

Hydrogen Molecule Ion - Graphical Display of Orbitals

Optimum scale factor and internuclear separation: $\alpha := 1.238$ $R := 2.0033$

Overlap integral:
$$S(\alpha, R) := \exp(-\alpha \cdot R) \cdot \left(1 + \alpha \cdot R + \frac{\alpha^2 \cdot R^2}{3} \right)$$

Bonding molecular orbital:
$$\Psi_{\text{bmo}}(x, y) := \frac{\sqrt{\frac{\alpha^3}{\pi}} \cdot \left[\exp(-\alpha \cdot \sqrt{x^2 + y^2}) + \exp[-\alpha \cdot \sqrt{(x - R)^2 + y^2}] \right]}{\sqrt{2 + 2 \cdot S(\alpha, R)}}$$

Anti-bonding molecular orbital:
$$\Psi_{\text{amo}}(x, y) := \frac{\sqrt{\frac{\alpha^3}{\pi}} \cdot \left[\exp(-\alpha \cdot \sqrt{x^2 + y^2}) - \exp[-\alpha \cdot \sqrt{(x - R)^2 + y^2}] \right]}{\sqrt{2 - 2 \cdot S(\alpha, R)}}$$

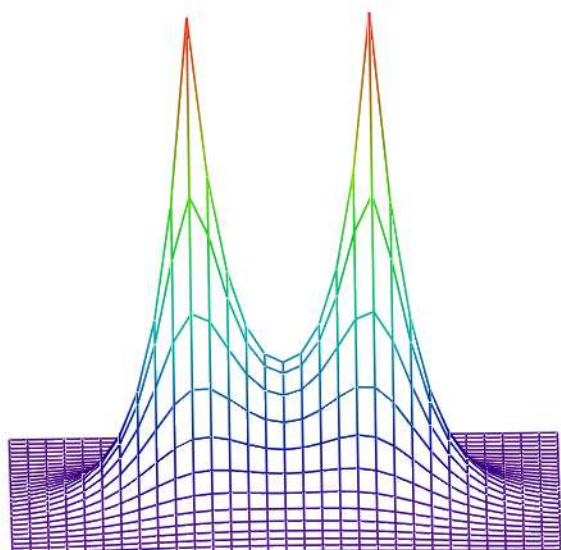
Non-bonding molecular orbital:
$$\Psi_{\text{nmo}}(x, y) := \frac{\sqrt{\frac{\alpha^3}{\pi}} \cdot \exp(-\alpha \cdot \sqrt{x^2 + y^2}) + i \cdot \exp[-\alpha \cdot \sqrt{(x - R)^2 + y^2}]}{\sqrt{2}}$$

Bonding electron density:
$$\rho_{\text{b}}(x, y) := \left(\left| \Psi_{\text{bmo}}(x, y) \right| \right)^2 - \left(\left| \Psi_{\text{nmo}}(x, y) \right| \right)^2$$

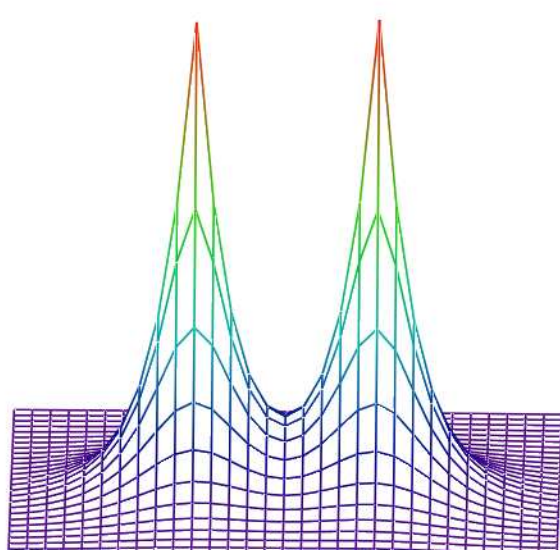
Graphical display of orbitals: $N := 30$ $i := 0..N$ $j := 0..N$ $x_i := -2 + i \cdot \frac{6}{N}$ $y_j := -3 + j \cdot \frac{6}{N}$

$$\text{TotalDensity}_{i,j} := \Psi_{\text{bmo}}(x_i, y_j)^2$$

$$\text{NonBondingDensity}_{i,j} := \left(\left| \Psi_{\text{nmo}}(x_i, y_j) \right| \right)^2$$

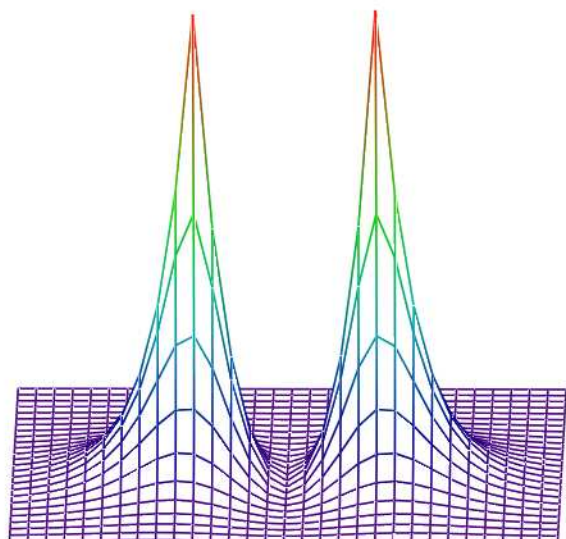


TotalDensity



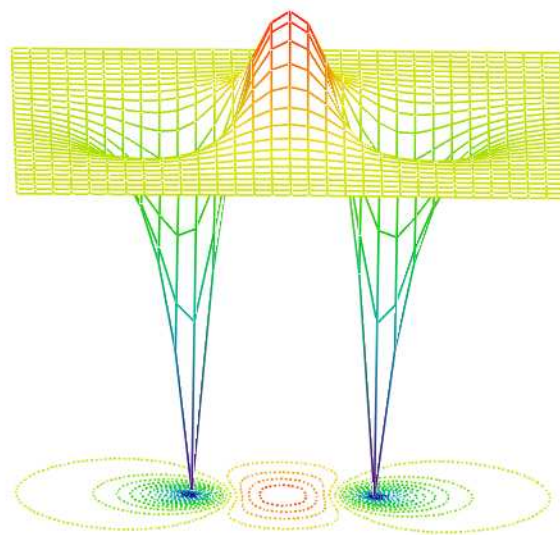
NonBondingDensity

$$\text{AntiBondingDensity}_{i,j} := \Psi_{\text{amo}}(x_i, y_j)^2$$



AntiBondingDensity

$$\text{BondingDensity}_{i,j} := \rho_b(x_i, y_j)$$



BondingDensity, BondingDensity