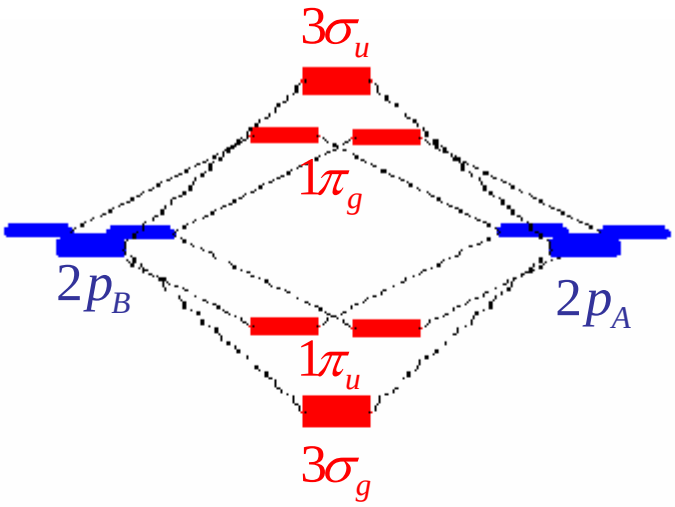
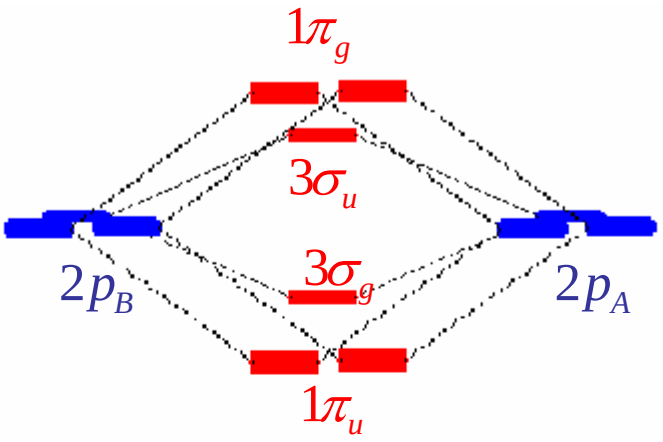
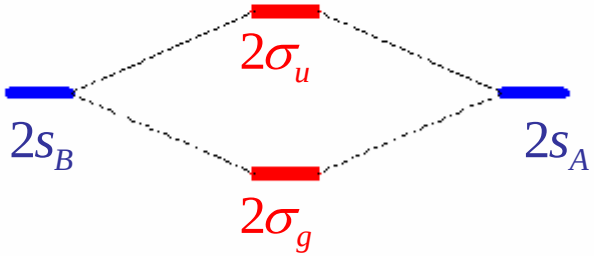
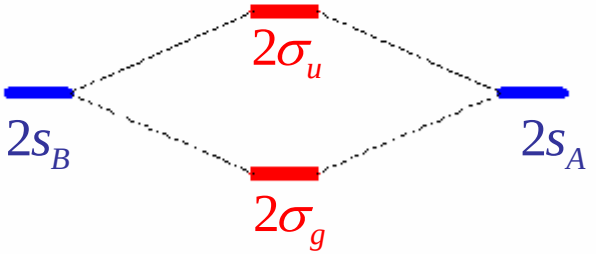
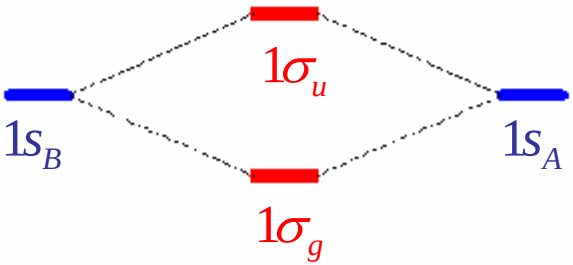
Molécules X_2

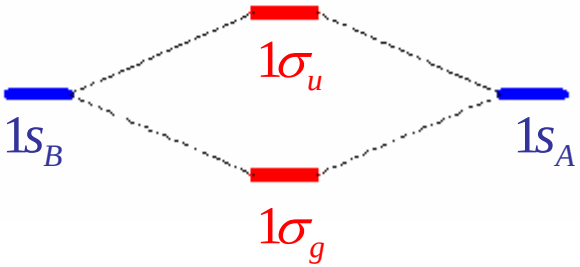












Molécules X_2

- Ordre de liaison: (ou indice de liaison)

$$n = \frac{1}{2}(n_{liant} - n_{antiliant})$$

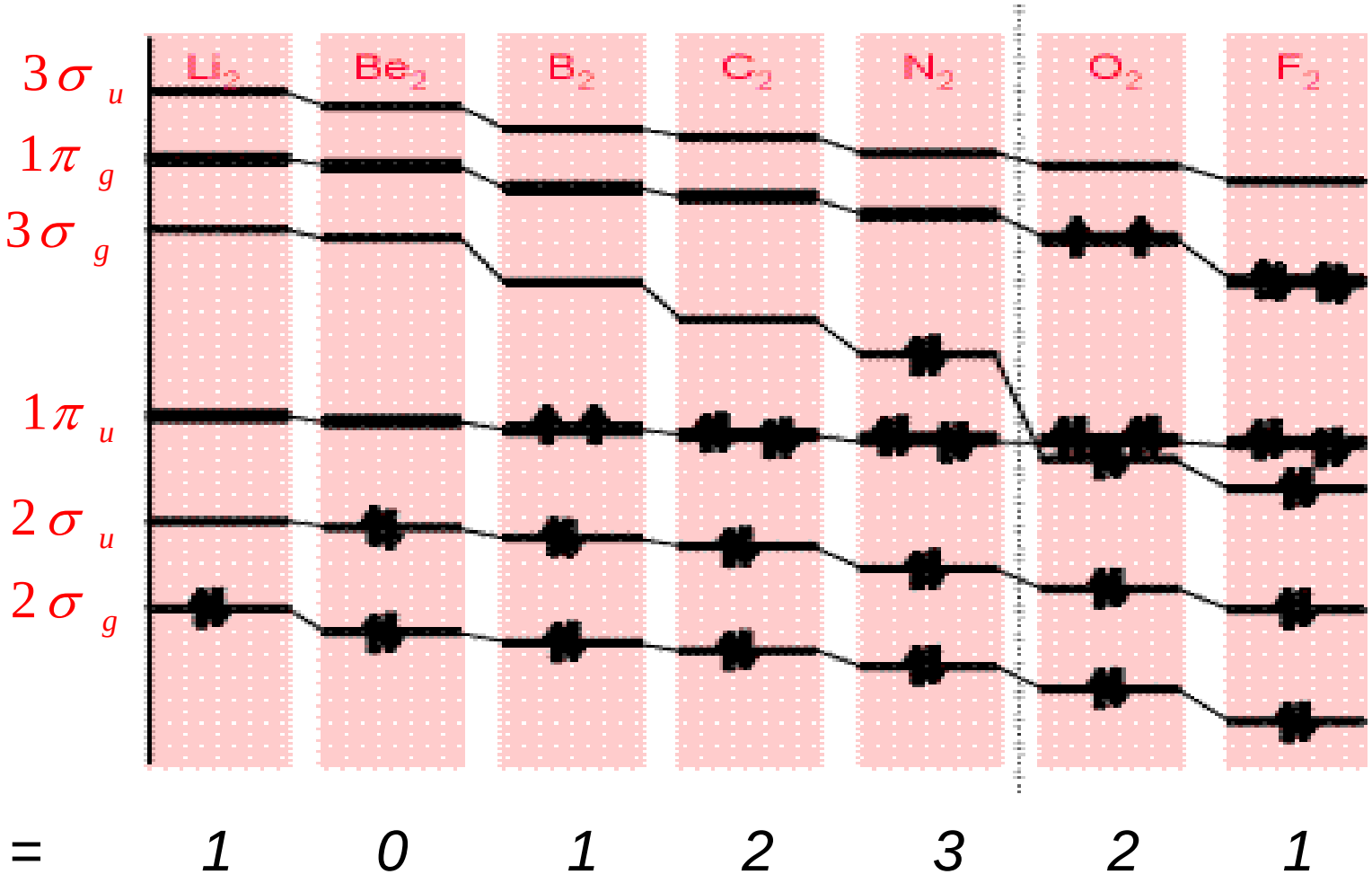
Exemples:

