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.

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

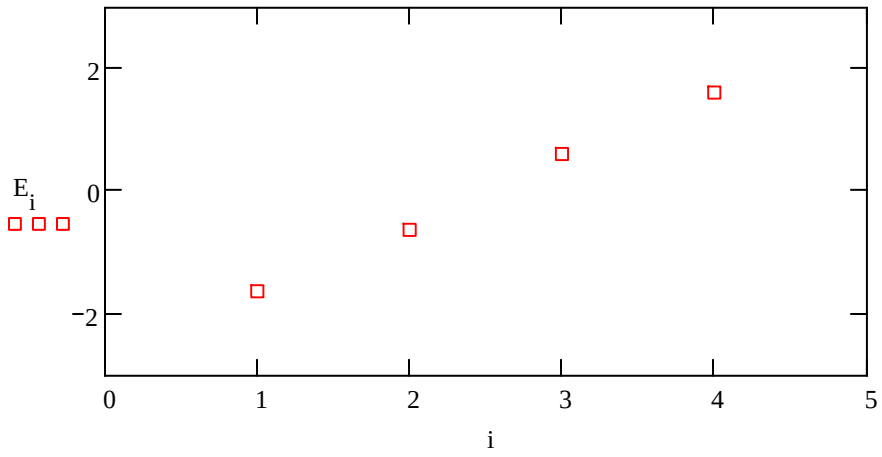
Calculate eigenvalues and eigenvectors:

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

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: $E := \text{sort}(E)$ $i := 1 .. \text{Natoms}$



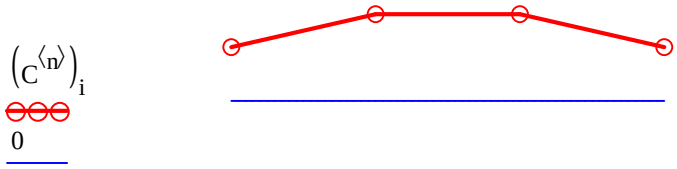
Calculate total π-electronic energy: $E_\pi := 2\cdot \sum_{i=1}^{Nocc} E_i$ $E_\pi = -4.472$

Calculate the delocalization energy: $E_{deloc} := E_\pi + 2\cdot Nocc$ $E_{deloc} = -0.472$

Calculate the delocalization energy per atom: $\frac{E_{deloc}}{Natoms} = -0.118$

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

Enter the number of the molecular orbital to be plotted: $n := 1$ $x := 1, 1.05 .. Natoms$



i, x

$r := 1$ $s := 1$ $2\cdot \sum_{i=1}^{Nocc} \left[(C^{\langle i \rangle})_r \cdot (C^{\langle i \rangle})_s \right] = 1$ π-electron density on carbon 1

$r := 1$ $s := 2$ $2\cdot \sum_{i=1}^{Nocc} \left[(C^{\langle i \rangle})_r \cdot (C^{\langle i \rangle})_s \right] = 0.894$ π-bond order between carbons 1 and 2

$r := 2$ $s := 3$ $2\cdot \sum_{i=1}^{Nocc} \left[(C^{\langle i \rangle})_r \cdot (C^{\langle i \rangle})_s \right] = 0.447$ π-bond order between carbons 2 and 3

$r := 3$ $s := 4$ $2\cdot \sum_{i=1}^{Nocc} \left[(C^{\langle i \rangle})_r \cdot (C^{\langle i \rangle})_s \right] = 0.894$ π-bond order between carbons 3 and 4