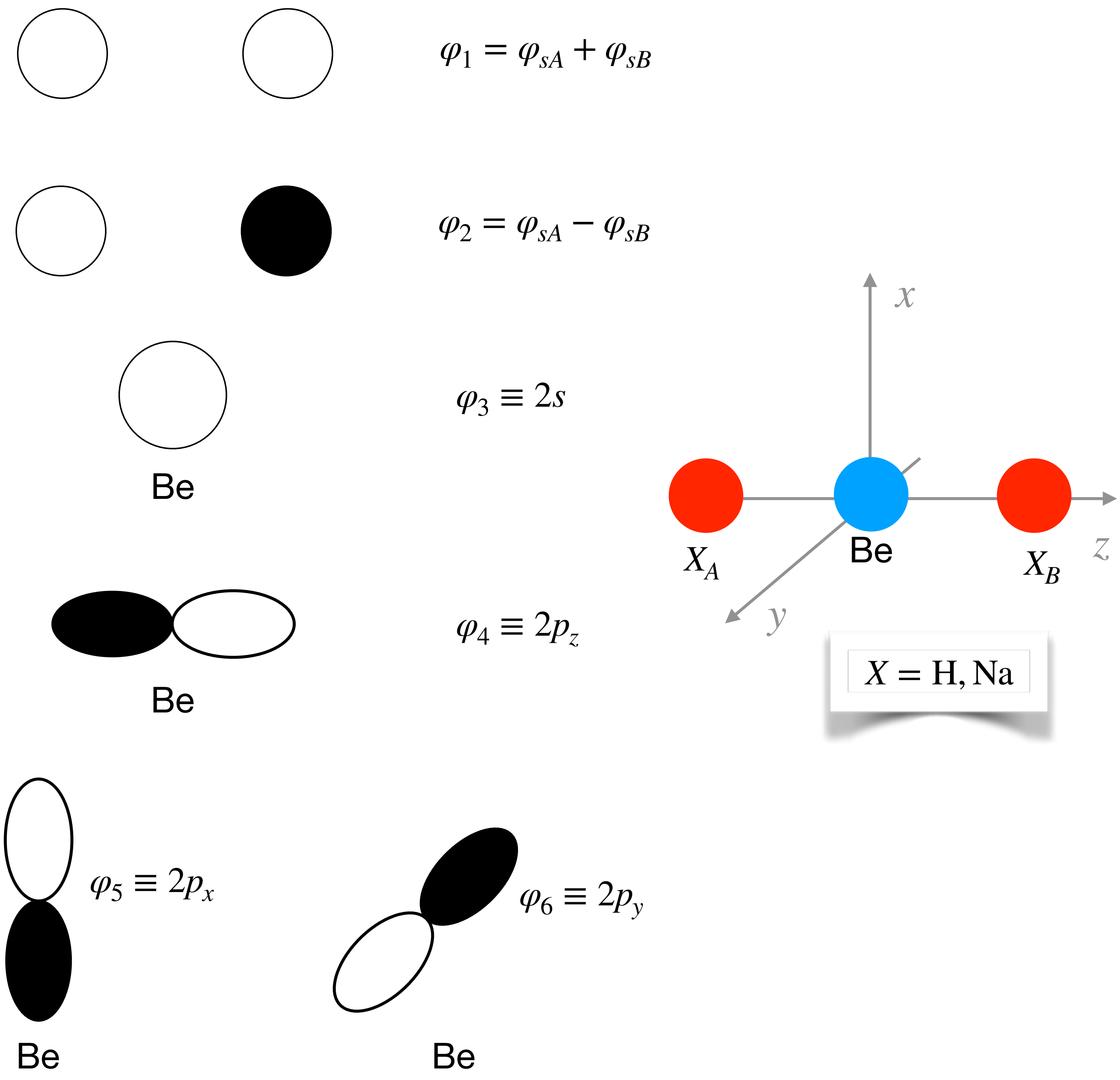
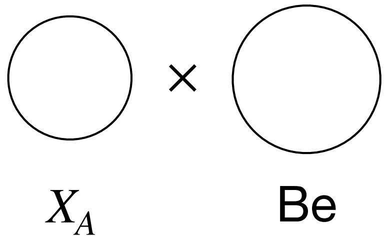
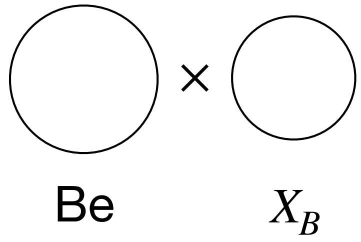


$\varphi_1 = \varphi_{sA} + \varphi_{sB}$
$\varphi_2 = \varphi_{sA} - \varphi_{sB}$
$\varphi_3 \equiv 2s$
Be
$\varphi_4 \equiv 2p_z$
Be
$\varphi_5 \equiv 2p_x$
Be
$\varphi_6 \equiv 2p_y$
Be
x
X_A
Be
X_B
z
y
$X =$ H, Na

$$\int d\mathbf{r}\,\varphi_3(\mathbf{r}) \times \varphi_{s_A}(\mathbf{r}) \equiv \int d\mathbf{r}$$

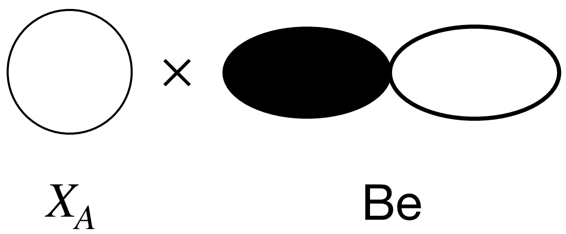


$$= \int d\mathbf{r}$$

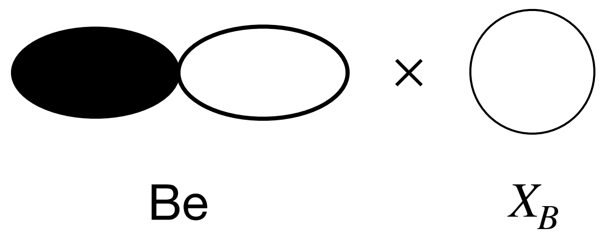


$$= \int d\mathbf{r}\,\varphi_3(\mathbf{r}) \times \varphi_{s_B}(\mathbf{r}) > 0$$