Li_2 $\quad 1\sigma_g^2 1\sigma_u^2 2\sigma_g^2$ $\qquad \{n_{liant} = 4, n_{antiliant} = 2\} \Rightarrow n = 1$

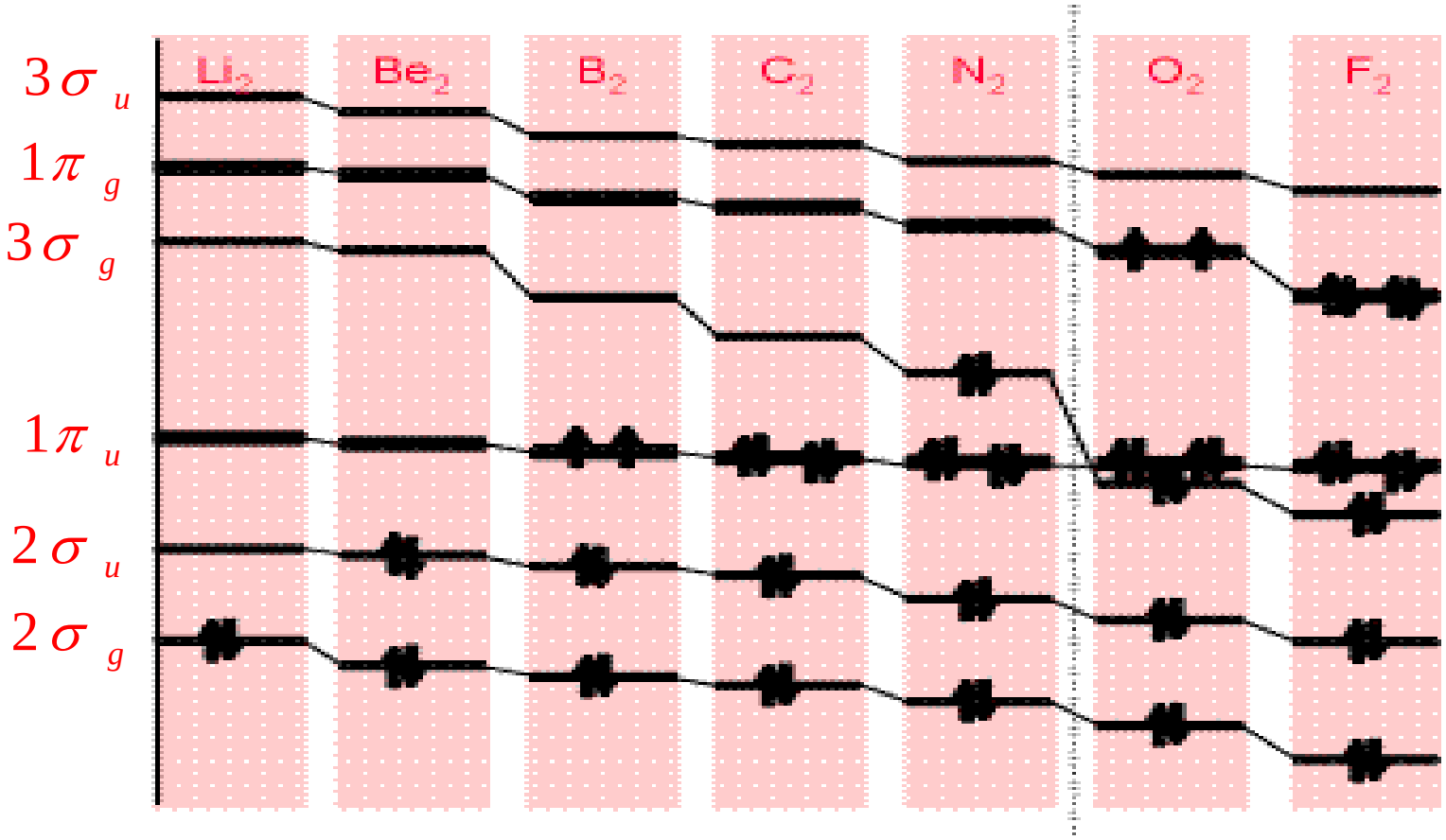
N_2 $\quad 1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 1\pi_{x,u}^2 1\pi_{y,u}^2 3\sigma_g^2$

