fonction n on linéaire en Z)? Voir Marinica Istres 2015.

$$E^i = E_{paire}^i + F(\rho_i)$$

Mendelev et al. (2003):

$$F(\rho_i) = -\sqrt{\rho_i} + a\rho_i^2$$

Au-delà du second moment



- ▶ Quand on tient compte de plus de moments (récursion) la densité d'états change mais pas tellement l'énergie de bande (intégrale)
- ▶ Second moment: précision de quelques 0.1 eV, à comparer à quelques eV pour l'énergie totale
- ▶ Meilleure précision nécessaire pour les variations d'énergie, entre structures par exemple

CFC-HCP

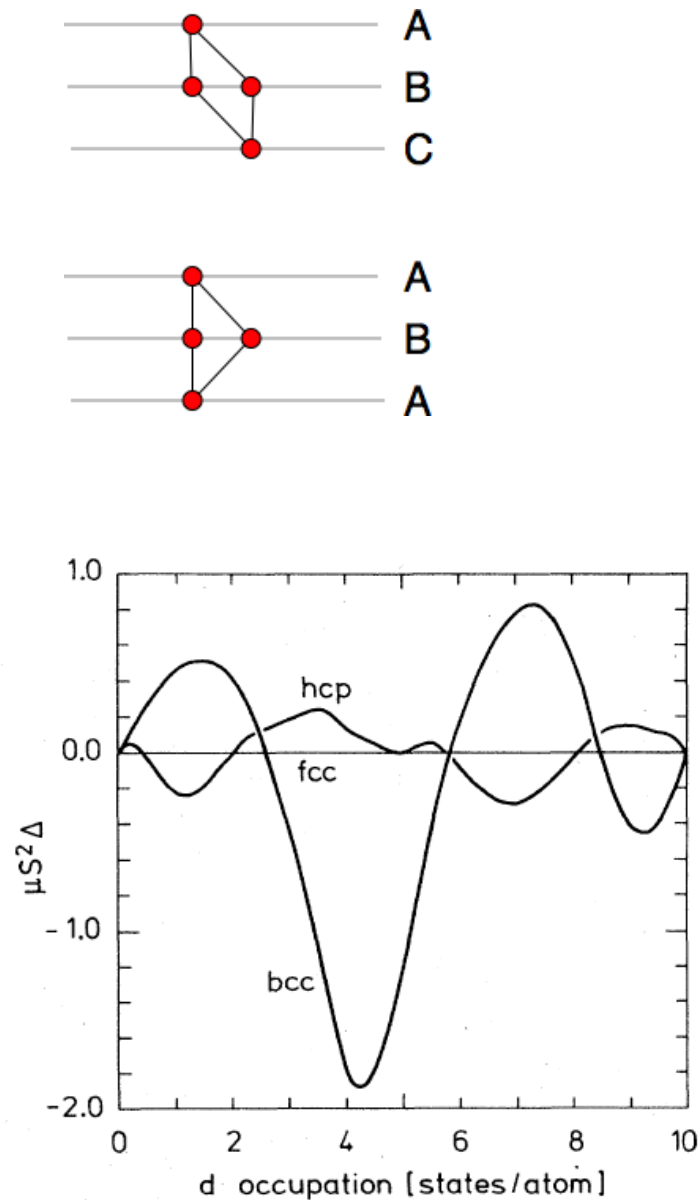
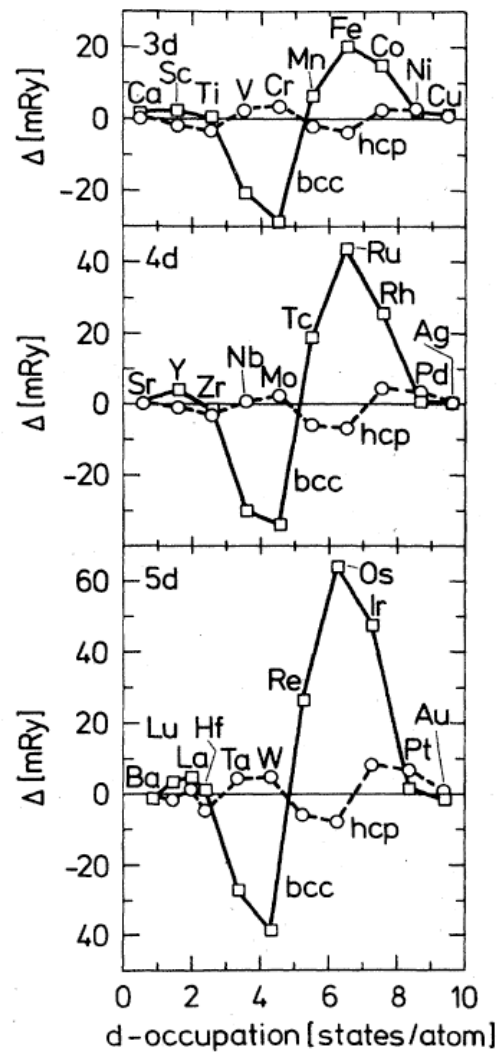


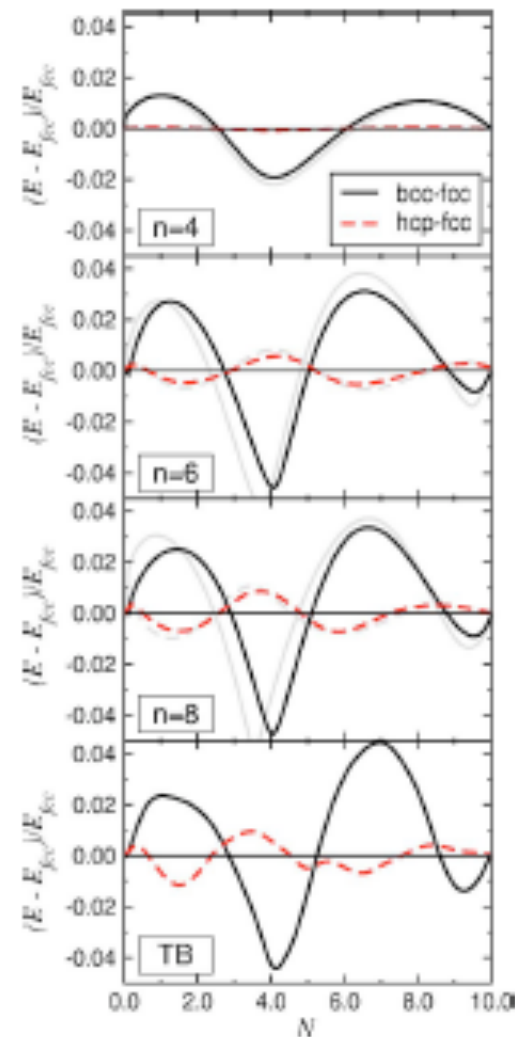
FIG. 2. Structural energy differences obtained from canonical d bands, by means of Eq. (4), as functions of the calculated canonical d occupation.