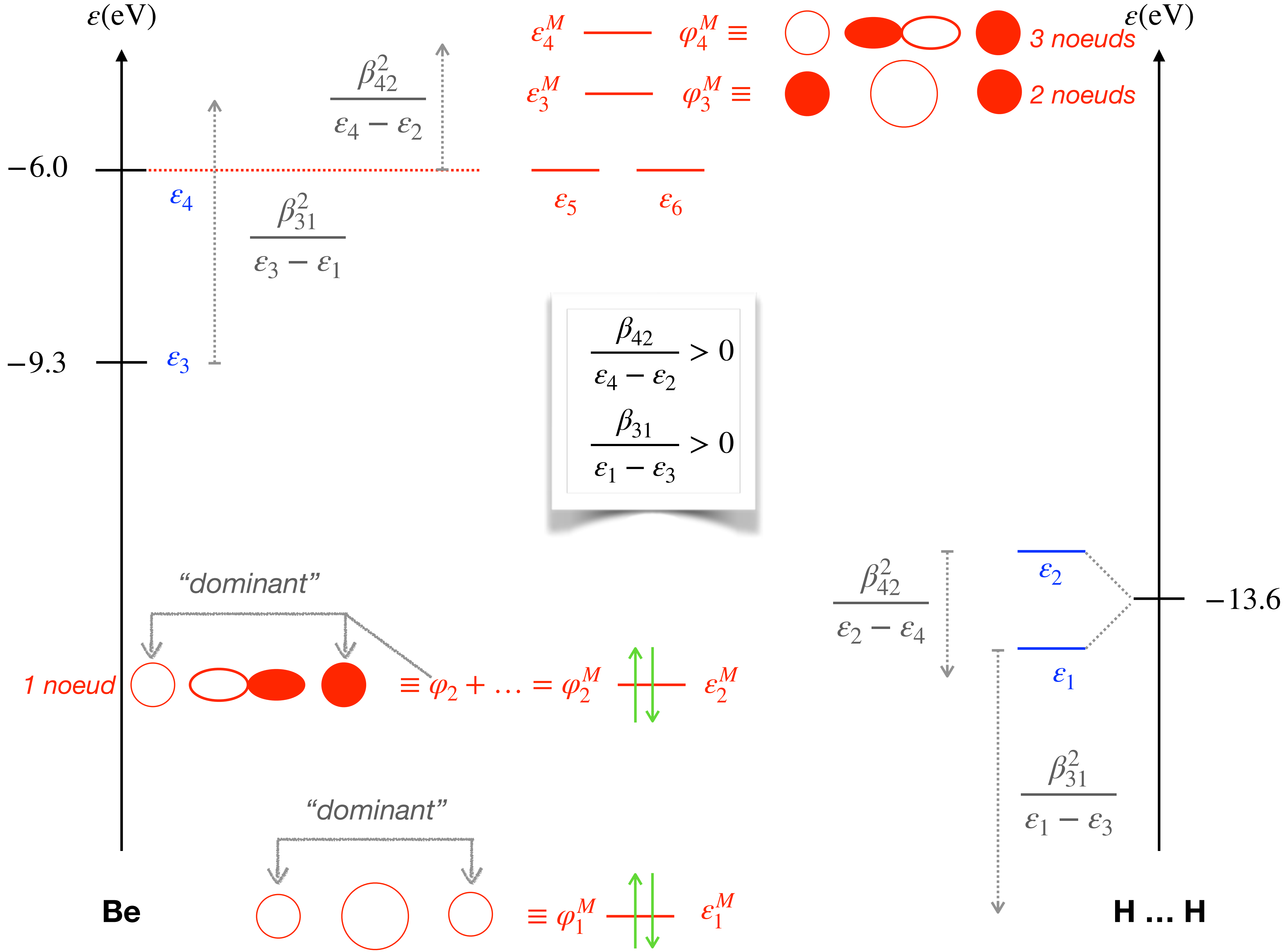
$$\int d\mathbf{r}\,\varphi_4(\mathbf{r}) \times \varphi_{s_A}(\mathbf{r}) \equiv \int d\mathbf{r}$$