$$\{n_{liant} = 10, n_{antiliant} = 4\} \Rightarrow n = 3$$

Molécules X_2

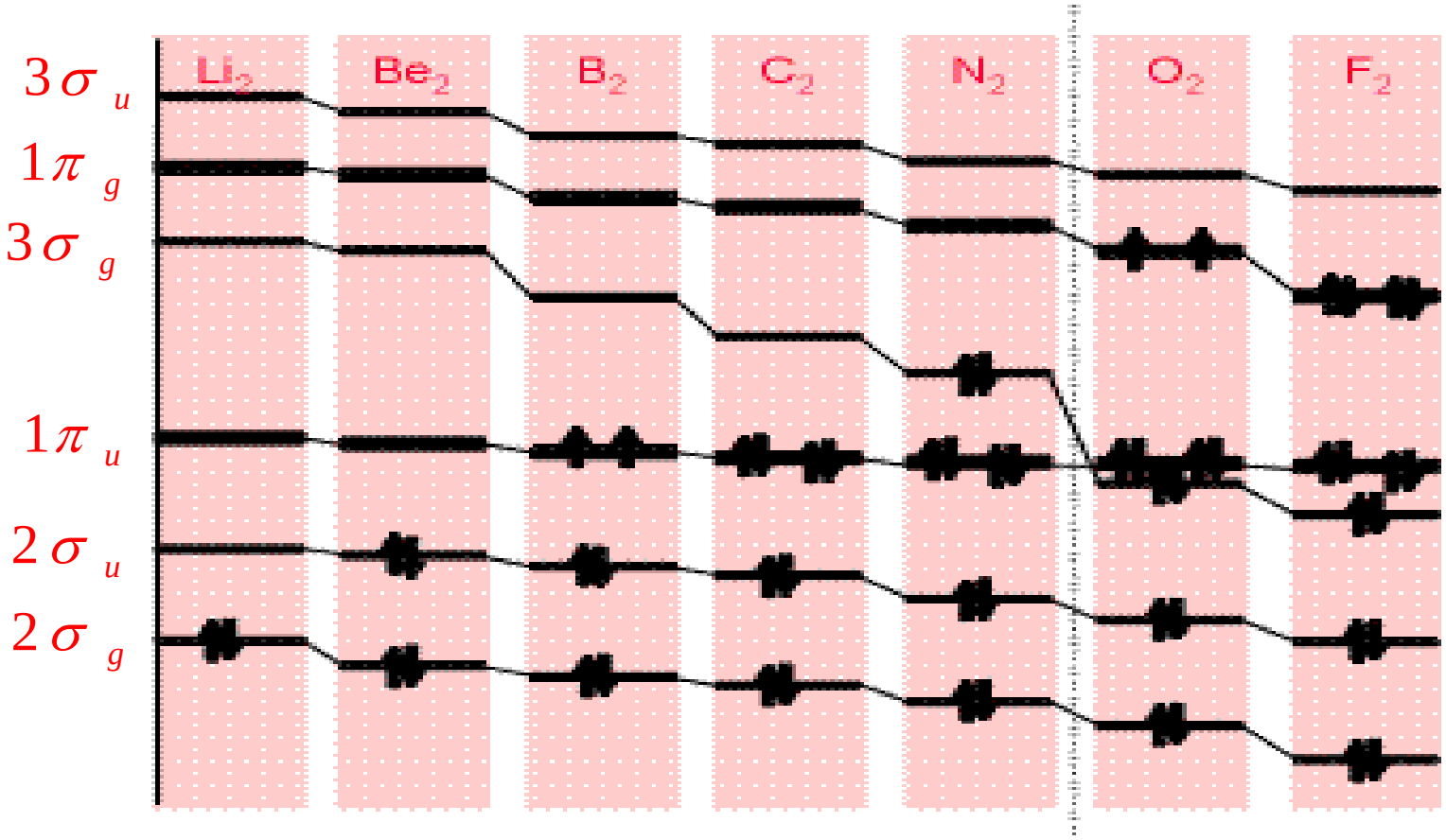


Molécules X_2



n =	*1*	*0*	*1*	*2*	*3*	*2*	*1*
R_e *(pm)* =	*267*	*245*	*159*	*124*	*110*	*121*	*141*

Molécules X_2



n =	*1*	*0*	*1*	*2*	*3*	*2*	*1*
D_e =	*105*	*9*	*289*	*599*	*942*	*494*	*154*

(kJ/mol)

Molécules AB faiblement polaires

SI $e_A \cong e_B$

Molécules AB faiblement polaires

SI $e_A \cong e_B$

Nomenclature des OM

A_2	AB
$1\sigma_g$	1σ
$1\sigma_u$	$1\sigma^*$
$2\sigma_g$	2σ
$2\sigma_u$	$2\sigma^*$
$3\sigma_g$	3σ
$3\sigma_u$	$3\sigma^*$
$1\pi_{u,x}$	$1\pi_x$
$1\pi_{g,x}$	$1\pi^*_x$
$1\pi_{u,y}$	$1\pi_y$
$1\pi_{g,y}$	$1\pi^*_y$

Molécules AB faiblement polaires

SI $e_A \cong e_B$

Nomenclature des OM

A_2	AB	caractère
$1\sigma_g$	1σ	*liante*
$1\sigma_u$	$1\sigma^*$	*antiliante*
$2\sigma_g$	2σ	*liante*
$2\sigma_u$	$2\sigma^*$	*antiliante*
$3\sigma_g$	3σ	*liante*
$3\sigma_u$	$3\sigma^*$	*antiliante*
$1\pi_{u,x}$	$1\pi_x$	*liante*
$1\pi_{g,x}$	$1\pi^*_x$	*antiliante*
$1\pi_{u,y}$	$1\pi_y$	*liante*
$1\pi_{g,y}$	$1\pi^*_y$	*antiliante*

Molécules AB faiblement polaires

SI $e_A \cong e_B$

Nomenclature des OM

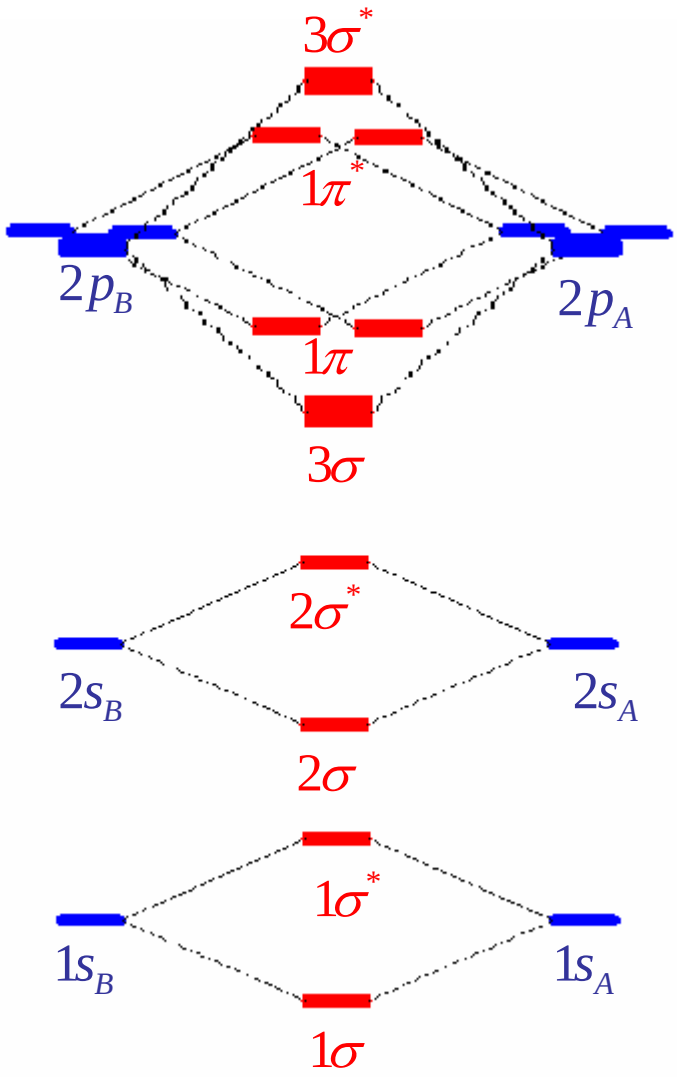
Ordre de liaison:

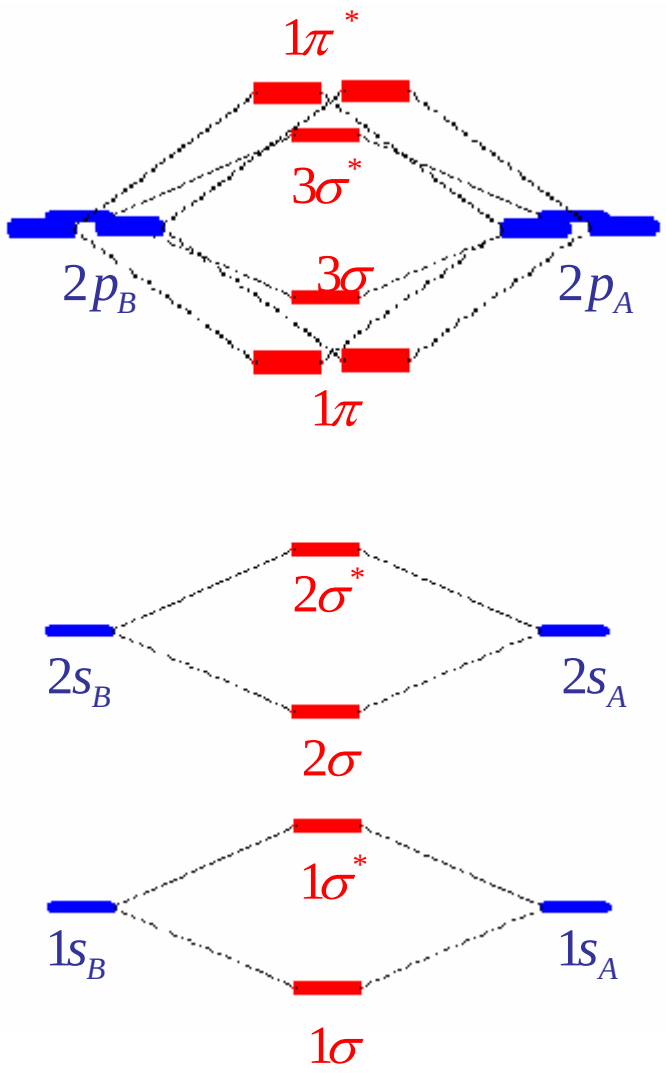
$$n = \frac{1}{2}(n_{liant} - n_{antiliant})$$

toujours

A_2	AB	caractère
$1\sigma_g$	1σ	*liante*
$1\sigma_u$	$1\sigma^*$	*antiliante*
$2\sigma_g$	2σ	*liante*
$2\sigma_u$	$2\sigma^*$	*antiliante*
$3\sigma_g$	3σ	*liante*
$3\sigma_u$	$3\sigma^*$	*antiliante*
$1\pi_{u,x}$	$1\pi_x$	*liante*
$1\pi_{g,x}$	$1\pi^*_x$	*antiliante*
$1\pi_{u,y}$	$1\pi_y$	*liante*
$1\pi_{g,y}$	$1\pi^*_y$	*antiliante*