- En examinant les chemins on se rend compte que les quatre premiers moments μ_0 à μ_3 sont identiques.
- Ceci implique des changements de signe de la différence d'énergie en fonction du remplissage

et CFC-CC

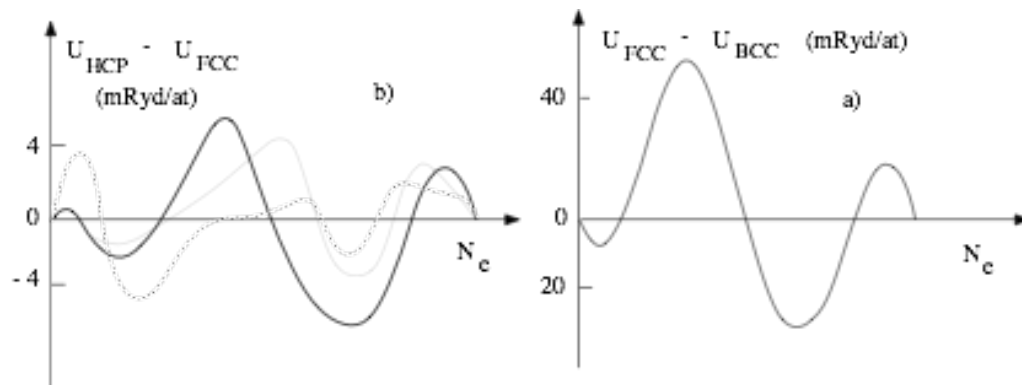


Skiver

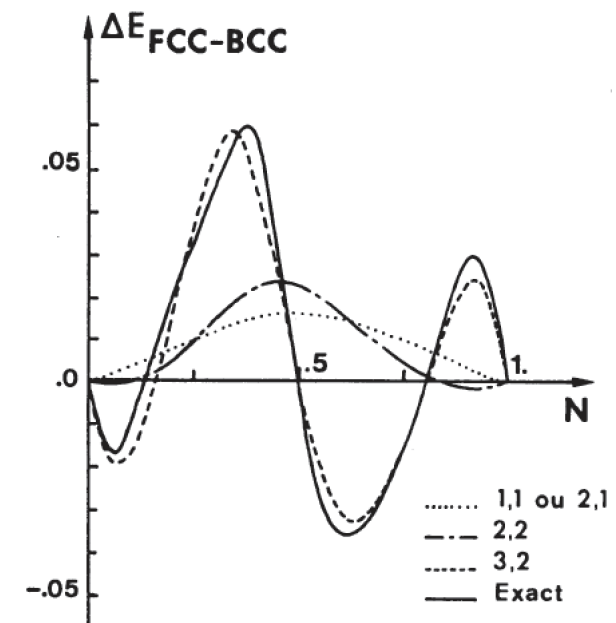


Dratz, Pettifor 2006

Les tendances calculées ab initio sont bien reproduites à condition d'aller au moins au cinquième moment

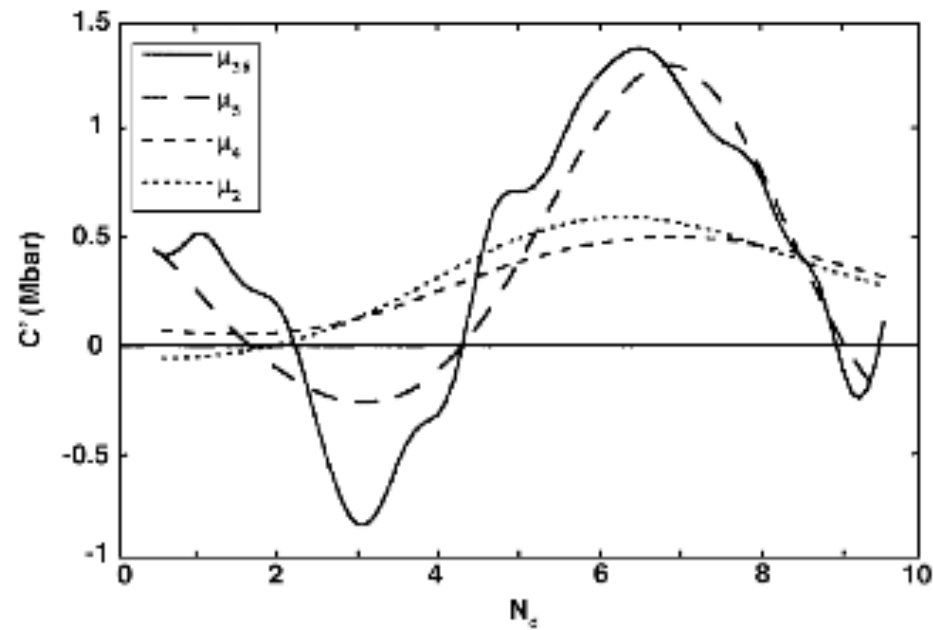


Legrand



Turchi, FD 1985

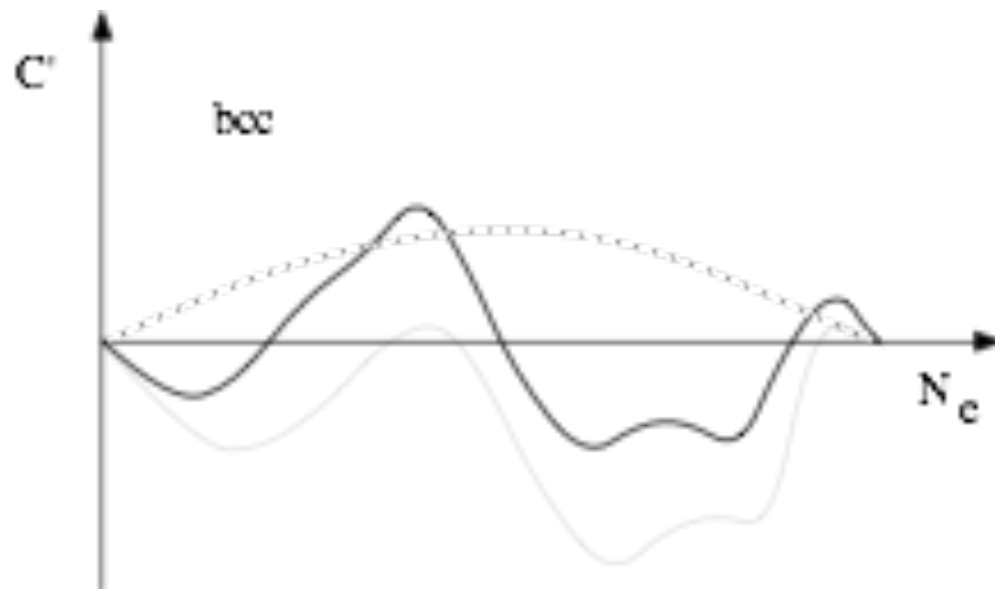
Constantes de cisaillement



► Pour les cubiques, C et C' ne varient pas de façon parabolique, et ne sont même pas toujours positives !

FIG. 4.5 – Effet du nombre de coefficients de fraction continue calculé exactement sur la reconstruction de C' dans une structure CFC en fonction du remplissage en électrons d. [93], [100]

Legrand, Nastar, Willaime



La méthode BOP: Bond Orbital Potential

PHYSICAL REVIEW B **72**, 144105 (2005)

Analytic bond-order potential for predicting structural trends across the *sp*-valent elements

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³*UKAEA Fusion, Culham Science Centre, Abingdon, OX14 3DB, UK*

(Received 6 May 2005; published 17 October 2005)

Analytic bond-order potentials for modelling the growth of semiconductor thin films

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H.N.G. Wadley^b, D.G. Pettifor^a

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^b *Department of Materials Science and Engineering, School of Engineering and Applied Science, University of Virginia, Charlottesville, VA 22904-4745, USA*

PHYSICAL REVIEW B **78**, 214108 (2008)



Binding-energy relations and equations of state for the 4*d* and 5*d* transition metals

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(Received 21 August 2008; published 22 December 2008)

PHYSICAL REVIEW B **83**, 224116 (2011)



Theory of structural trends within 4*d* and 5*d* transition metal topologically close-packed phases

B. Seiser,¹ T. Hammerschmidt,² A. N. Kolmogorov,¹ R. Drautz,² and D. G. Pettifor¹

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²*Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Stiepelers Strasse 129, D-44801 Bochum, Germany*

- Re-écriture systématique de la méthode TB + moments + récursion
- Développement explicite de l'énergie de bande en fonction du nombre de moments pris en compte
- Forces



David Pettifor
1945-2017

Bond-order potentials: derivation and parameterization for refractory elements

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¹ ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany

² Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK

PHYSICAL REVIEW B **87**, 094105 (2013)

A new method for development of bond-order potentials for transition bcc metals

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² Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstrasse 11, 79108 Freiburg, Germany

Analytic bond-order potential expansion of recursion-based methods

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PHYSICAL REVIEW B **83**, 224116 (2011)



Theory of structural trends within 4d and 5d transition metal topologically close-packed phases