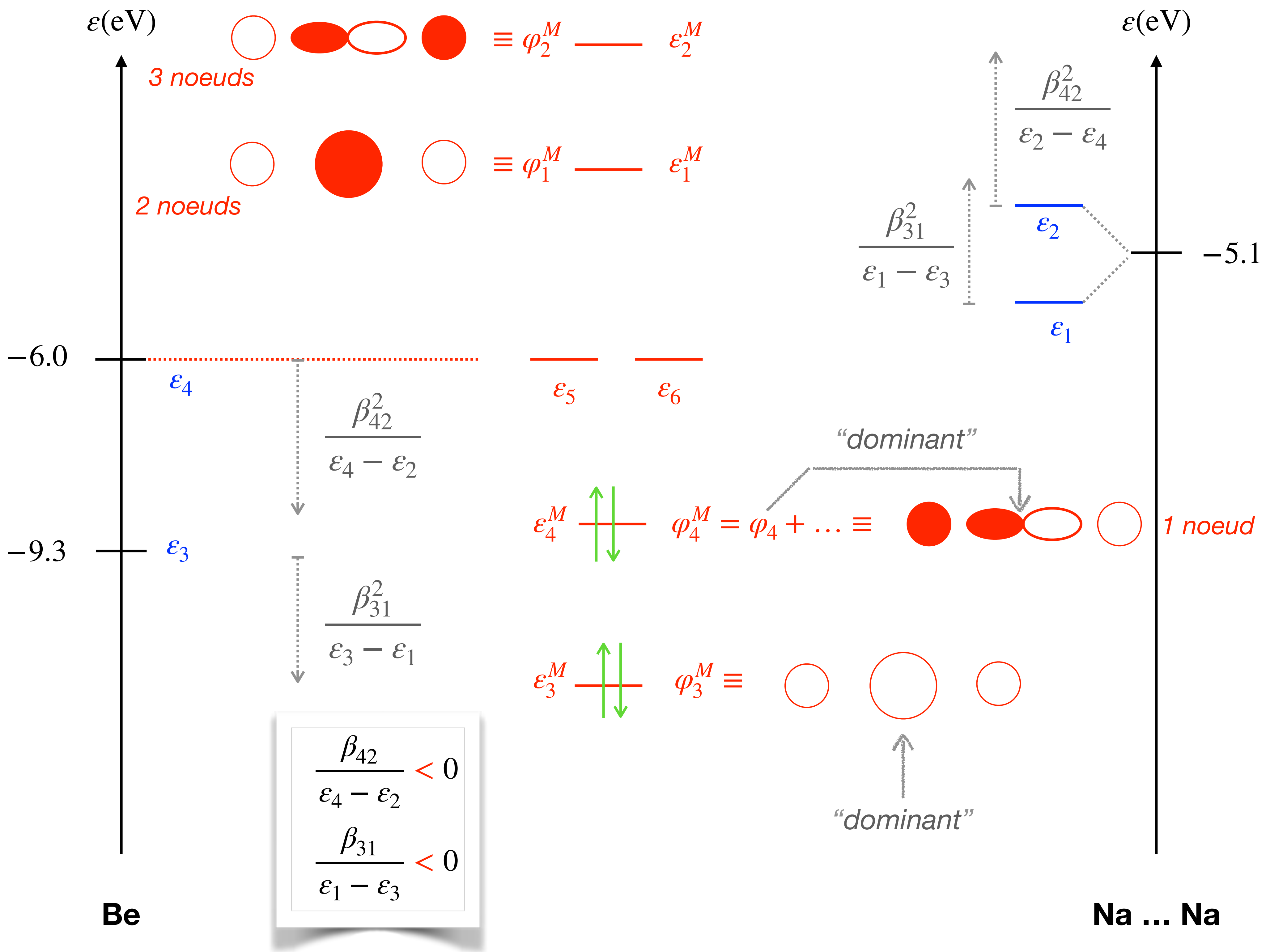
$$= - \int d\mathbf{r}$$



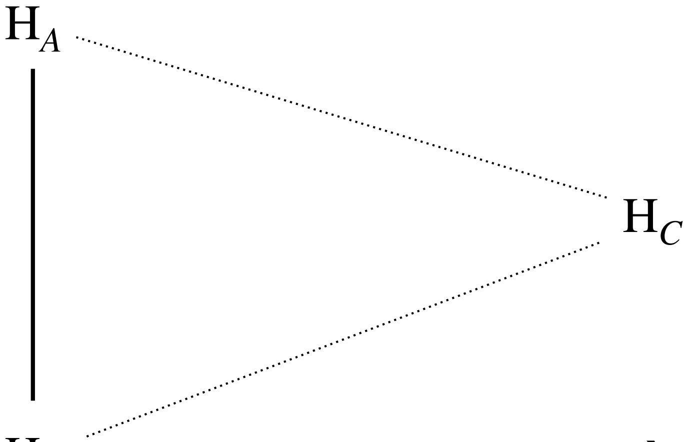
$$= - \int d\mathbf{r}\,\varphi_4(\mathbf{r}) \times \varphi_{s_B}(\mathbf{r}) < 0$$



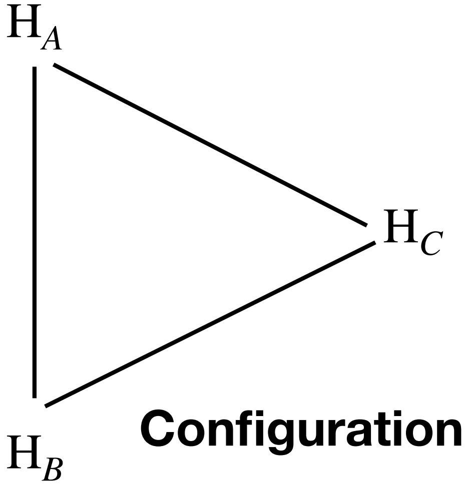
ε(eV)
ε(eV)
−6.0
−9.3
−13.6
3 noeuds
2 noeuds
1 noeud
"dominant"
"dominant"
Be
H … H



ε(eV)
$\equiv \varphi_2^M$
ε_2^M
3 noeuds
$\equiv \varphi_1^M$
ε_1^M
2 noeuds
-6.0
ε_4
ε_5
ε_6
$\frac{\beta_{42}^2}{\varepsilon_4 - \varepsilon_2}$
-9.3
ε_3
$\frac{\beta_{31}^2}{\varepsilon_3 - \varepsilon_1}$
$\frac{\beta_{42}}{\varepsilon_4 - \varepsilon_2} < 0$
$\frac{\beta_{31}}{\varepsilon_1 - \varepsilon_3} < 0$
Be
ε(eV)
$\frac{\beta_{42}^2}{\varepsilon_2 - \varepsilon_4}$
$\frac{\beta_{31}^2}{\varepsilon_1 - \varepsilon_3}$
ε_2
-5.1
ε_1
"dominant"
ε_4^M
$\varphi_4^M = \varphi_4 + \ldots \equiv$
1 noeud
ε_3^M
$\varphi_3^M \equiv$
"dominant"
Na ... Na

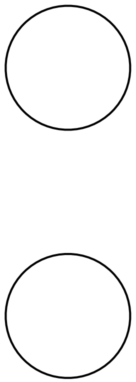


Configuration isocèle

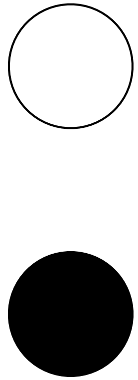


Configuration équilatérale

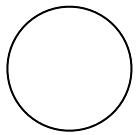
$$\varphi_1 = \varphi_{sA} + \varphi_{sB} \equiv$$