Molécules AB faiblement polaires





Molécules AB (fortement) polaires

SI $e_A \prec e_B$

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- considérer cas par cas

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- noter généralement:
  - l'existence d'orbitales non-liantes, dites OM de cœur

Molécules AB (fortement) polaires

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- considérer cas par cas
- respecter règles LCAO
- noter généralement:
  - l'existence d'orbitales non-liantes, dites OM de cœur
  - des interactions d'OA de valence seulement

Molécules AB (fortement) polaires

Exemple HF $e_H \prec e_F$

Molécules AB (fortement) polaires

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$$E(1s_H) = -Ry = -0.5 \text{ u.a.}$$

1 u.a. = 27.2 eV

Molécules AB (fortement) polaires

Exemple HF $\quad e_H \prec e_F$

$$E(1\mathrm{s}_{\mathrm{H}}) = -Ry = -0.5 \text{ u.a.}$$

1 u.a. = 27.2 eV

$$E(1s_{\mathrm{F}}) \cong -38 \ u.a.$$

$$E(2s_{\mathrm{F}}) \cong -1.44 \, u.a.$$

$$E(2p_{\mathrm{F}}) \cong -0.68 \, u.a.$$

Molécules AB (fortement) polaires

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$$E(1s_F) \cong -38 \; u.a.$$

$$E(2s_F) \cong -1.44 \, u.a.$$

$$E(2p_F) \cong -0.68 \, u.a.$$

$$\boxed{E(1s_F) < E(2s_F) << E(1s_H) \cong E(2p_F)}$$

Molécules AB (fortement) polaires

Exemple HF $e_H \prec e_F$

$\psi_1 \cong 1s_F$ OM de coeur **1 u.a. = 27.2 eV**

Molécules AB (fortement) polaires

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$\psi_1 \cong 1s_F$ OM de coeur **1 u.a. = 27.2 eV**

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$\psi_3 \cong 2p_{\mathrm{z,F}} + t1s_H \quad 0 < t < 1$ OM liante

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$\psi_4 \cong 2p_{x,F} \quad \psi_5 \cong 2p_{y,F}$ OM non-liante

Molécules AB (fortement) polaires

Exemple HF $\boxed{e_H \prec e_F}$

$\psi_1 \cong 1s_{\mathrm{F}}$ OM de coeur **1 u.a. = 27.2 eV**

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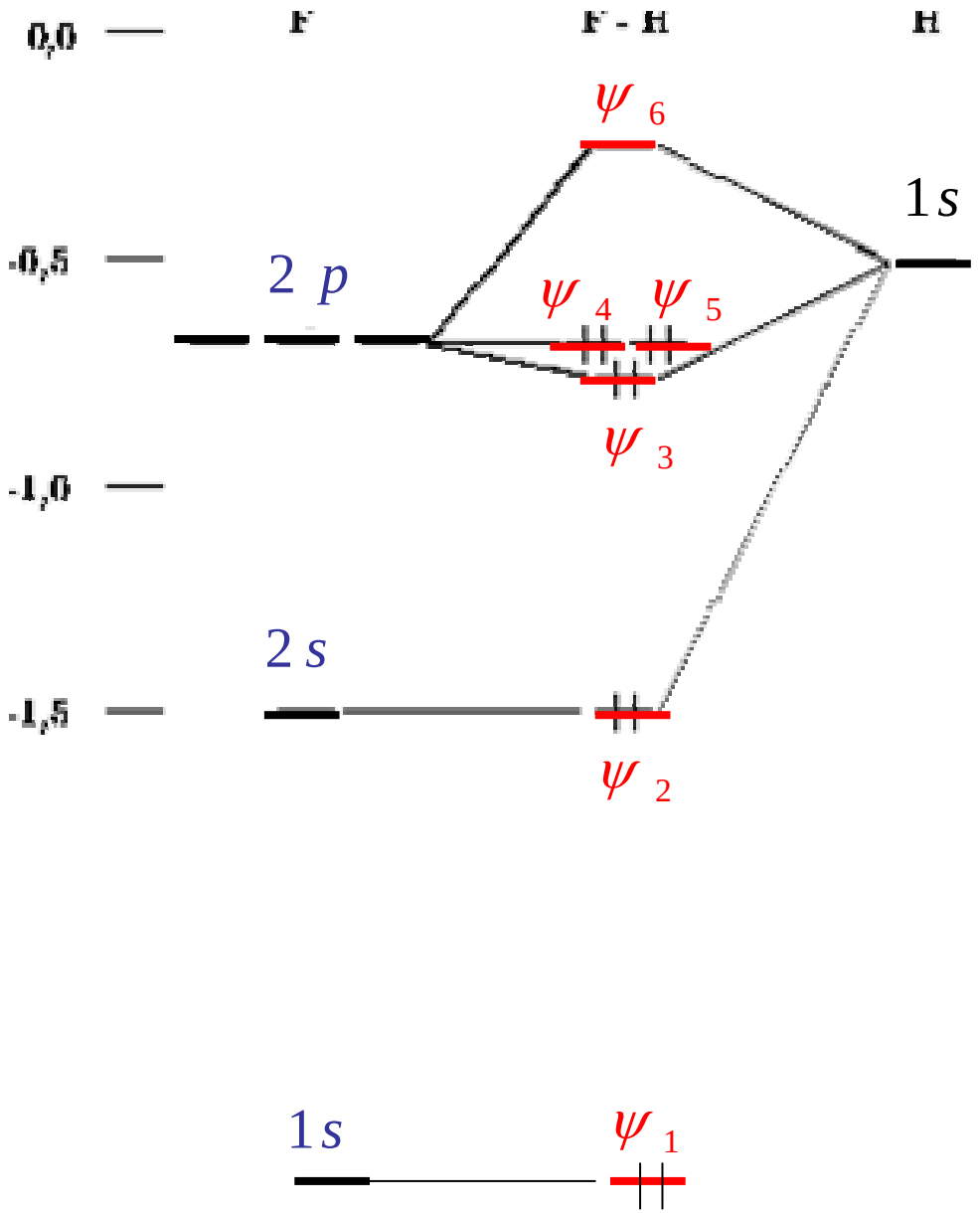
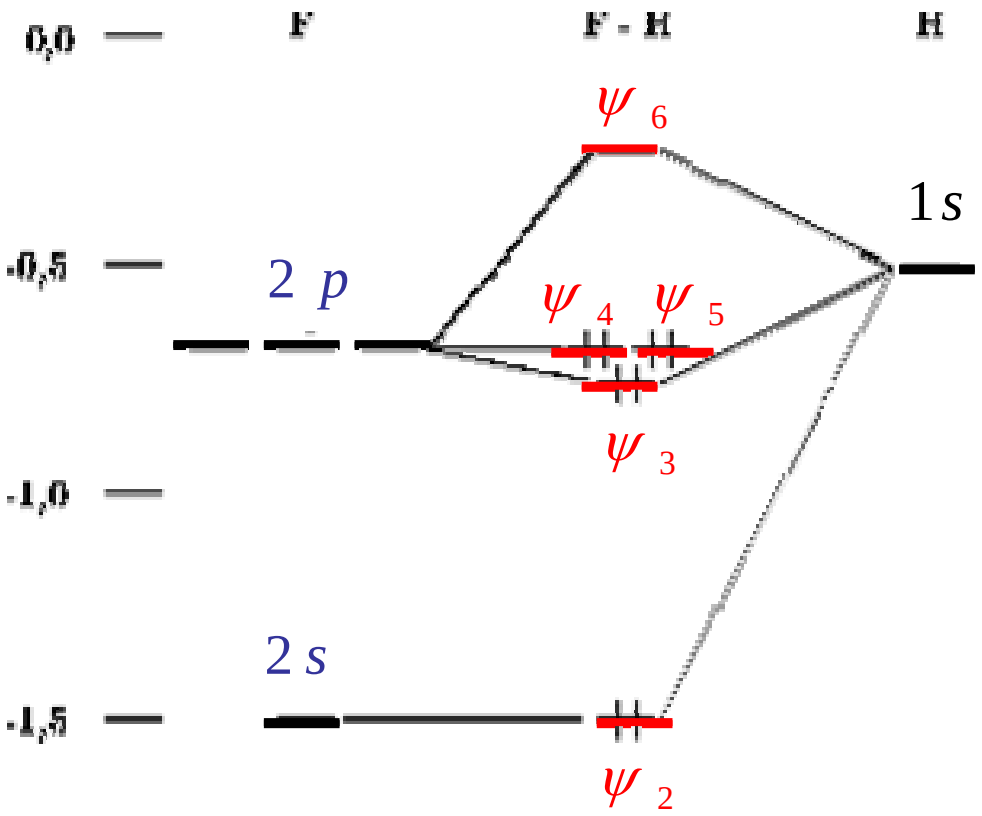
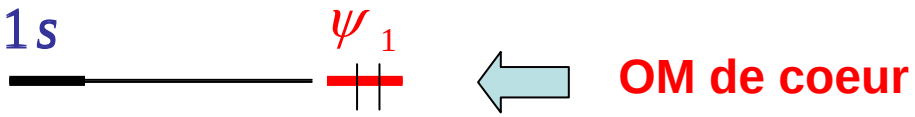
$\psi_3 \cong 2p_{\mathrm{z,F}} + t1s_H \quad 0 < t < 1$ OM liante

