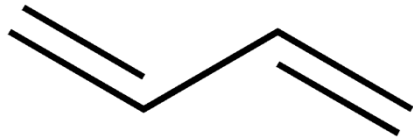


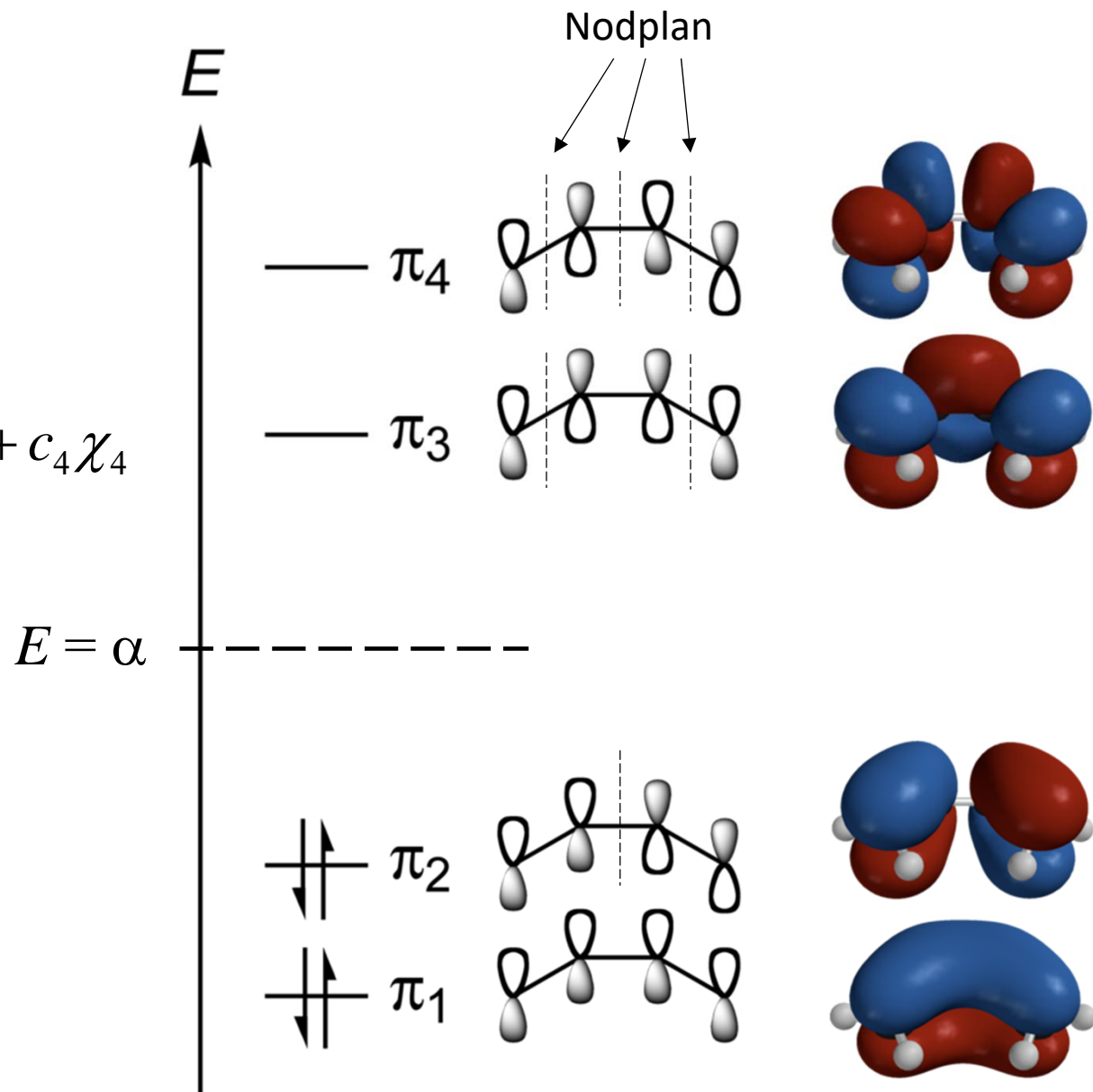
# MO för Butadien



$$\psi = c_1\chi_1 + c_2\chi_2 + c_3\chi_3 + c_4\chi_4$$

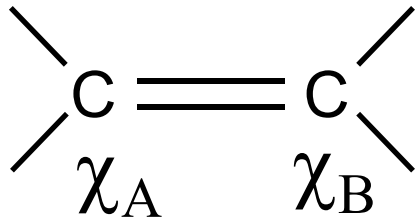
$$E = \alpha \pm 0,62 \beta$$

$$E = \alpha \pm 1,62 \beta$$



# Delokaliseringsenergi (Resonansenergi)

Eten:  $\pi$ -orbitaler, men *ingen* delokalisering

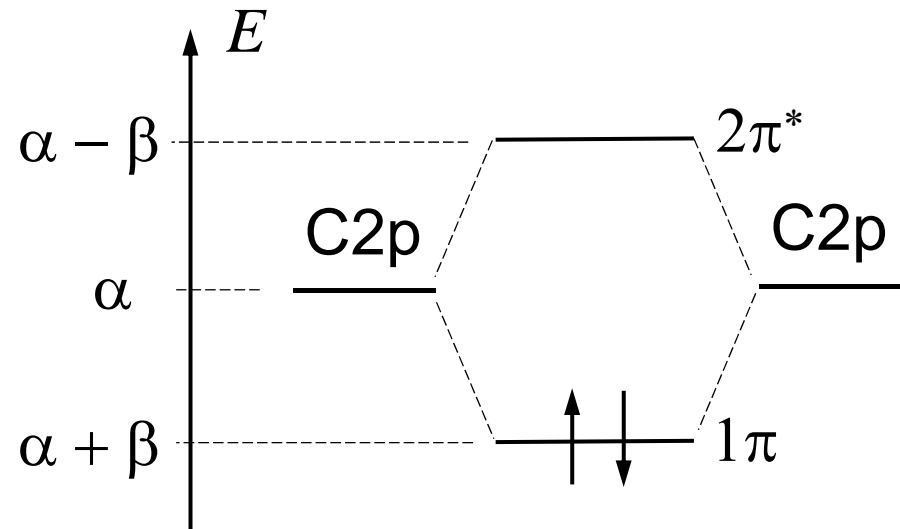