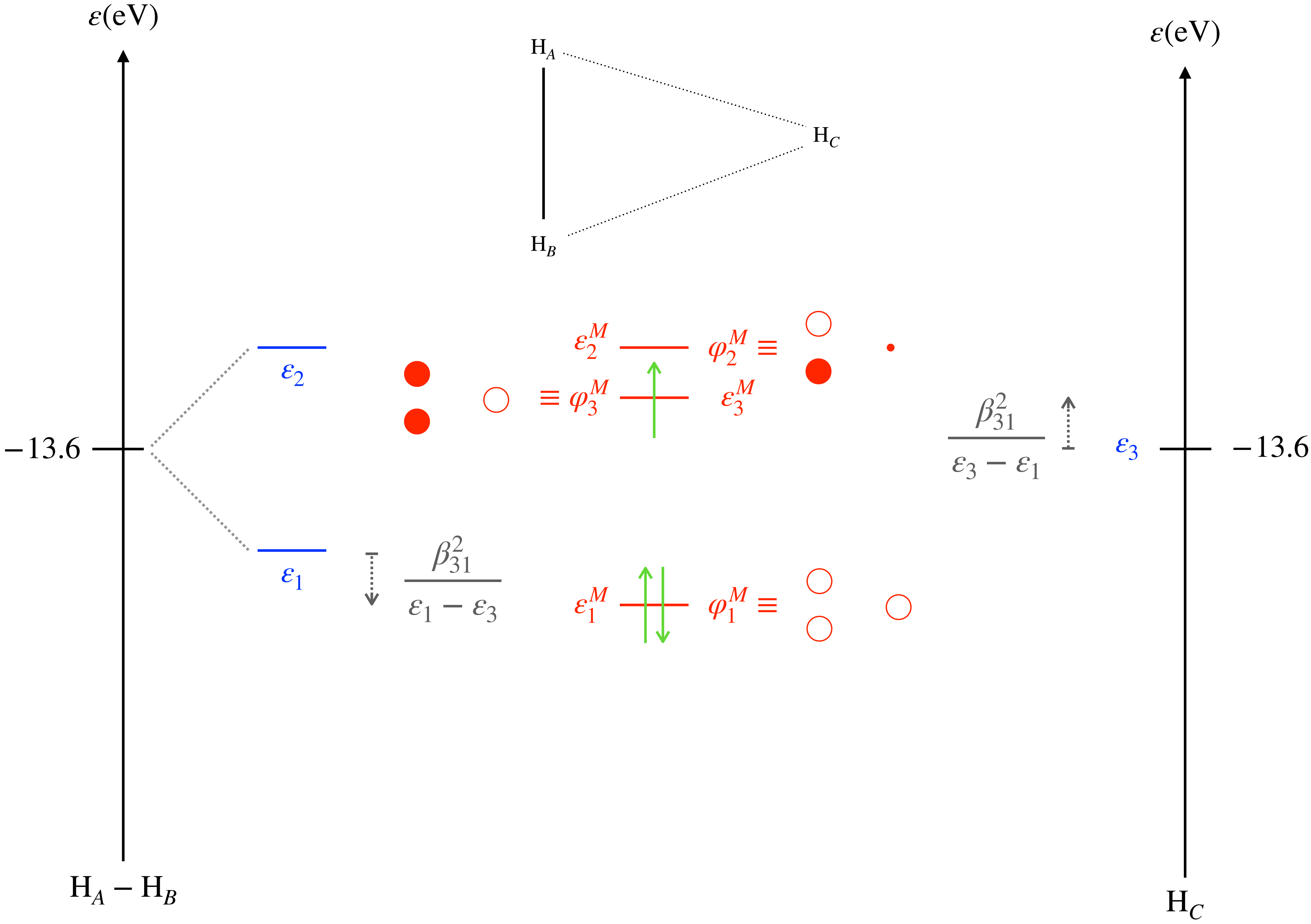


$$\varphi_2 = \varphi_{sA} - \varphi_{sB} \equiv$$

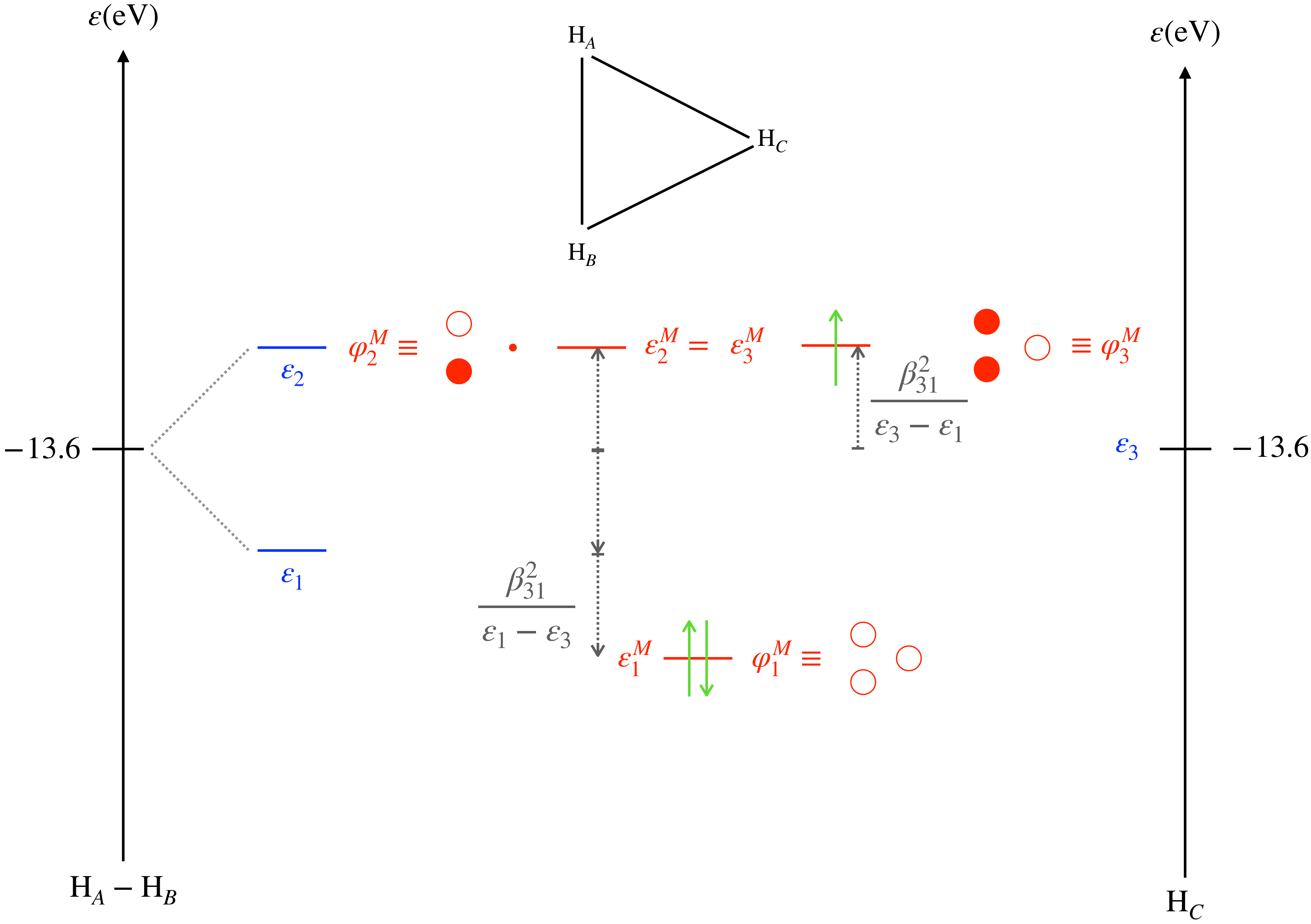


$$\varphi_3 = \varphi_{s_C} \equiv$$

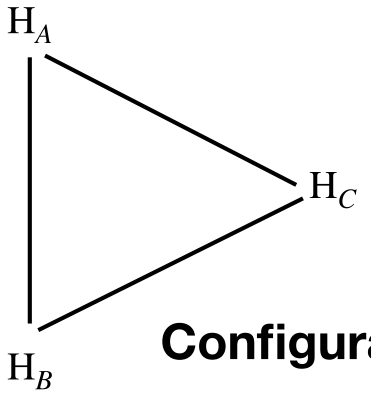




ε(eV)
H_A
H_B
H_C
−13.6
ε_2
ε_1
ε_2^M
ε_3^M
ε_1^M
≡ φ_3^M