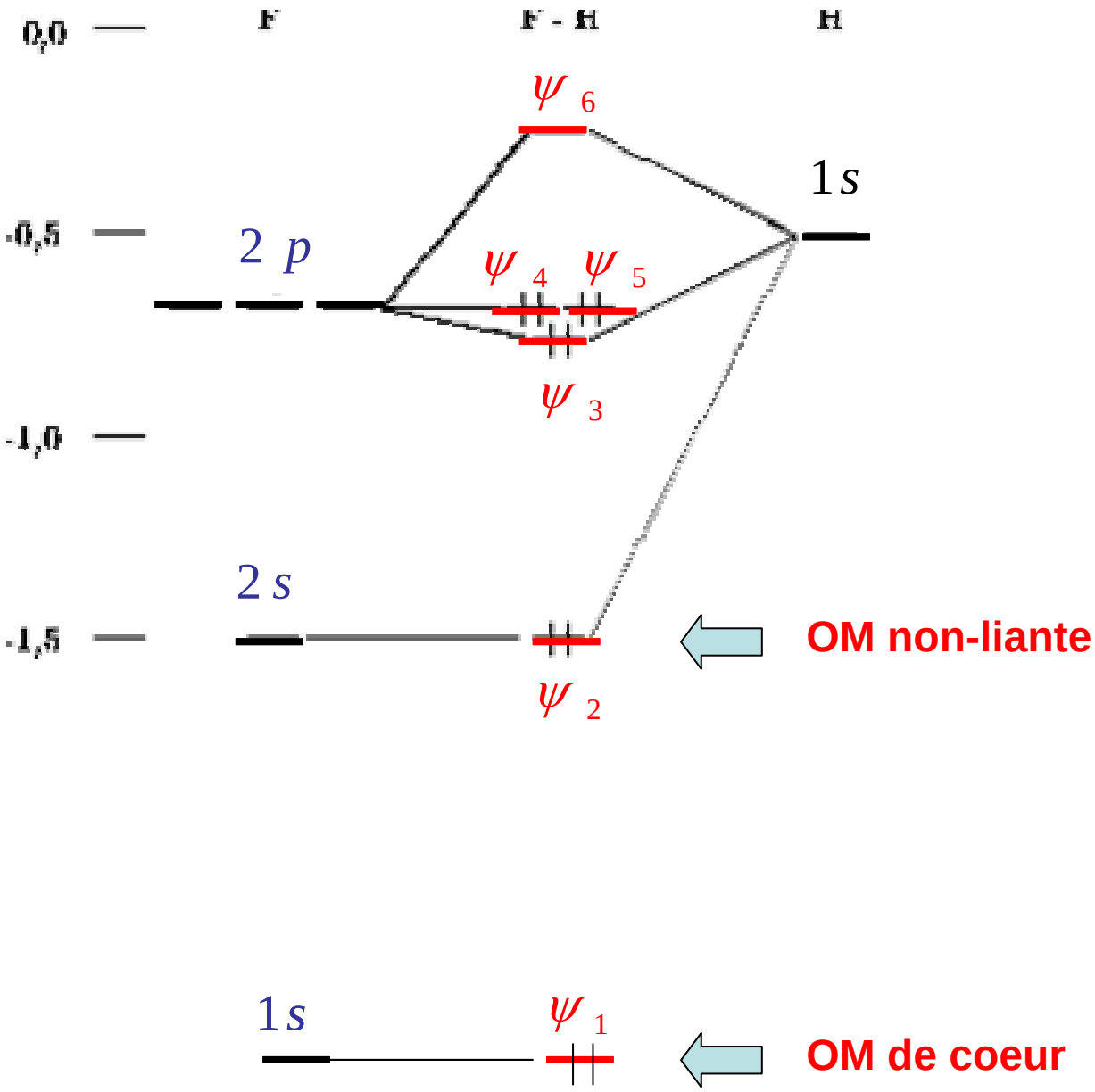
$\psi_4 \cong 2p_{\mathrm{x,F}} \quad \psi_5 \cong 2p_{\mathrm{y,F}}$ OM non-liante

