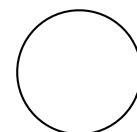
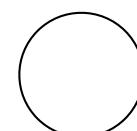


$$\varphi_1 = \varphi_{sA} + \varphi_{sB} \equiv$$

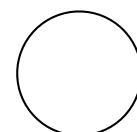


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$$\varphi_2 = \varphi_{sA} - \varphi_{sB} \equiv$$

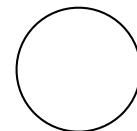


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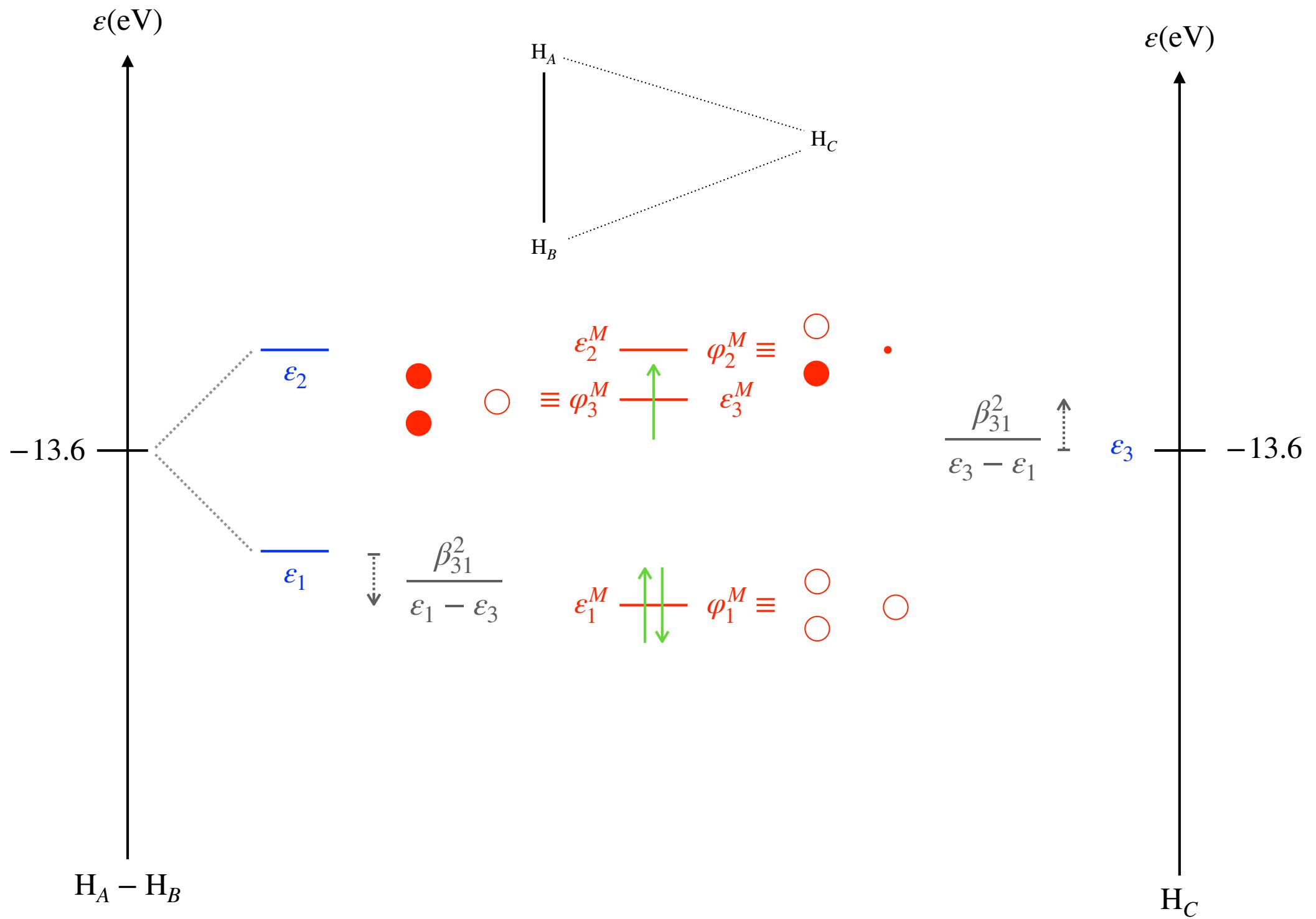