φ_2^M ≡
φ_1^M ≡
β_31^2 / (ε_1 − ε_3)
β_31^2 / (ε_3 − ε_1)
ε_3
−13.6
ε(eV)
H_A − H_B
H_C



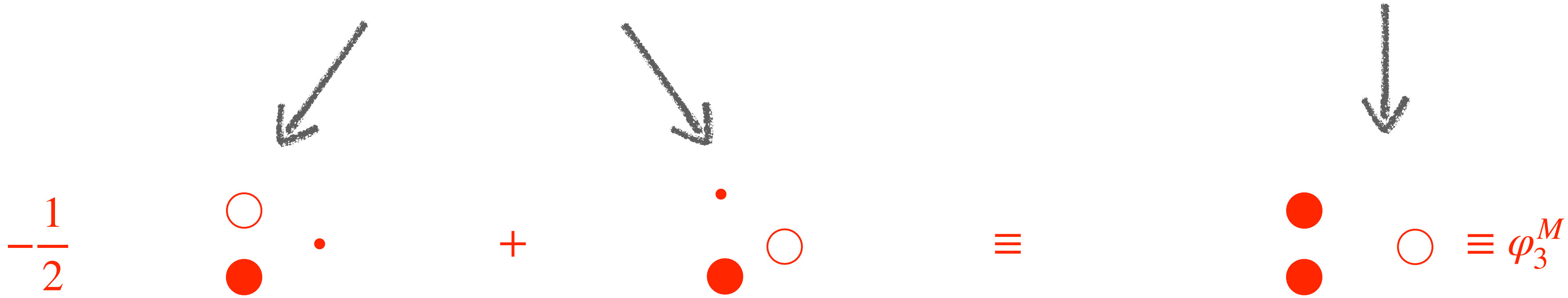
ε(eV)
H_A
H_B
H_C
ε(eV)
φ_2^M ≡
ε_2^M = ε_3^M
≡ φ_3^M
ε_2
−13.6
β_31^2 / (ε_3 − ε_1)
ε_3
−13.6
ε_1
β_31^2 / (ε_1 − ε_3)
ε_1^M
φ_1^M ≡
H_A − H_B
H_C