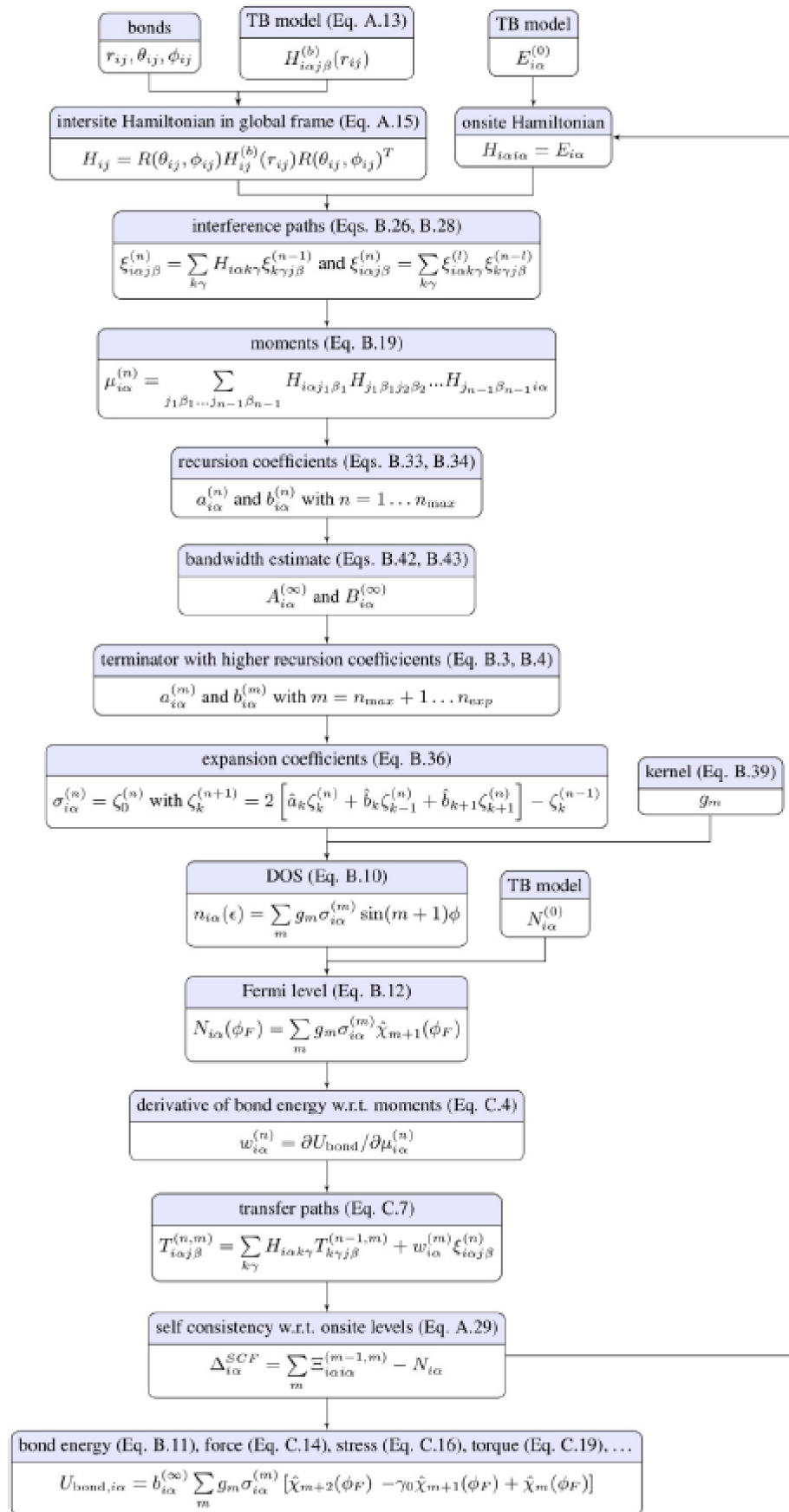
B. Seiser,¹ T. Hammerschmidt,² A. N. Kolmogorov,¹ R. Drautz,² and D. G. Pettifor¹

¹Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

²Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Stiepel Strasse 129, D-44801 Bochum, Germany

{110} planar faults in strained bcc metals: Origins and implications of a commonly observed artifact of classical potentials

Johannes J. Möller,^{1,2,*} Matous Mrovec,³ Ivan Bleskov,⁴ Jörg Neugebauer,⁴ Thomas Hammerschmidt,³ Ralf Drautz,³ Christian Elsässer,^{2,5} Tilmann Hickel,⁴ and Erik Bitzek¹



BOPfox program for tight-binding and analytic bond-order potential calculations

T. Hammerschmidt ^{a,b,*}, B. Seiser ^{a,b}, M.E. Ford ^{a,b}, A.N. Ladines ^a, S. Schreiber ^a, N. Wang ^a, J. Jenke ^a, Y. Lysogorskiy ^a, C. Teijeiro ^c, M. Mrovec ^a, M. Cak ^a, E.R. Margine ^{b,d}, D.G. Pettifor ^b, R. Drautz ^{a,b}

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www.bopfox.de

Etapas

- Structure
- TB hamiltonien
- Calcul des moments
- Calcul des coefficients de récursion
- Prolongement de la fraction continue
- Densité d'états
- Energie
- Auto-cohérence

Fig. 1. Overview of the calculation of the bond energy for a non-magnetic system with analytic BOPs in BOPfox.

Exemples: Carbone

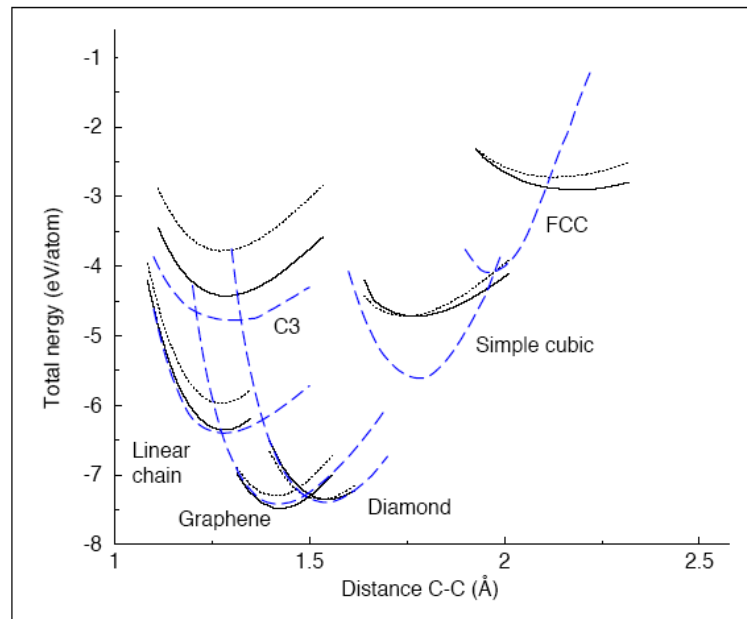
$$E_{rep}^i = F\left(\sum_{j \neq i} \phi(r_{ij})\right),$$

where $F(x)$ is a polynomial function :

$$F(x) = C_1x + C_2x^2 + C_3x^3 + C_4x^4 + C_5x^5$$

and $\phi(r_{ij})$ is a repulsive pairwise potential

$$\phi(r) = \phi_0(d_0/r)^m \exp\{m[-(r/d_c)^{m_c} + (d_0/d_c)^{m_c}]\}$$



BOP dédiés au carbone :