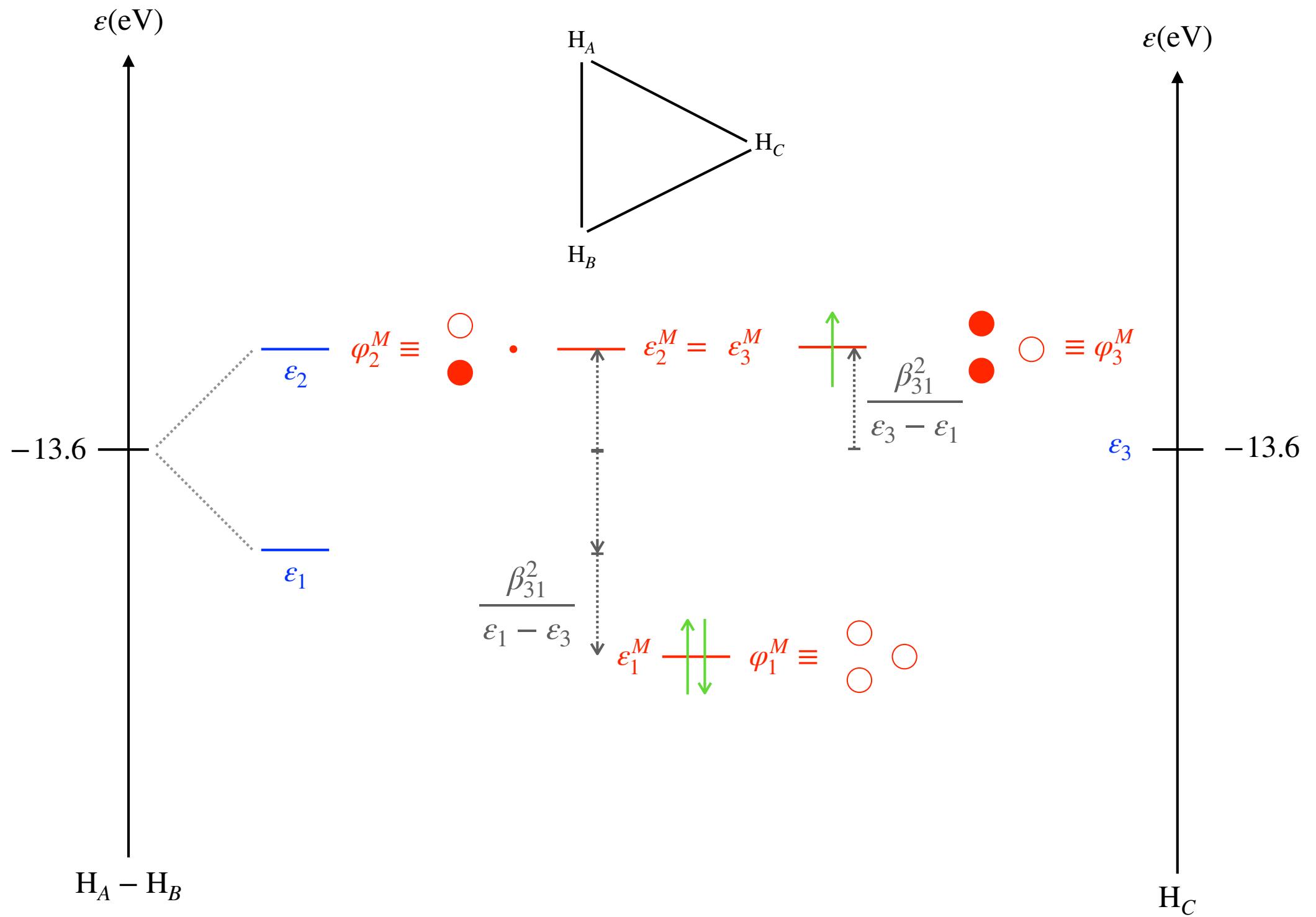
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$$\varphi_3 = \varphi_{sC} \equiv$$

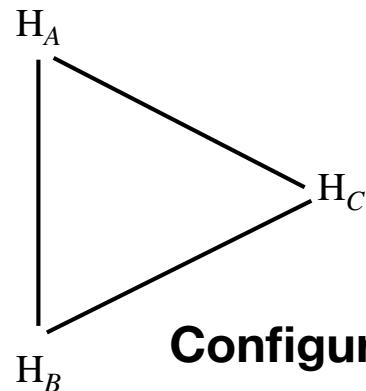


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Identification de l'orbitale φ_3^M