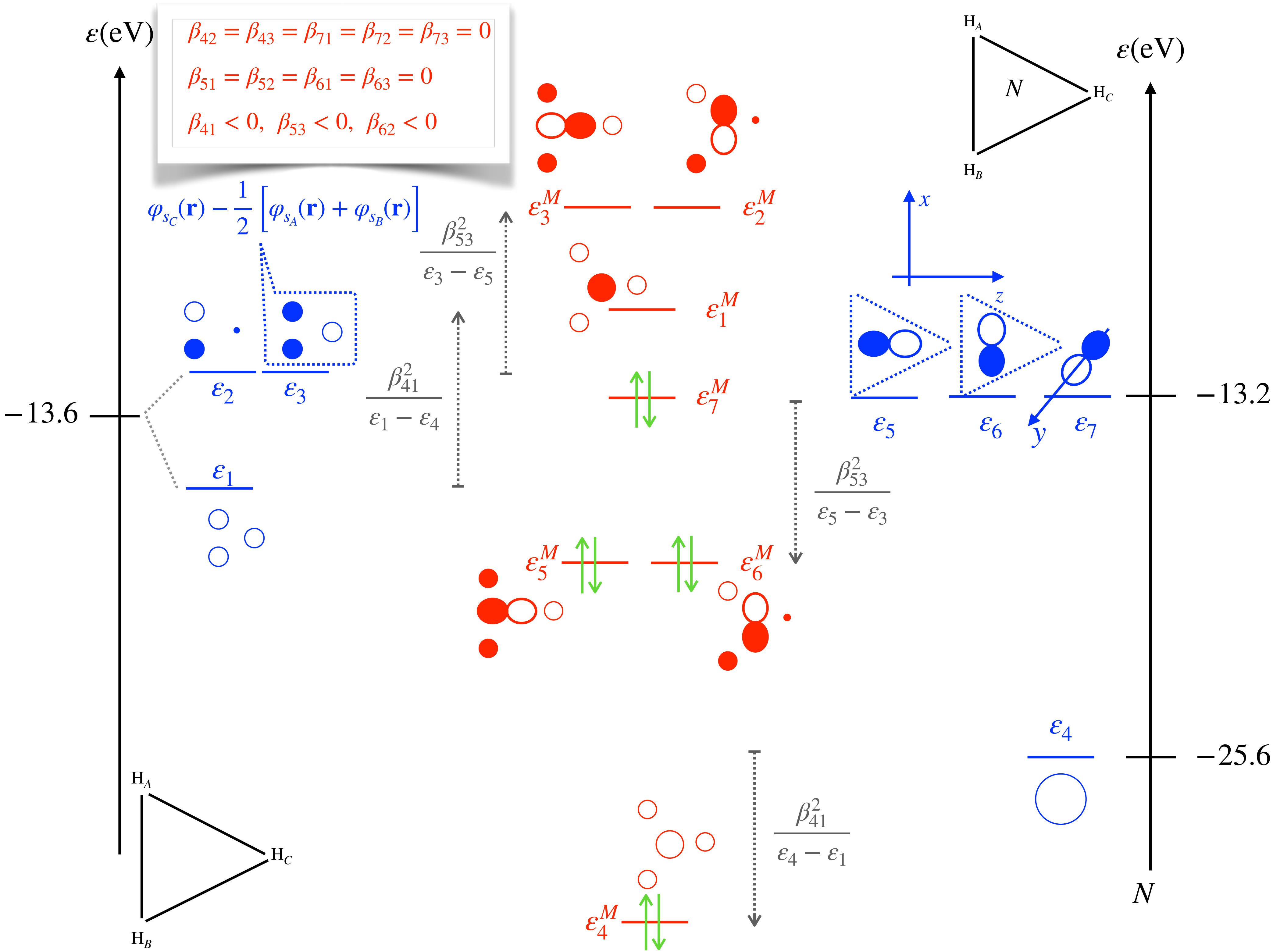
Configuration équilatérale

Orbitales "équivalentes" (et donc combinables) d'énergie ε_2^M

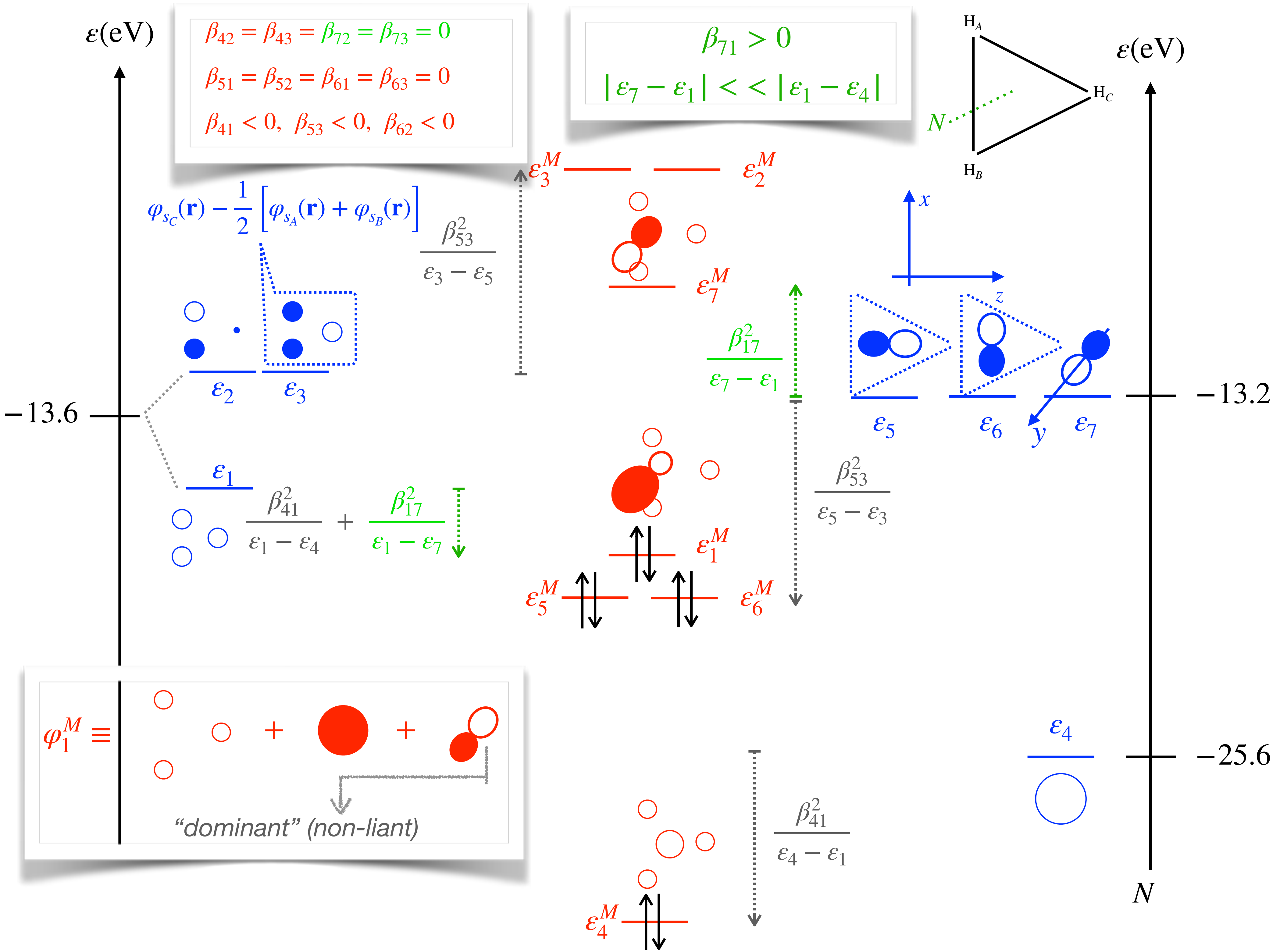
Orbitale de même énergie $\varepsilon_3^M = \varepsilon_2^M$