$$\psi = c_A \chi_A + c_B \chi_B$$

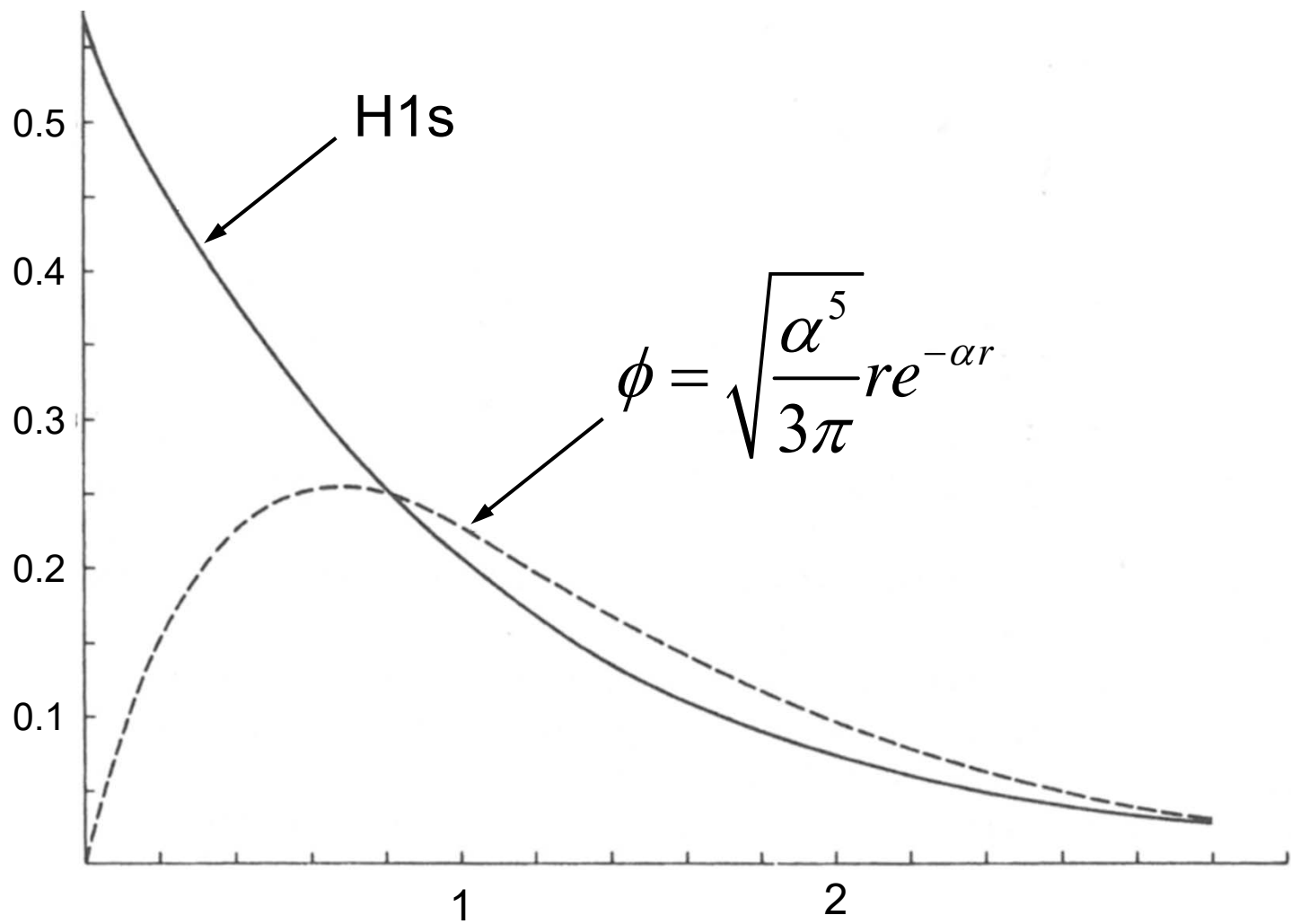
$$\begin{vmatrix} \alpha - E & \beta \\ \beta & \alpha - E \end{vmatrix} = 0$$

$$(\alpha - E)^2 - \beta^2 = 0$$

$$E_{\pm} = \alpha \pm \beta, \quad \beta < 0$$



**Delokaliseringsenergi:**  
Energisänkning utöver  $\pi$ -elektron-  
energin för elektronerna i eten.



# Allylradikal