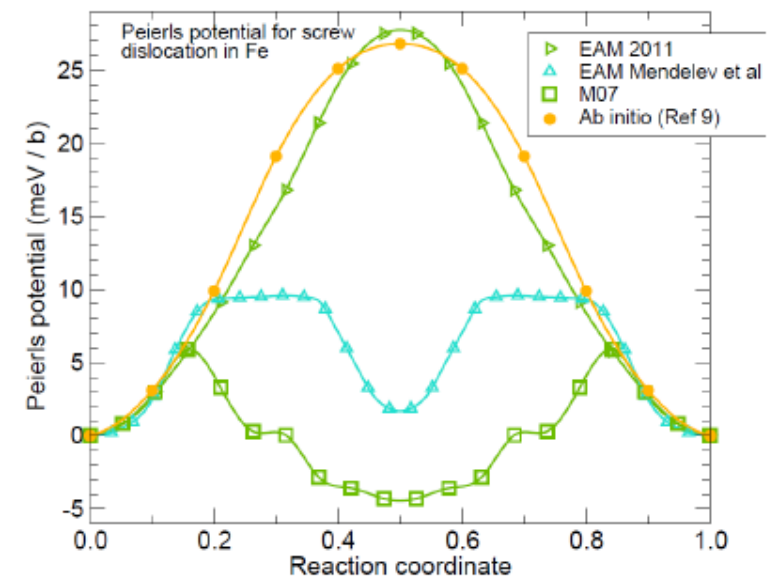
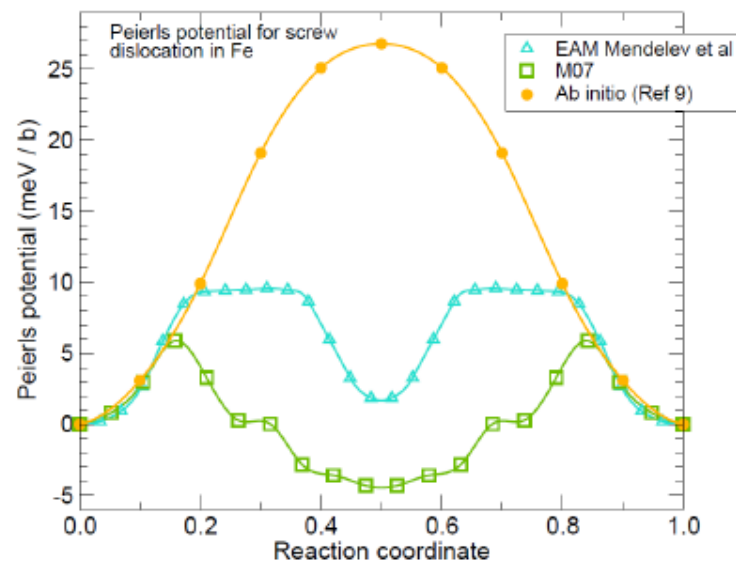
Potentiel	Année	Nature	Portée	Références
Stillinger-Weber	1985	Empirique	courte	F.H. Stillinger and T.A. Weber, Phys. Rev. B 31, 5262 (1985)
Tersoff	1989	BOP	courte	J. Tersoff, Phys. Rev. B 37, 6991 (1988)
Brenner	1990	BOP	courte	D.W. Brenner, Phys. Rev. B 42, 9458 (1990)
REBO	2002	BOP	courte	D.W. Brenner et al, J. Phys. Cond. Matt 14, 783 (2002)
Tersoff-LB	2010	BOP	courte	L. Lindsay, D.A. Broido, Phys. Rev. B 81, 205441 (2010)
REBO-LB	2010	BOP	courte	L. Lindsay, D.A. Broido, Phys. Rev. B 81, 205441 (2010)
LBOP	2002	BOP	medium	J.H. Los, A. Fasolino, Comp. Phys. Comm. 147, 178 (2002)
LCBOP	2003	BOP	medium	J.H. Los et al, Phys. Rev. B 68, 024107 (2003)
GEEBOD	1999	BOP	longue	J. Che et al, Theor. Chem. Acc. 102, 346 (1999)
AIREBO	2000	BOP	longue	S.J. Stuart et al, J. Chem. Phys. 112, 6472 (2002)

- ▶ Pas trop de problèmes pour la partie attractive (bande)
- ▶ Problèmes pour la partie répulsive
- ▶ Beaucoup de potentiels plus ou moins empiriques
- ▶ BOP différent ici du précédent
- ▶ Voir Magnin, Istres 2015

Fer



Fe EAM potentials: screw dislocation



	SIA		VAC		Surfaces		Phonons		Screw d	
	1,2	N>2	1,2	N>2					P	Gp
Fe-Mendelev 2003	+/-	+/-	+/-	+/-	+	+/-	+	-	-	+
Fe-Marinica 2007	+	+	+	+	+	+	+	+	-	-
Fe-Ackland-Mendelev 2004	+/-	+/-	+/-	+/-	+	+/-	+	+	-	-
Fe-Proville 2012	-	-	+	+	+	+/-	+/-	+/-	+	+

{110} planar faults in strained bcc metals: Origins and implications of a commonly observed artifact of classical potentials

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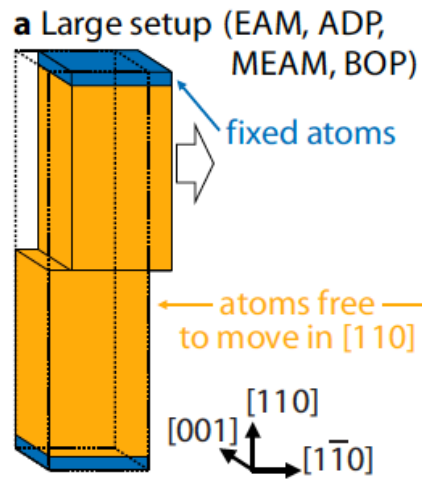


TABLE I. Summary of contributions for modeling atomic interactions explicitly included (●) or not taken into account (○) in the different material models.

Model	Radial distance	Directional bonding	Bond order	Magnetism	Electronic structure
EAM/FS	●	○	○	○	○
MEAM	●	●	○	○	○
ADP	●	●	○	○	○
Tersoff	●	●	●	○	○
BOP	●	●	●	●	● ^a
DFT	●	●	●	●	●