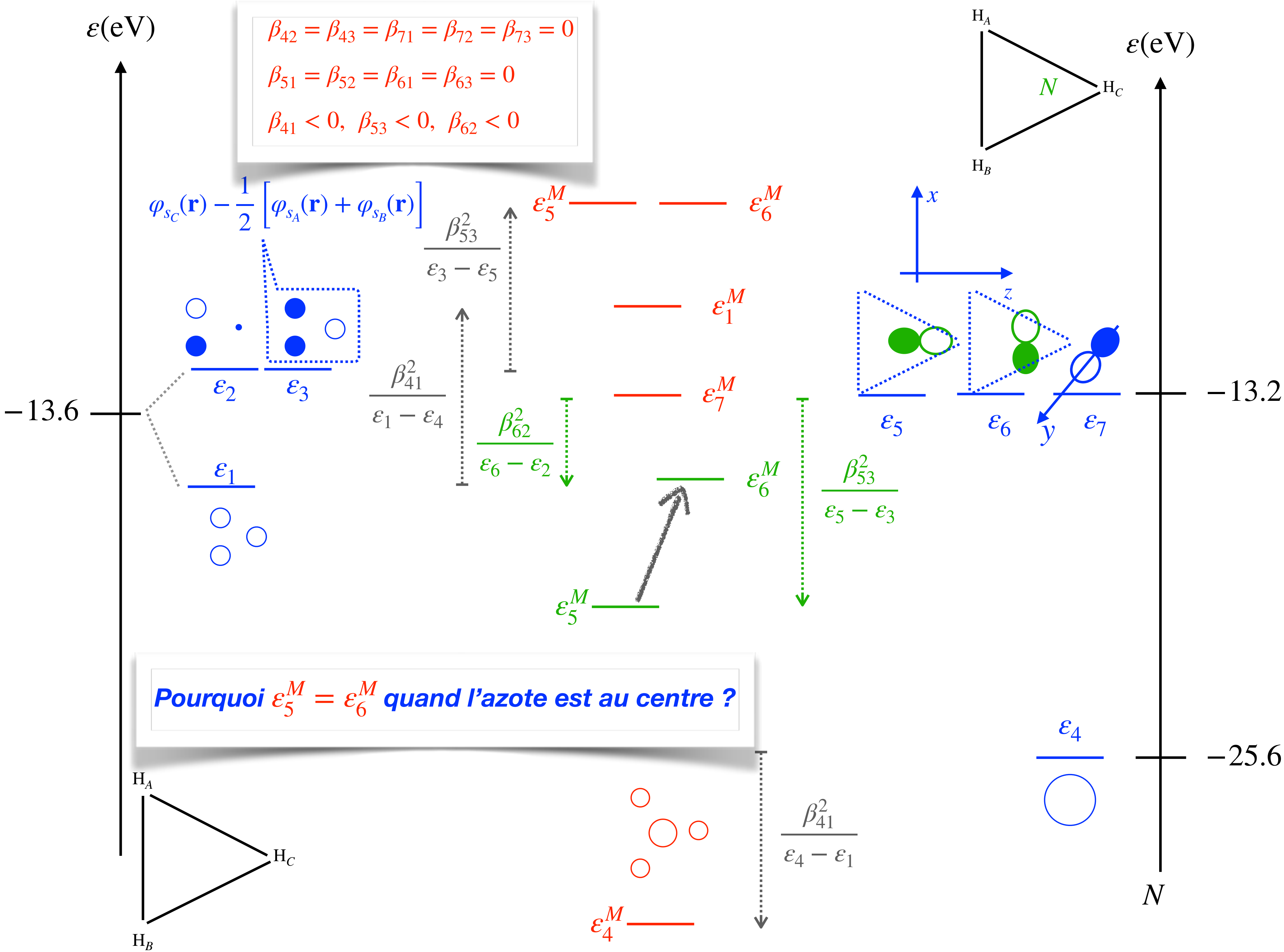
$$\varphi_{s_A}(\mathbf{r}) - \varphi_{s_B}(\mathbf{r}) \qquad \varphi_{s_C}(\mathbf{r}) - \varphi_{s_B}(\mathbf{r}) \qquad \varphi_{s_C}(\mathbf{r}) - \frac{1}{2}\left[\varphi_{s_A}(\mathbf{r}) + \varphi_{s_B}(\mathbf{r})\right]$$



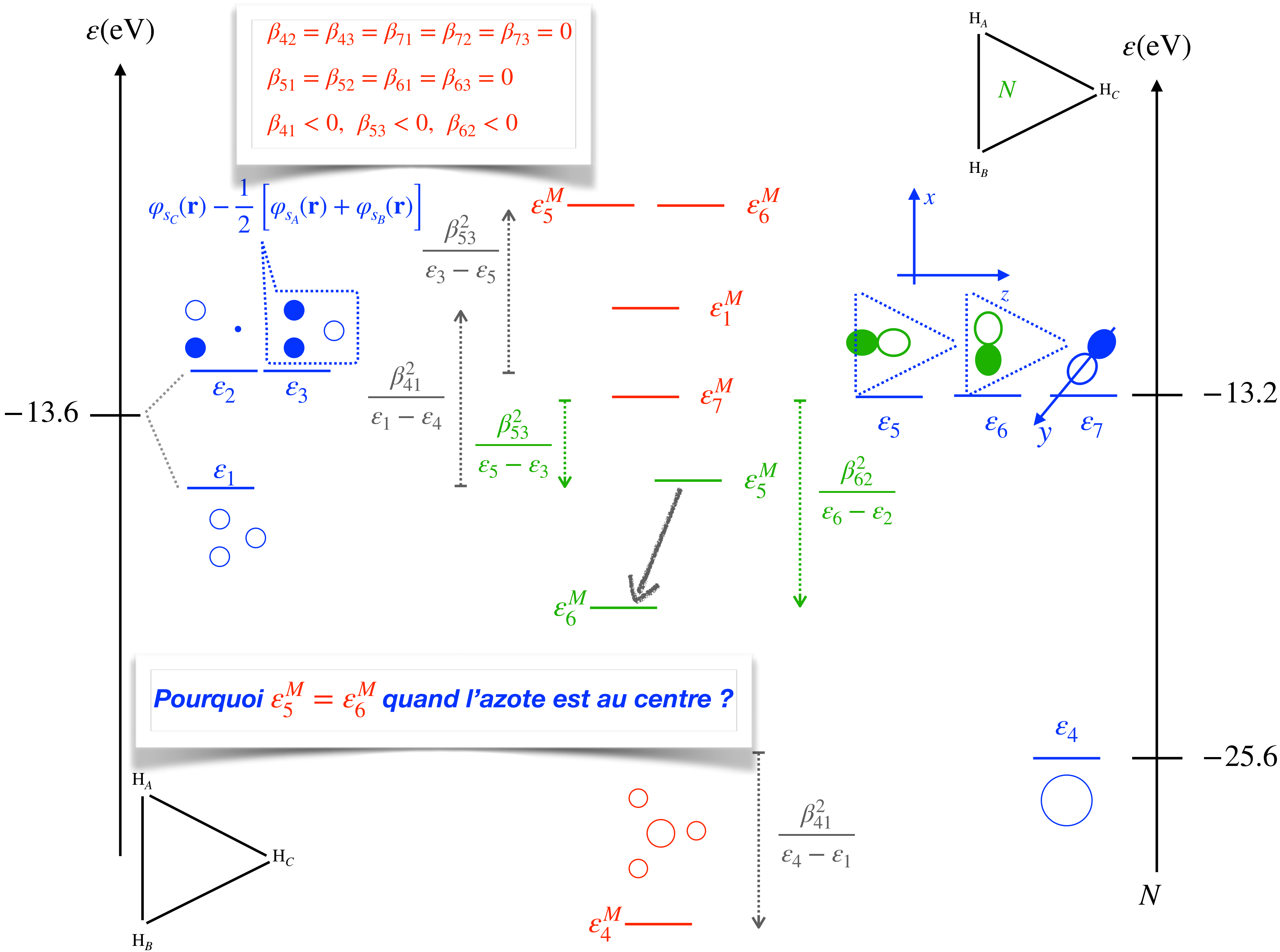
ε(eV)
$\beta_{42} = \beta_{43} = \beta_{71} = \beta_{72} = \beta_{73} = 0$
$\beta_{51} = \beta_{52} = \beta_{61} = \beta_{63} = 0$
$\beta_{41} < 0,\ \beta_{53} < 0,\ \beta_{62} < 0$
$\varphi_{s_C}(\mathbf{r}) - \frac{1}{2}\left[\varphi_{s_A}(\mathbf{r}) + \varphi_{s_B}(\mathbf{r})\right]$
$\frac{\beta_{53}^2}{\varepsilon_3 - \varepsilon_5}$
$\frac{\beta_{41}^2}{\varepsilon_1 - \varepsilon_4}$
$\frac{\beta_{53}^2}{\varepsilon_5 - \varepsilon_3}$
$\frac{\beta_{41}^2}{\varepsilon_4 - \varepsilon_1}$
−13.6
−13.2
−25.6
ε_1 ε_2 ε_3 ε_4 ε_5 ε_6 ε_7
ε_1^M ε_2^M ε_3^M ε_4^M ε_5^M ε_6^M ε_7^M
H_A H_B H_C
N
x y z