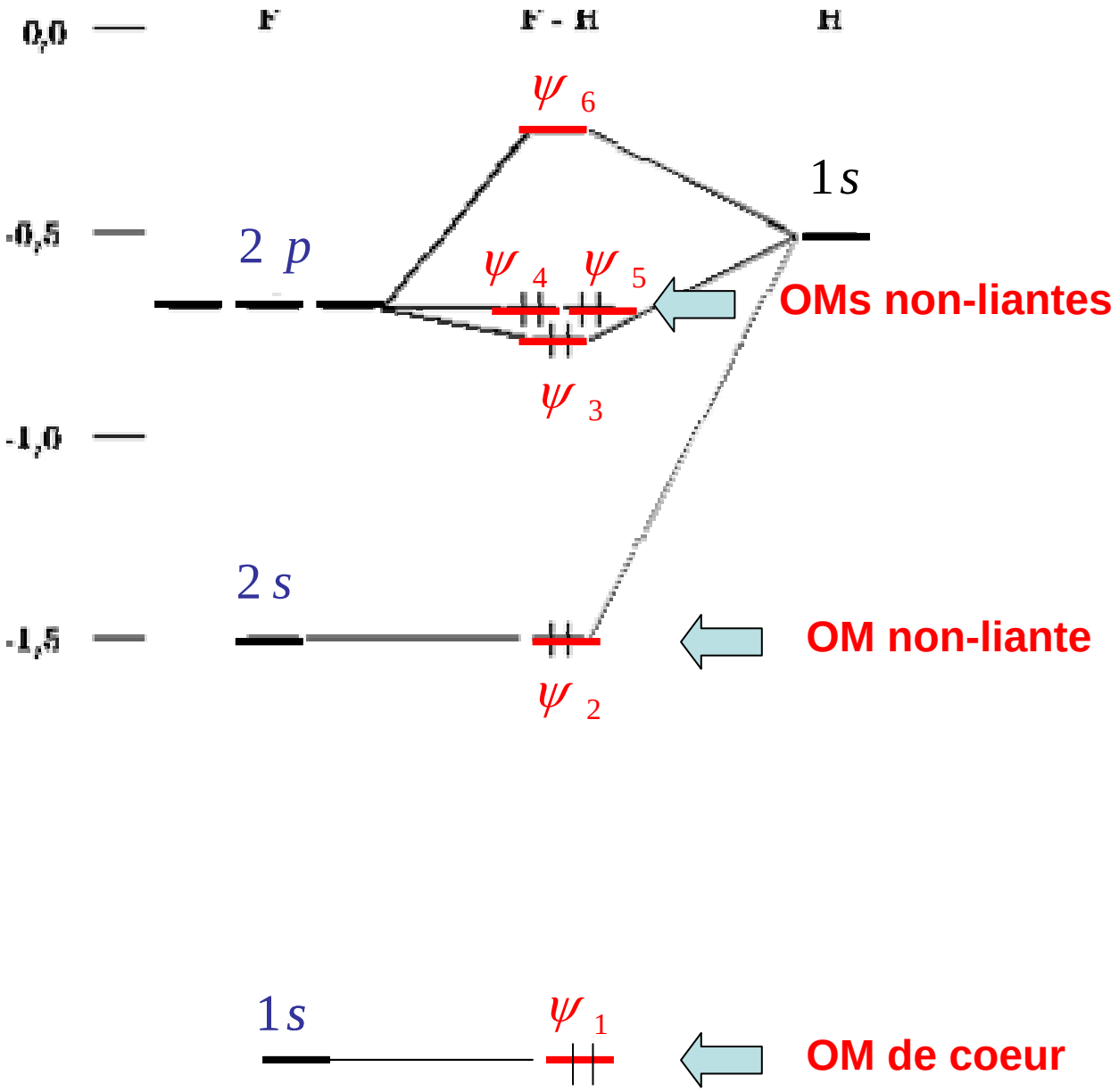
$\psi_6 \cong 1s_H - t2p_{\mathrm{z,F}} \quad 0 < t < 1$ OM anti-liante