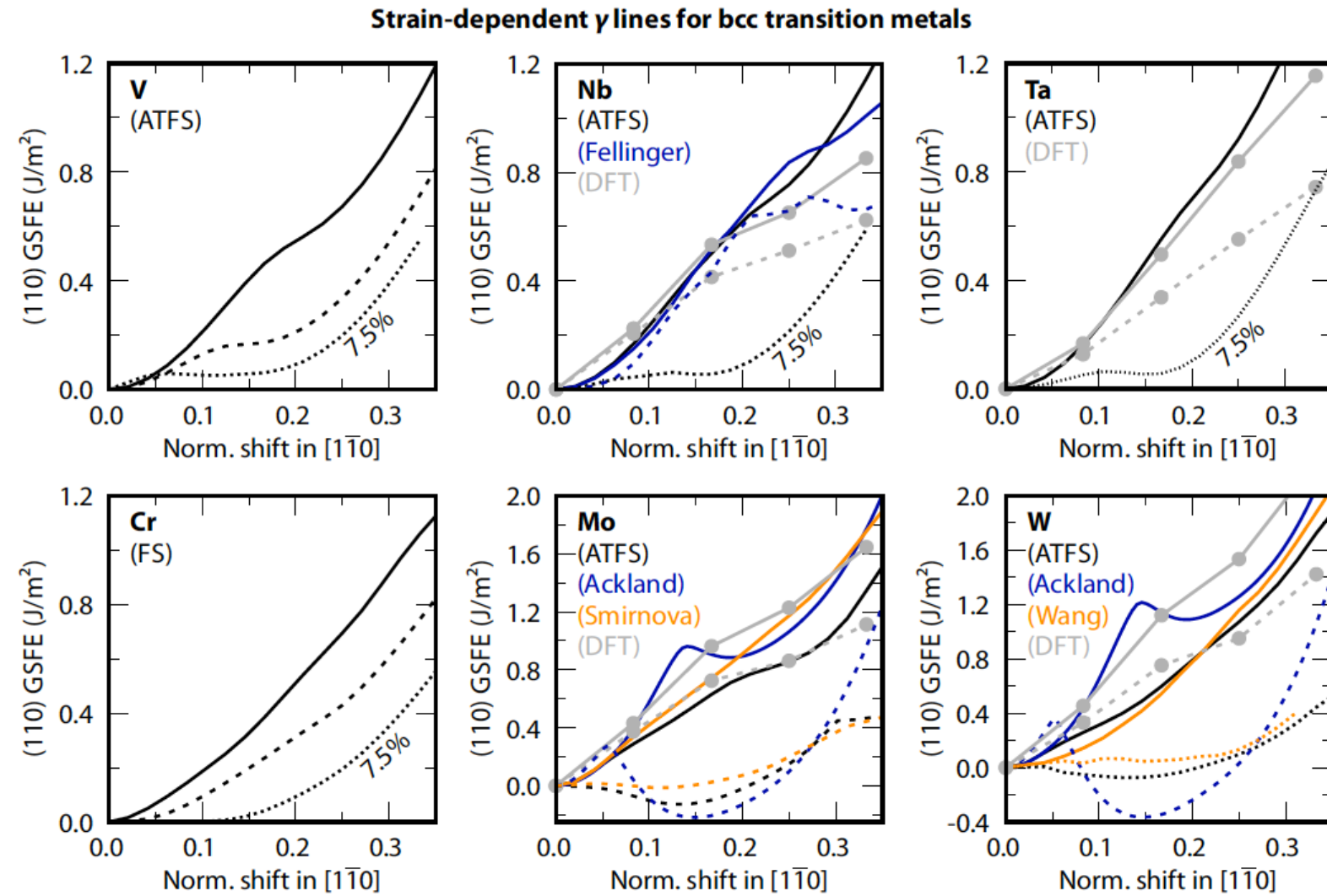


FIG. 5. Strain-dependent γ lines of various EAM potentials for the bcc metals V, Nb, Ta, Cr, Mo, and W. The GSFE data are plotted for 0% (solid lines), 5% (dashed), and 7.5% (dotted) applied equi-biaxial strain parallel to both the (110) plane normal and the [1 $\bar{1}$ 0] shearing direction. The shift in [1 $\bar{1}$ 0] direction is normalized, i.e., divided by the corresponding periodicity distance $\sqrt{2}a_0$. Relaxed stacking fault energies for Nb, Ta, Mo, and W were additionally calculated using DFT.

Entre la DFT et le potentiel Lennard-Jones plein de méthodes intermédiaires à choisir après s'être donné un cahier de charges précis:
précision désirée, ressources de calcul, quantités recherchées, transférabilité, ...

On peut deviner que les méthodes complètement empiriques vont être remplacées par des techniques d'IA (apprentissage automatique)

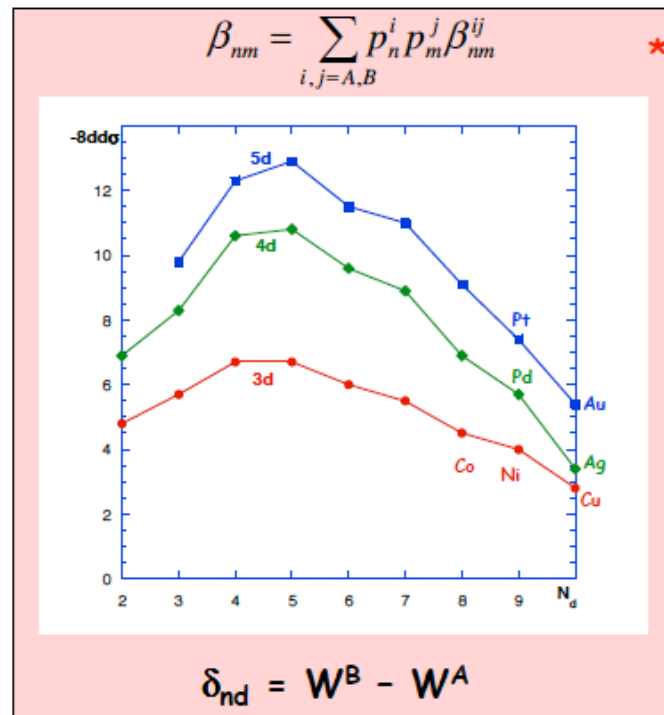
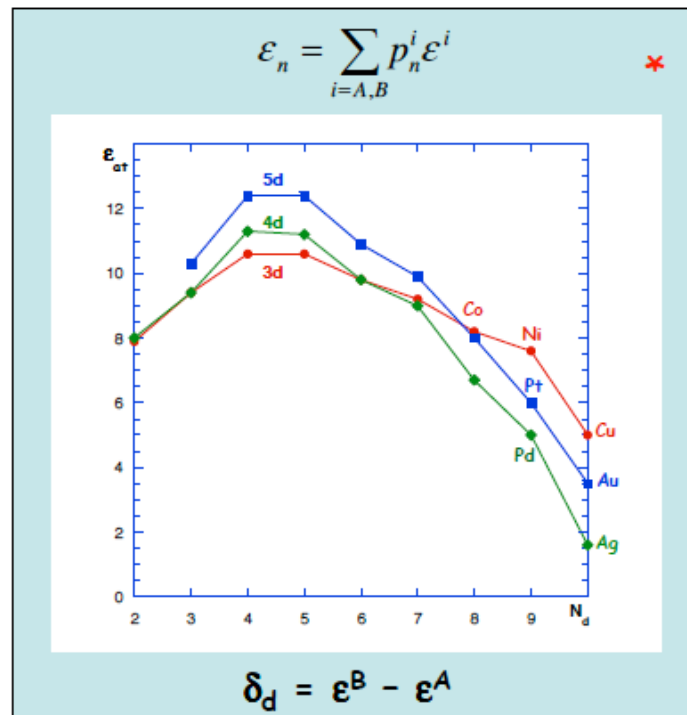
Alliages

Alliages: les paramètres

Hamiltonien de Liaisons Fortes

$$H = \sum_n |n\rangle \varepsilon_n \langle n| + \sum_{n,m} |n\rangle \beta_{nm} \langle m|$$