Configuration équilatérale

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



+



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



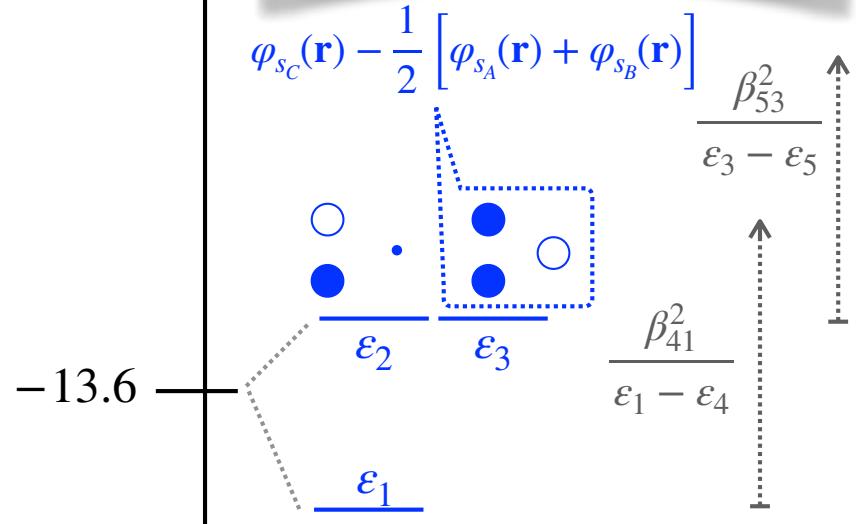
$$-\varphi_{s_A}(\mathbf{r}) + \varphi_{s_C}(\mathbf{r})$$

$$\varphi_{s_C}(\mathbf{r}) - \varphi_{s_B}(\mathbf{r})$$

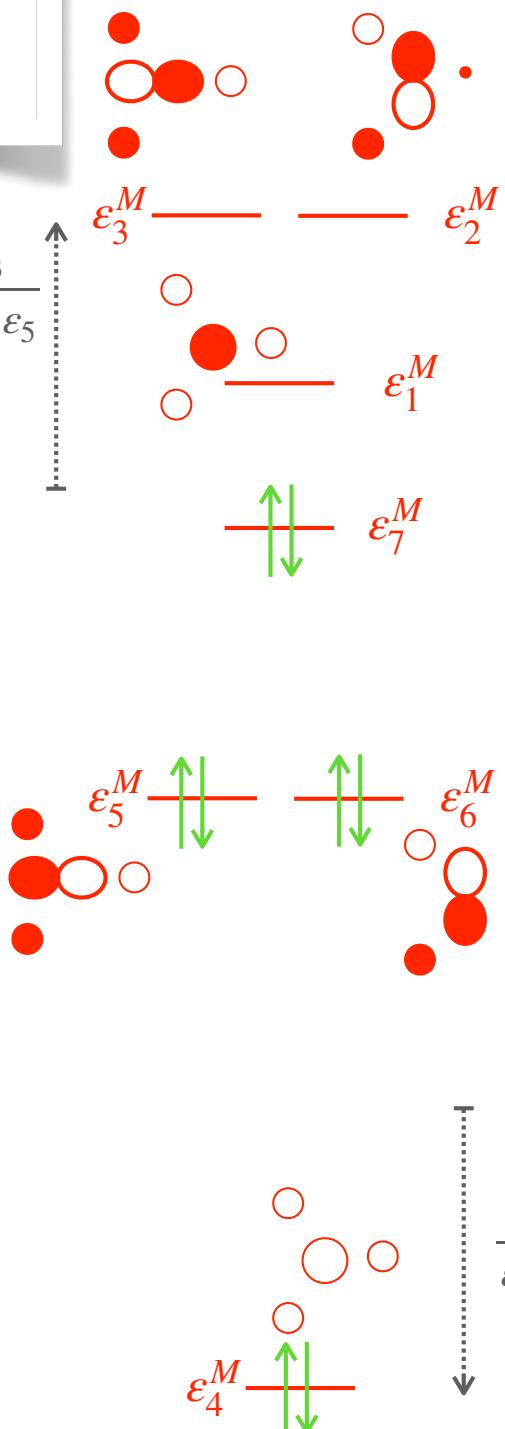
$$2 \left(\varphi_{s_C}(\mathbf{r}) - \frac{1}{2} [\varphi_{s_A}(\mathbf{r}) + \varphi_{s_B}(\mathbf{r})] \right)$$

$\varepsilon(\text{eV})$

$$\begin{aligned}\beta_{42} &= \beta_{43} = \beta_{71} = \beta_{72} = \beta_{73} = 0 \\ \beta_{51} &= \beta_{52} = \beta_{61} = \beta_{63} = 0 \\ \beta_{41} &< 0, \quad \beta_{53} < 0, \quad \beta_{62} < 0\end{aligned}$$



Géométrie plane

 H_A H_B H_C $\varepsilon(\text{eV})$ N x y z -13.2 -25.6 