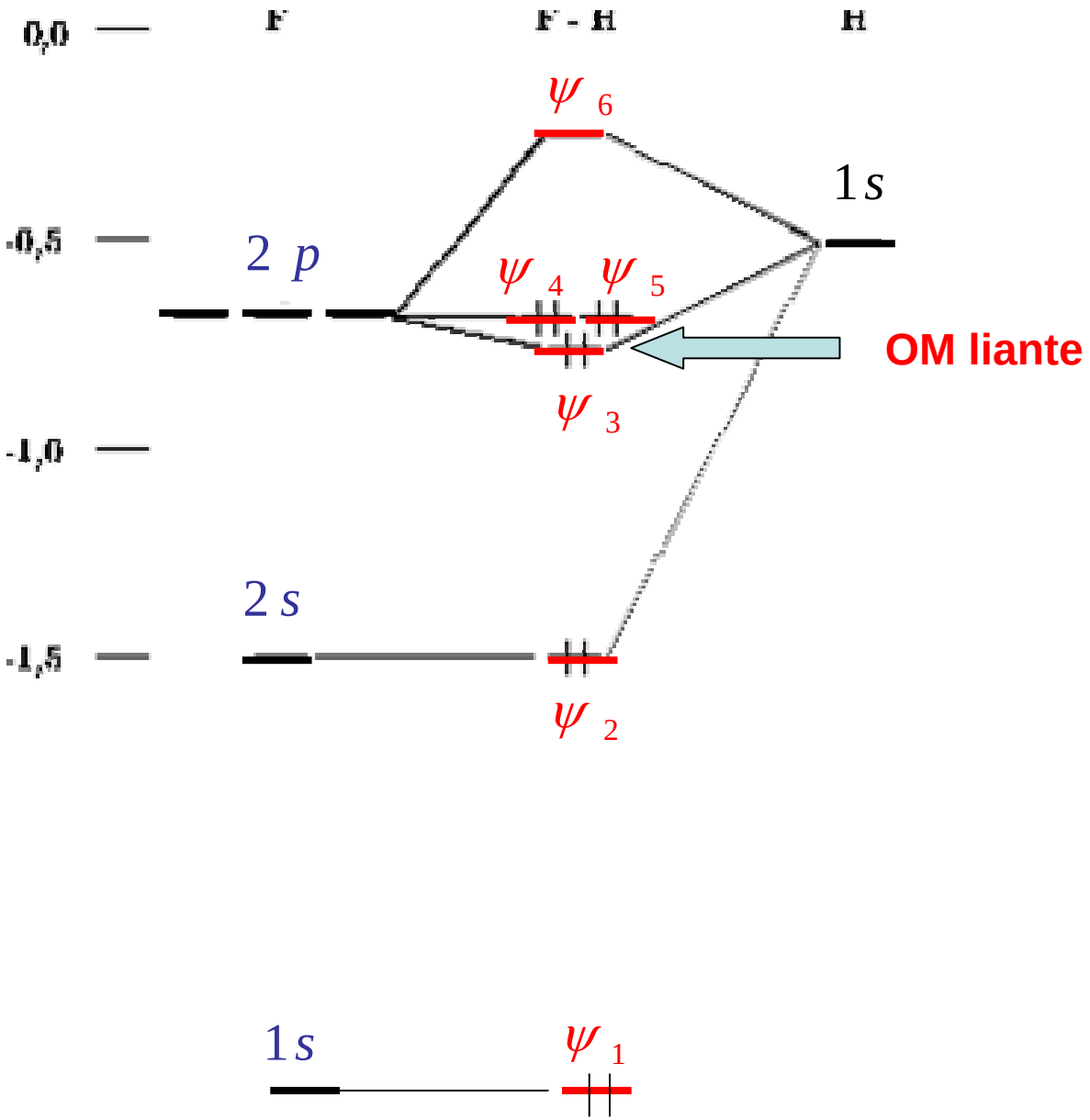

0,0
-0,5
-1,0
-1,5
F
F - H
H
ψ 6
1s
2 p
ψ 4
ψ 5
ψ 3
2 s
ψ 2
1s
ψ 1

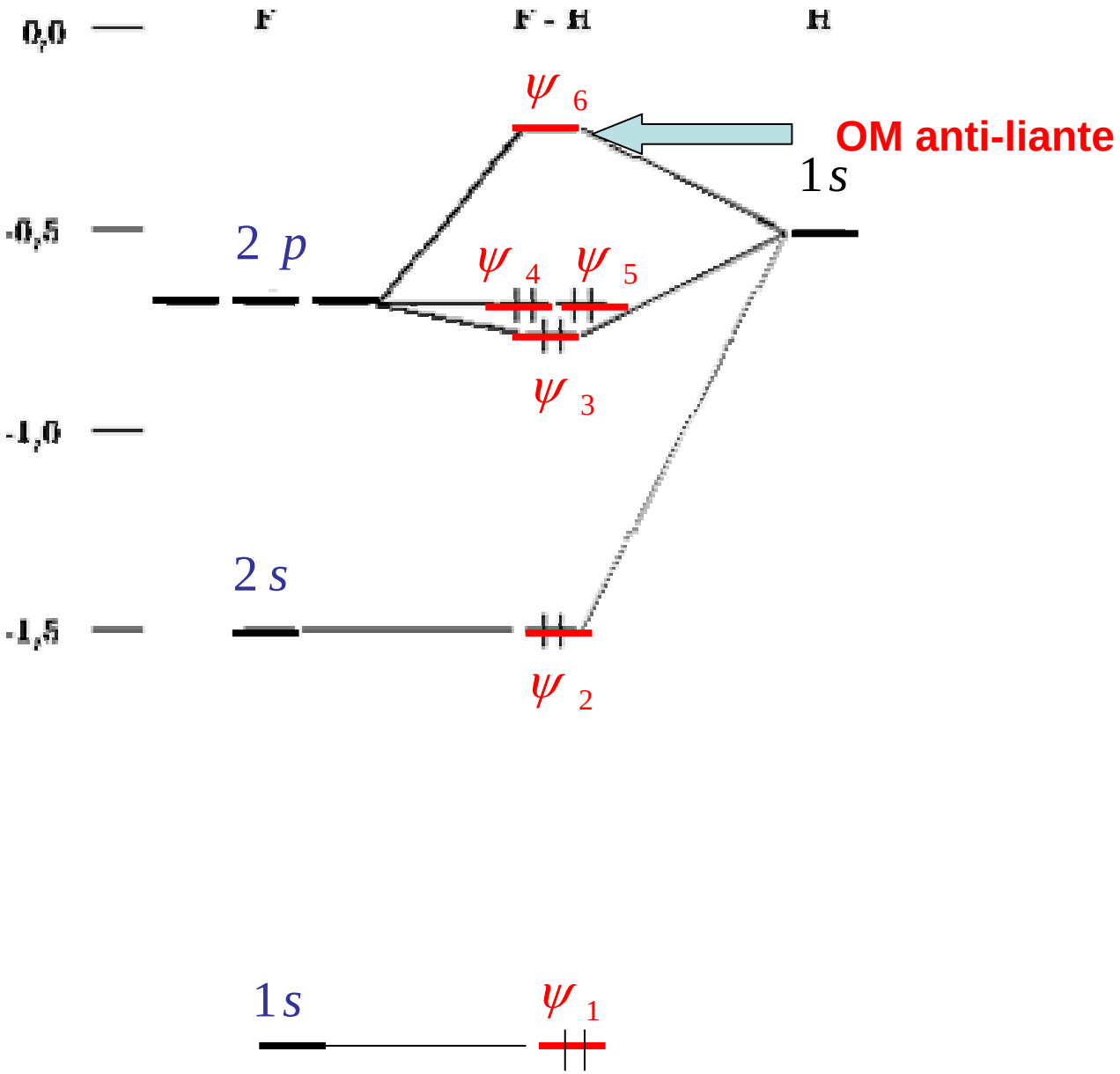

0,0
-0,5
-1,0
-1,5
F
F - H
H
ψ 6
1 s
2 p
ψ 4
ψ 5
ψ 3
2 s
ψ 2


1 s
ψ 1
OM de coeur


0,0
-0,5
-1,0
-1,5
F
F - H
H
ψ 6
1s
2 p
ψ 4
ψ 5
ψ 3
2 s
ψ 2
OM non-liante
1s
ψ 1
OM de coeur

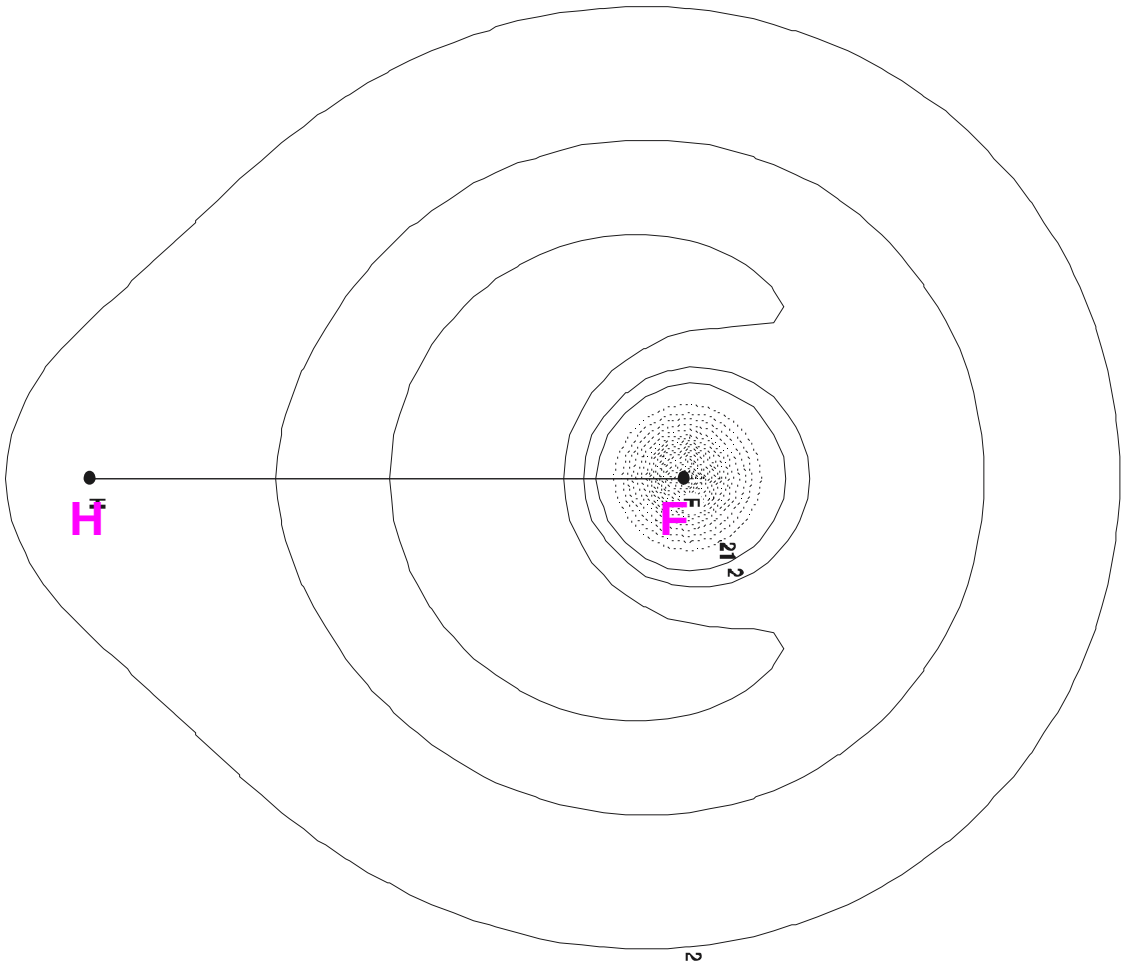

0,0
-0,5
-1,0
-1,5
F
F - H
H
ψ 6
1s
2 p
ψ 4
ψ 5
OMs non-liantes
ψ 3
2 s
OM non-liante
ψ 2
1s
ψ 1
OM de coeur