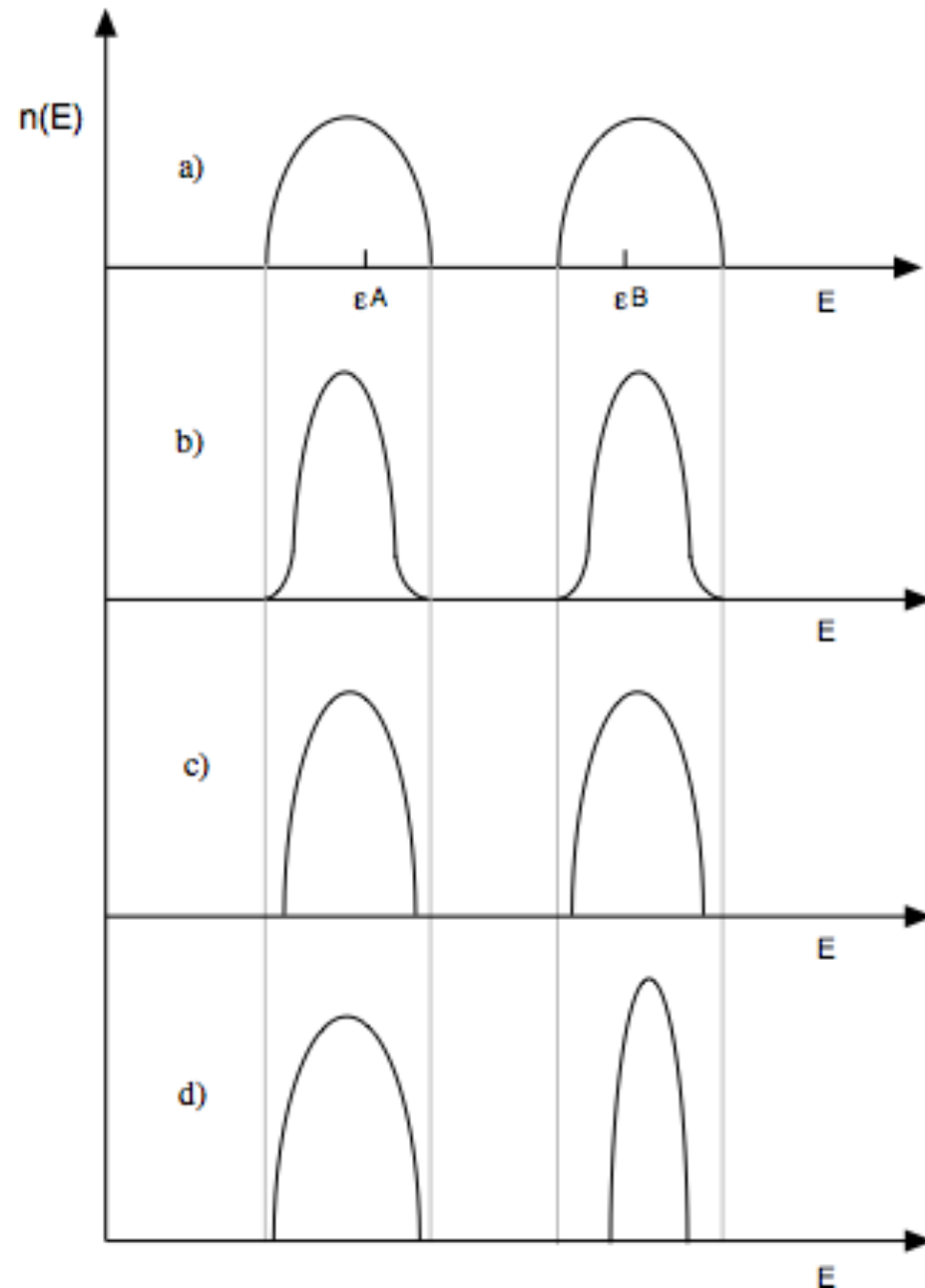
**from "Papaconstantopoulos compil"*



$\delta_d / W \gg \delta_{nd} / W \dots$ dans la plupart des cas ?

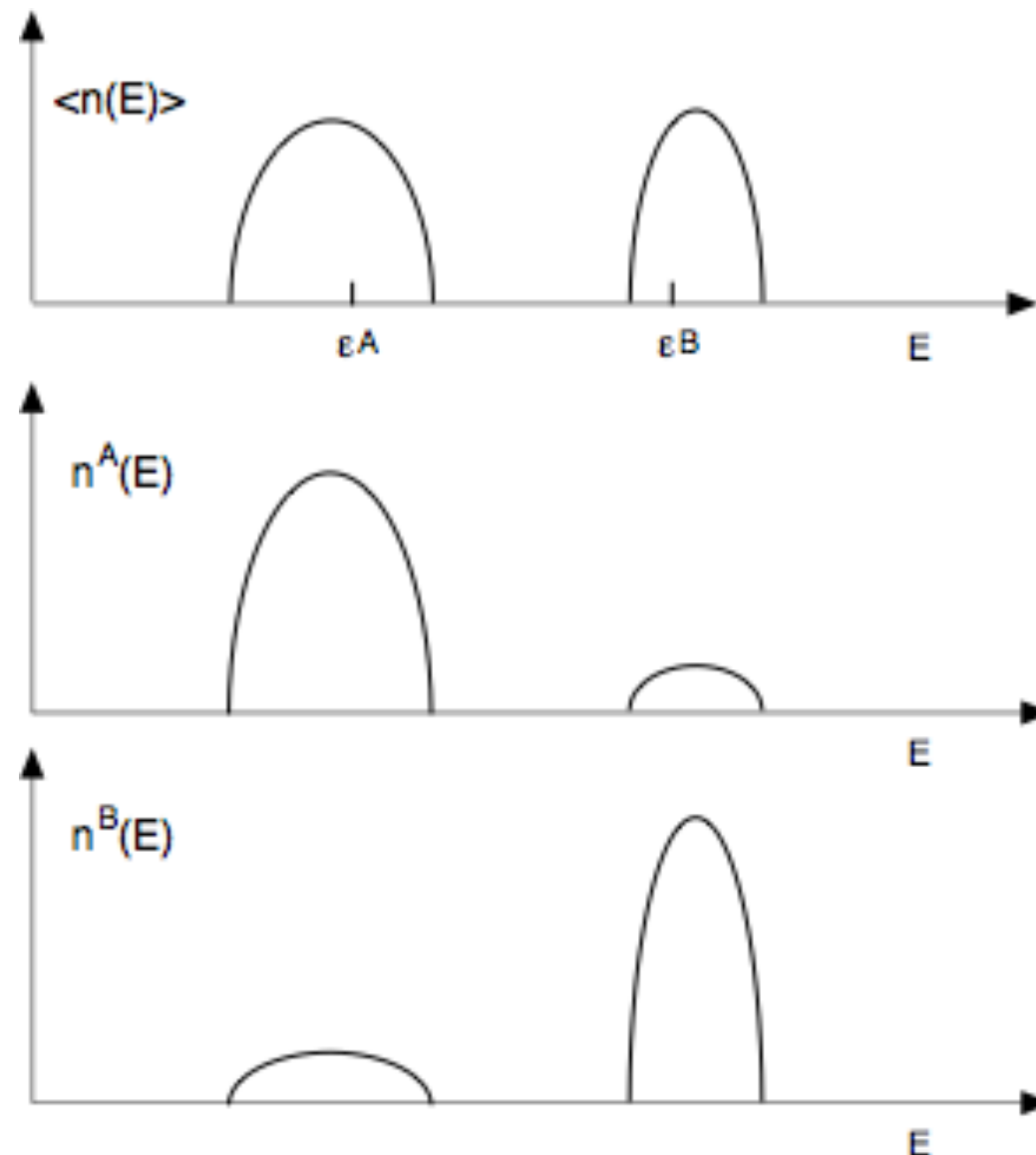
- On étend le modèle liaisons fortes en supposant dans un premier temps que les paramètres ne dépendent pas de l'environnement
- Si le contraste est faible (alliage binaire) modèle de bandes rigides (cristal moyen)
- Sinon, bandes séparées

Fort désordre



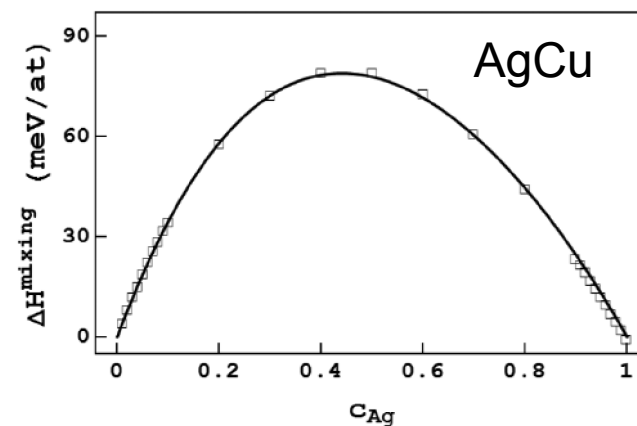
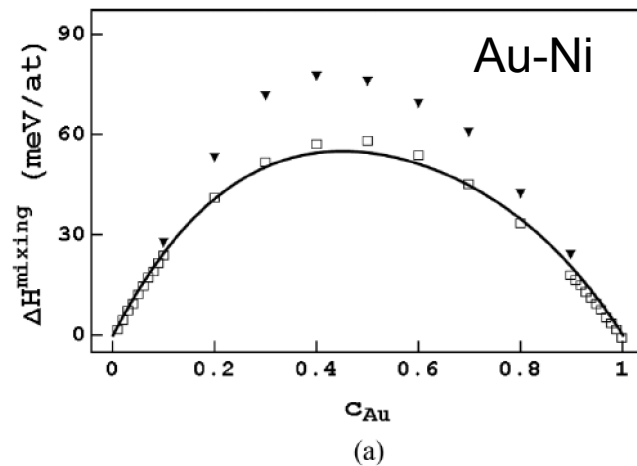
- ▶ Superposition des densités d'états; $c=1/2$
- ▶ Théorème sur la « localisation » en énergie des états !
- ▶ Alliages désordonné
- ▶ Alliages ordonné
- ▶ $c \neq 1/2$