ε(eV)
β42 = β43 = β72 = β73 = 0
β51 = β52 = β61 = β63 = 0
β41 < 0, β53 < 0, β62 < 0
β71 > 0
|ε7 − ε1| << |ε1 − ε4|
HA
HB
HC
N
ε(eV)
φsC(r) − 1/2 [φsA(r) + φsB(r)]
β53² / (ε3 − ε5)
ε3M
ε2M
ε7M
x
z
y
β17² / (ε7 − ε1)
ε2
ε3
−13.6
ε1
β41² / (ε1 − ε4) + β17² / (ε1 − ε7)
ε5
ε6
ε7
−13.2
β53² / (ε5 − ε3)
ε1M
ε5M
ε6M
φ1M ≡
+
+
“dominant” (non-liant)
ε4
−25.6
β41² / (ε4 − ε1)
ε4M
N



ε(eV)
$\beta_{42} = \beta_{43} = \beta_{71} = \beta_{72} = \beta_{73} = 0$
$\beta_{51} = \beta_{52} = \beta_{61} = \beta_{63} = 0$
$\beta_{41} < 0, \ \beta_{53} < 0, \ \beta_{62} < 0$
$\varphi_{s_C}(\mathbf{r}) - \frac{1}{2}\left[\varphi_{s_A}(\mathbf{r}) + \varphi_{s_B}(\mathbf{r})\right]$
$\frac{\beta_{53}^2}{\varepsilon_3 - \varepsilon_5}$
ε_5^M
ε_6^M
ε_1^M
ε_7^M
ε_6^M
ε_5^M
ε_4^M
ε_2
ε_3
ε_1
-13.6
$\frac{\beta_{41}^2}{\varepsilon_1 - \varepsilon_4}$
$\frac{\beta_{62}^2}{\varepsilon_6 - \varepsilon_2}$
$\frac{\beta_{53}^2}{\varepsilon_5 - \varepsilon_3}$
$\frac{\beta_{41}^2}{\varepsilon_4 - \varepsilon_1}$
H_A
H_B
H_C
N
x
z
y
ε_5
ε_6
ε_7
ε_4
-13.2
-25.6
Pourquoi $\varepsilon_5^M = \varepsilon_6^M$ quand l'azote est au centre ?



$\varepsilon(\text{eV})$
$\beta_{42} = \beta_{43} = \beta_{71} = \beta_{72} = \beta_{73} = 0$
$\beta_{51} = \beta_{52} = \beta_{61} = \beta_{63} = 0$
$\beta_{41} < 0,\ \beta_{53} < 0,\ \beta_{62} < 0$
H_A
N
H_C
H_B
$\varepsilon(\text{eV})$
$\varphi_{s_C}(\mathbf{r}) - \frac{1}{2}\left[\varphi_{s_A}(\mathbf{r}) + \varphi_{s_B}(\mathbf{r})\right]$
$\frac{\beta_{53}^2}{\varepsilon_3 - \varepsilon_5}$
ε_5^M
ε_6^M
x
z
ε_1^M
$\frac{\beta_{41}^2}{\varepsilon_1 - \varepsilon_4}$
ε_2
ε_3
-13.6
$\frac{\beta_{53}^2}{\varepsilon_5 - \varepsilon_3}$
ε_7^M
ε_5
ε_6
y
ε_7
-13.2
ε_1
ε_5^M
$\frac{\beta_{62}^2}{\varepsilon_6 - \varepsilon_2}$
ε_6^M
Pourquoi $\varepsilon_5^M = \varepsilon_6^M$ *quand l'azote est au centre ?*
ε_4
-25.6
H_A
H_C
H_B
$\frac{\beta_{41}^2}{\varepsilon_4 - \varepsilon_1}$
ε_4^M
N