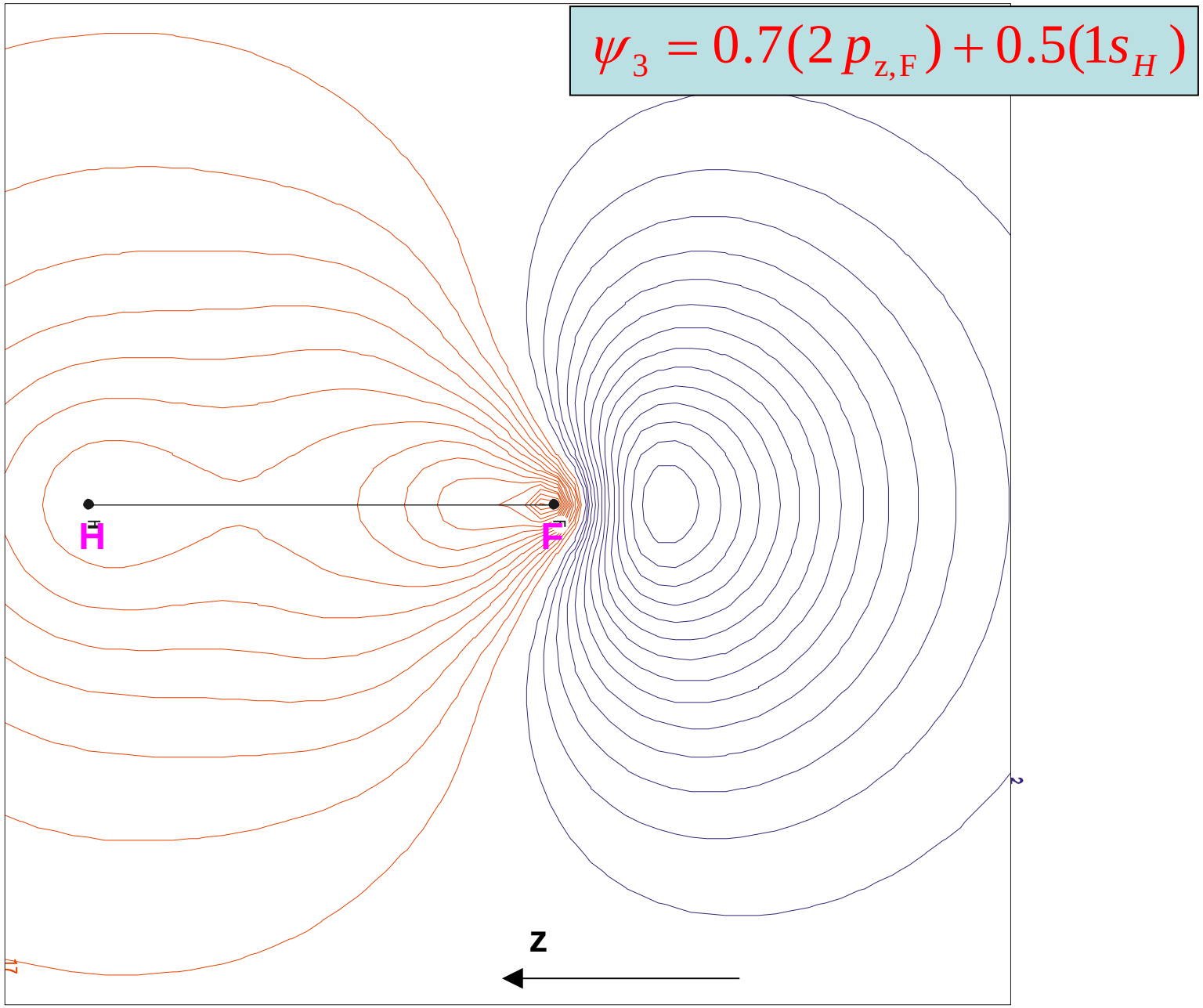

0,0
-0,5
-1,0
-1,5
F
F - H
H
ψ 6
1s
2 p
ψ 4
ψ 5
OM liante
ψ 3
2 s
ψ 2
1s
ψ 1


0,0
-0,5
-1,0
-1,5
F
F - H
H
ψ 6
OM anti-liante
1 s
2 p
ψ 4
ψ 5
ψ 3
2 s
ψ 2
1 s
ψ 1

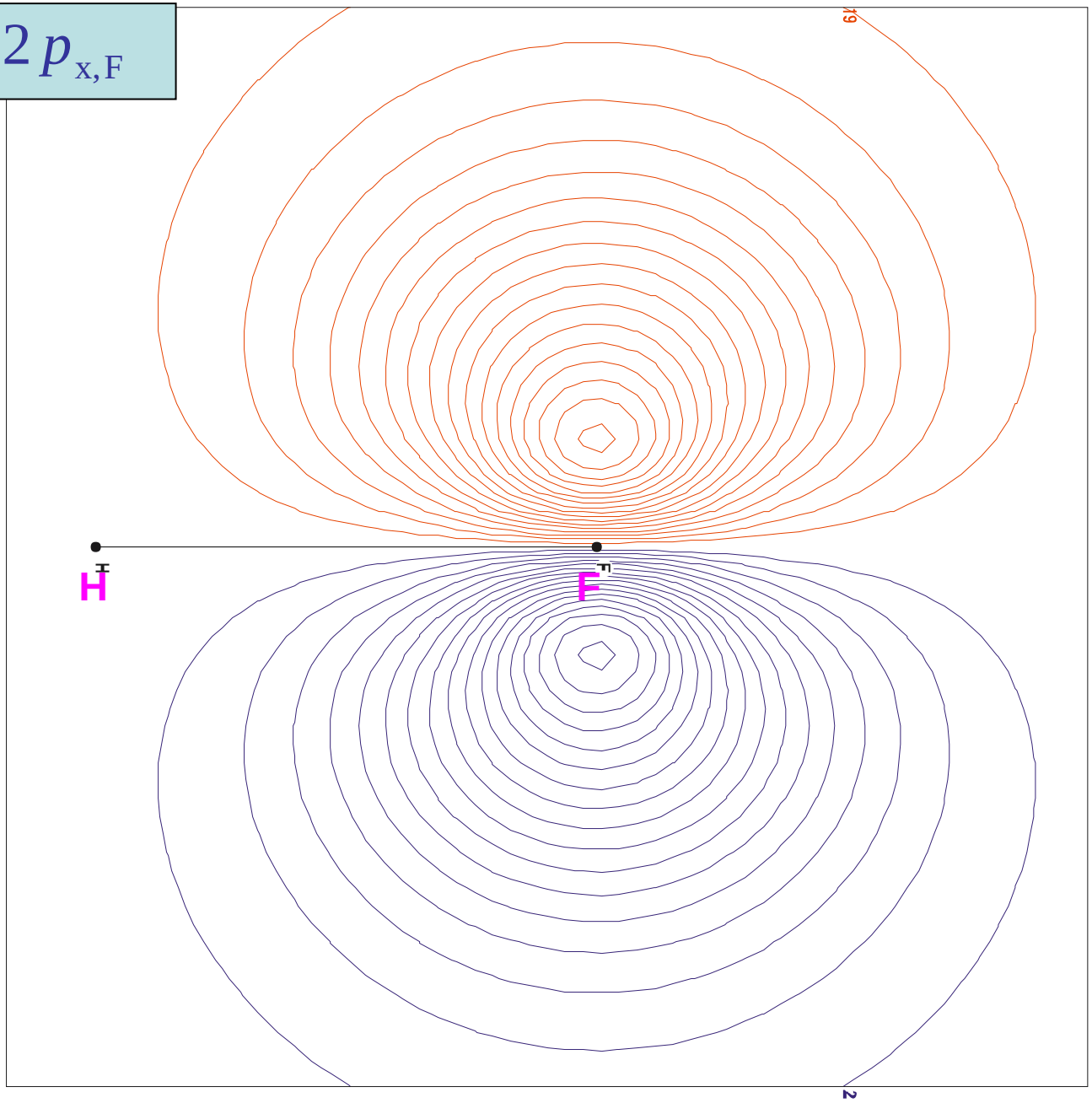
$$\psi_1 \cong 1s_F$$

$\psi_2 \cong 2s_F$




$\psi_3 = 0.7(2p_{z,F}) + 0.5(1s_H)$
H
F
z

$$\psi_4 \cong 2p_{x,F}$$



$$\psi_6 \cong 1s_H - 0.8(2p_{z,F})$$