Densités d'états partielles

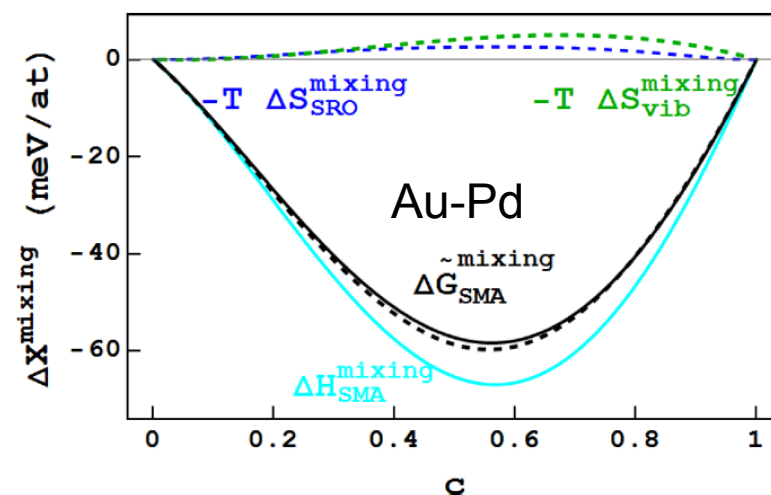


- La densité d'états locale minoritaire est d'autant plus faible que le désordre diagonal δ/W est fort
- Ceci a tendance à réduire δ car ϵ^i est décalé de $U Q^i$ où Q^i est le transfert de charge. Reste vrai dans la limite U infini, Q^i nul !
- δ doit donc être considéré comme un paramètre

SMA pour alliages



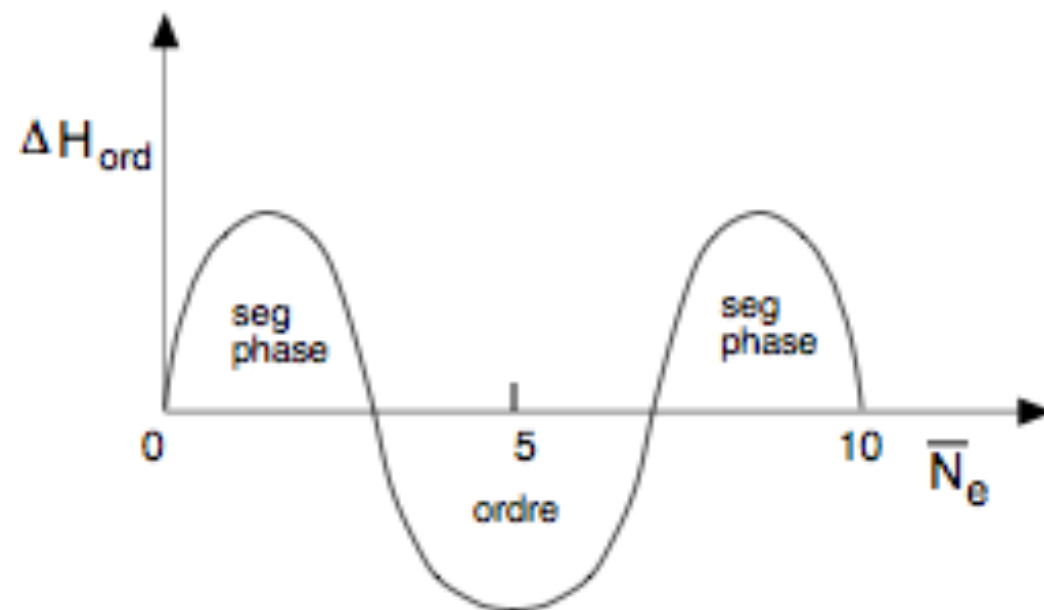
Berthier et al.
2017 - 2019



- En utilisant des densités d'états « centrées », on peut utiliser le modèle de second moment (y compris avec termes répulsifs).
- Le terme principal provient de l'élargissement de la bande qui donne une contribution négative pour des remplissages de bande d intermédiaires.
- Modèle plus empiriques pour les alliages de métaux nobles à faible δ/W et désordre non-diagonal, mais qui permet de discuter des effets de taille

Au delà du second moment

$$E_{coh}(\{p_n^i\}) = \bar{E}(c) + \frac{1}{2} \sum_{n,m,i,j} p_n^i p_m^j V_{nm}^{ij}$$

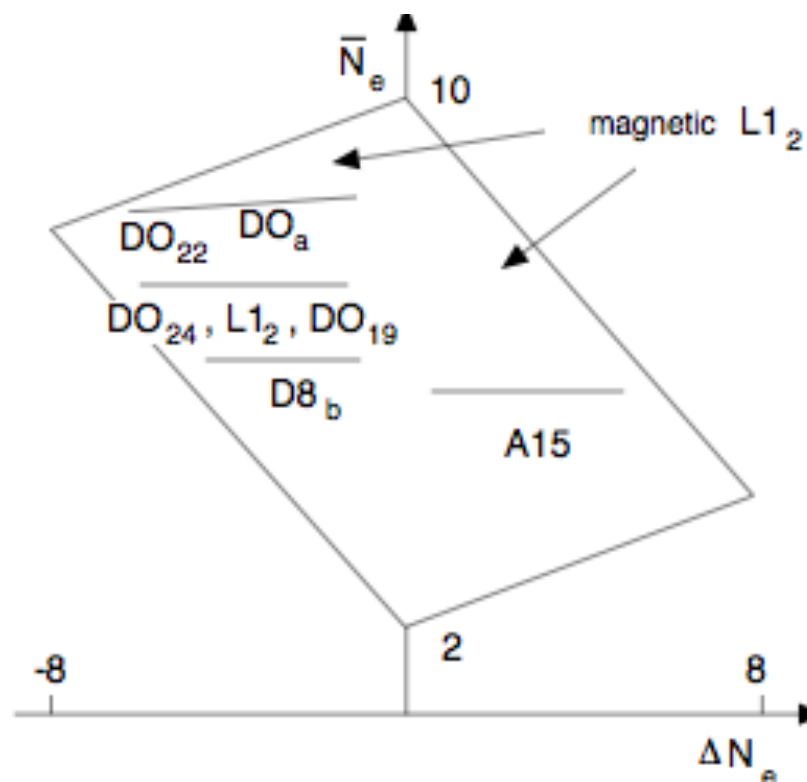


- ▶ On décompose l'énergie en énergie du système désordonné et énergie d'ordre
- ▶ Au plus bas ordre en perturbation, interactions de paire effectives: modèle d'Ising effectif
- ▶ Analyse de moments: avec désordre diagonal, il faut aller au moins au quatrième moment
- ▶ Extension au cas du désordre non-diagonal

Cartes structurales

Table 1
Transition metal alloys for which an $L1_2$ OS has been experimentally observed at low temperatures [13]. The alloys which are also magnetically ordered (MO) at low temperatures [132,134], have large values of $\bar{N}_d$ and are outside the predicted range for the stability of the $L1_2$ structure (see fig. 1) whereas those which are non-magnetically ordered (NMO) are correctly predicted to be chemically ordered according to an $L1_2$ OS (F and AF indicate ferromagnetic and antiferromagnetic order respectively [133]). $\bar{N}_d$ is the average "d" band filling: $\bar{N} = \bar{N}_d + 1$

NMO			MO				
AB_2	$\bar{N}_d$	ΔN	AB_2			$\bar{N}_d$	ΔN
ScRh	6.5	-6	CrIr	F	[137]	7.25	-3
ScPd	6.5	-6	CrPt	F	[138]	8	-4
ScPt	6.5	-6	MnNi	F	[139]	8.25	-3
YPd	6.5	-6	MnPt	F	[140]	8.25	-3
YPt	6.5	-6	FeNi	F	[141]	8.5	-2
LaPd	6.5	-6	FePd	F	[142]	8.5	-2
LaPt	6.5	-6	FePt	AF	[140]	8.5	-2
TiCo	6.75	-5	CoPt	F	[143]	8.75	1
TiRh	6.75	-5					
TiIr	6.75	-5	RhMn	AF	[144]	6.5	+2
ZrRh	6.75	5	IrMn	AF	[145]	6.5	+2
ZrIr	6.75	-5	PtMn	AF	[140]	6.75	+3
HfRh	6.75	-5	PtFe	F	[140]	7.5	+2
HfIr	6.75	-5	PtCu	F	[145]	8.25	+1
VRh	7	-4	PtNi	F	[146]	9	0
VIr	7	-4					
NbRh	7	-4					
NbIr	7	-4					
TaRh	7	-4					
TaIr	7	-4					
TiPt	7.5	-6					



- On classe bien les structures observées en utilisant comme paramètres, N , ΔN et c
- Ici c est fixé pour une structure cristalline de base donnée : CFC

Three-Parameter Crystal-Structure Prediction for *sp-d*-Valent Compounds

Arthur F. Bialon, Thomas Hammerschmidt,* and Ralf Drautz

Cartes structurales
pour alliages
ternaires ...

