

## Huckel Molecular Orbital Theory

Enter the number of carbon atoms.

Natoms := 4

Enter the number of occupied molecular orbitals.

Nocc := 2

Enter the Huckel matrix.

$$H := \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad H := -H$$

Calculate eigenvalues and eigenvectors:

$$E := \text{eigenvals}(H) \quad \text{Display} := \text{rsort}(\text{stack}(E^T, \text{eigenvecs}(H)), 1)$$

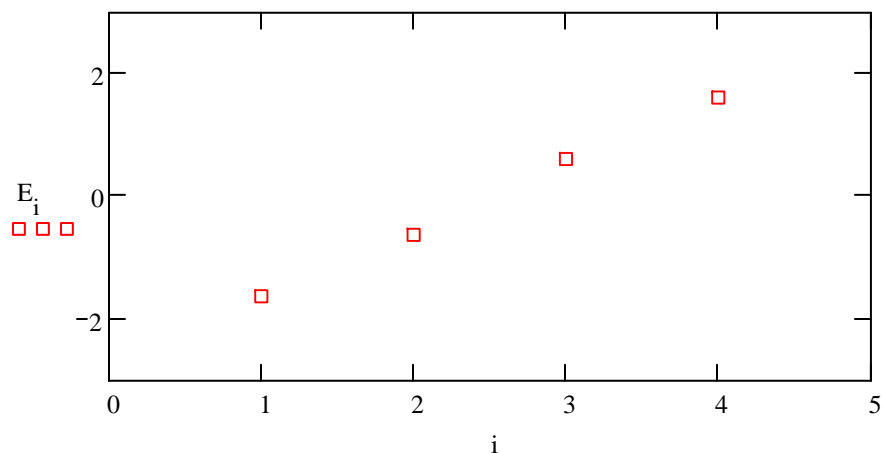
Display eigenvalues and eigenvectors:

$$\text{Display} = \begin{pmatrix} -1.618 & -0.618 & 0.618 & 1.618 \\ 0.372 & -0.602 & 0.602 & -0.372 \\ 0.602 & -0.372 & -0.372 & 0.602 \\ 0.602 & 0.372 & -0.372 & -0.602 \\ 0.372 & 0.602 & 0.602 & 0.372 \end{pmatrix}$$

Display energy level diagram:

$E := \text{sort}(E)$

$i := 1.. \text{Natoms}$



Calculate total  $\pi$ -electronic energy:

$$E_{\pi} := 2 \cdot \sum_{i=1}^{\text{Nocc}} E_i \quad E_{\pi} = -4.472$$

Calculate the delocalization energy:

$$E_{\text{deloc}} := E_{\pi} + 2 \cdot \text{Nocc} \quad E_{\text{deloc}} = -0.472$$

Calculate the delocalization energy per atom:

$$\frac{E_{\text{deloc}}}{\text{Natoms}} = -0.118$$

C := submatrix(Display, 2, Natoms + 1, 1, Natoms)

Enter the number of the molecular orbital to be plotted:

n := 1

x := 1, 1.05 .. Natoms

$$\begin{array}{c} (c^{(n)})_i \\ \text{---} \text{---} \text{---} \\ 0 \\ \text{---} \end{array}$$



i, x

$$r := 1 \quad s := 1 \quad 2 \cdot \sum_{i=1}^{\text{Nocc}} [(c^{(i)})_r \cdot (c^{(i)})_s] = 1 \quad \pi\text{-electron density on carbon 1}$$

$$r := 1 \quad s := 2 \quad 2 \cdot \sum_{i=1}^{\text{Nocc}} [(c^{(i)})_r \cdot (c^{(i)})_s] = 0.894 \quad \pi\text{-bond order between carbons 1 and 2}$$

$$r := 2 \quad s := 3 \quad 2 \cdot \sum_{i=1}^{\text{Nocc}} [(c^{(i)})_r \cdot (c^{(i)})_s] = 0.447 \quad \pi\text{-bond order between carbons 2 and 3}$$

$$r := 3 \quad s := 4 \quad 2 \cdot \sum_{i=1}^{\text{Nocc}} [(c^{(i)})_r \cdot (c^{(i)})_s] = 0.894 \quad \pi\text{-bond order between carbons 3 and 4}$$