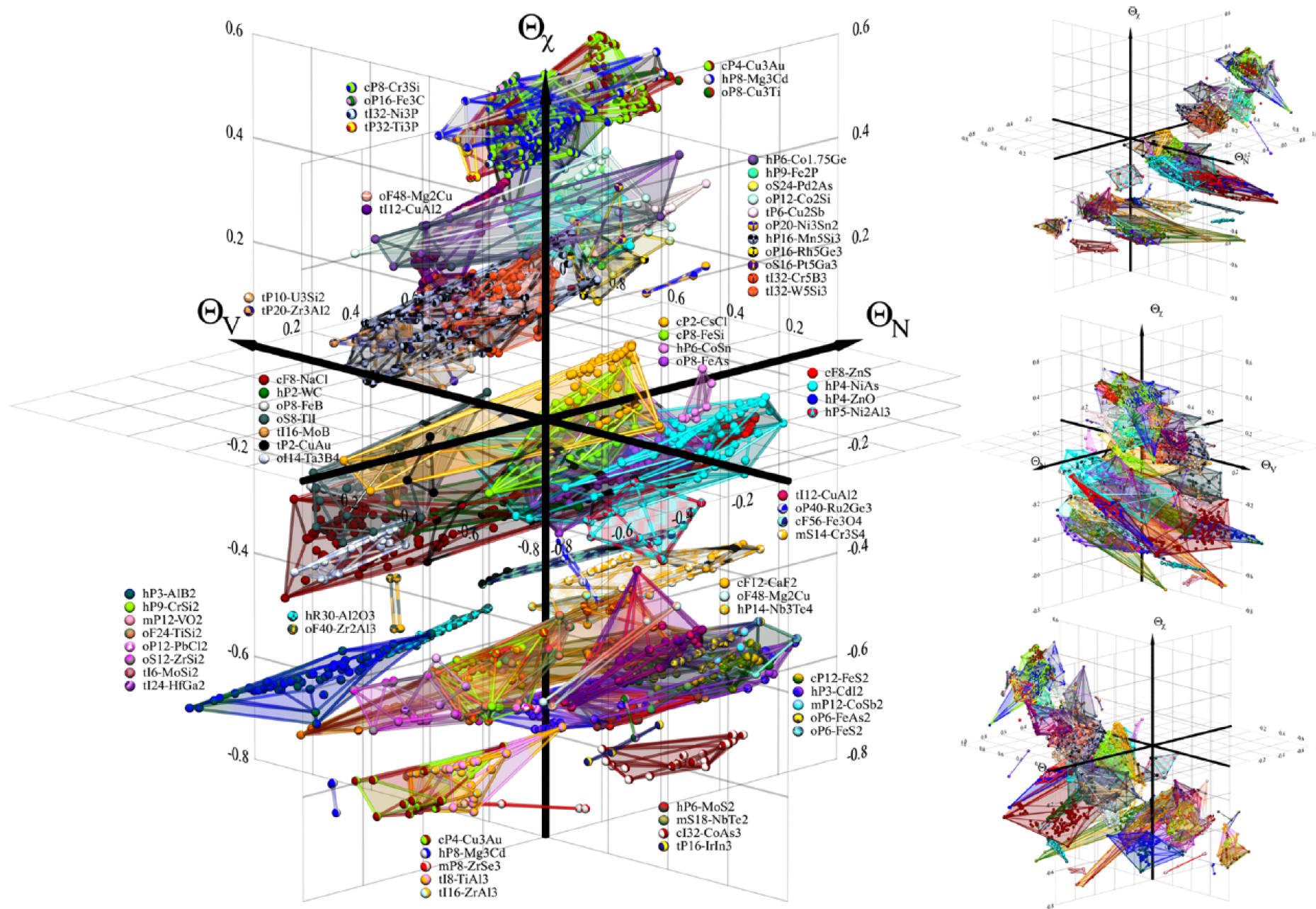


Figure 3. Three-dimensional structure map for 64 prototypical crystal structures in the *sp-d*-valent systems. The data set is highlighted with small spheres, the crystal structure domains as polyhedra. Side panel shows rotation along Θ_χ with $\Phi = 90^\circ, 180^\circ, 270^\circ$.

MIX Ab initio-méthodes empiriques

- ▶ On postule un développement de l'énergie en interactions de paires, triplets, multiplets, ..., Cluster Expansion
- ▶ On calcule ensuite l'énergie par des méthodes ab initio pour un certain nombre de structures ordonnées définies, par exemple L_{12} , L_{10} sur un réseau cfc.
- ▶ En retour on obtient les interactions par inversion d'un système linéaire
- ▶ on recalcule avec le développement, des énergies de structures non incluses dans le jeu initial; on compare avec un calcul ab initio
- ▶ Si ça ne marche pas, on modifie la base d'interactions et on recommence
- ▶ On peut aussi engendrer des états désordonnés
- ▶ POUR: quelques valeurs ab initio; utilisation de méthodes IA: données, analyse
- ▶ CONTRE: instabilité des bases; pas toujours justifié; pas de « physique » pour la hiérarchie des interactions

Vers les alliages complexes, à haute entropie, ... ?

Ab initio phase stabilities and mechanical properties of multicomponent alloys: A comprehensive review for high entropy alloys and compositionally complex alloys

Yuji Ikeda^{a,b,*}, Blazej Grabowski^a, Fritz Körmann^{a,c}

JPhys Materials

TOPICAL REVIEW

From DFT to machine learning: recent approaches to materials science—a review

Gabriel R Schleder^{1,2,3} , Antonio C M Padilha² , Carlos Mera Acosta^{1,2} , Marcio Costa²  and Adalberto Fazzio^{1,2,3} 

Quelques livres

F. Seitz	The Modern Theory of Solids	MC Graw Hill
Ch. Kittel	Physique de l'état solide	Dunod
N. W. Ashcroft et N. D. Mermin	Physique des solides	EDP
A. P. Sutton	Electronic Structure of Materials	Oxford
D. G. Pettifor	Bonding and Structure of Molecule and Solids	Oxford
J. K. Burdett	Chemical Bonding in Solids	Oxford
J.-L. Rivail	Éléments de chimie quantique	EDP
W. A. Harrison	Electronic Structure and the Properties of Solids	Dover
S. Elliott	The Physics and Chemistry of Solids	Wiley
M. Gerl et J.-P. Issi	Physique des matériaux	PUPR
M. Lannoo et P. Friedel	Atomic and Electronic Structure of Surfaces	Springer
M.-C. Desjonquères et D. Spanjaard	Concepts in Surface Physics	Springer
(beaucoup de choses sur les liaisons fortes et les covalents, y compris dans le volume)		

Et aussi, pour la structure électronique,

R. M. Martin	Electronic Structure: Basic Theory and Practical Methods	Cambridge
R. M. Martin, L. Reining, D. M. Ceperley	Interacting Electrons: Theory and Computational Approaches	Cambridge