Quiz 9.1 – Valence Bond Theory

Name: Key

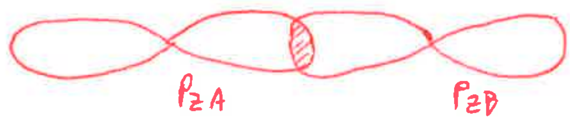
Valence Bond Theory

Consider an F_2 molecule from the perspective of valence bond theory. Draw the orbital overlap which leads to the covalent bond in F_2

$\frac{1\downarrow}{}\ \frac{1\downarrow}{}\ \frac{1}{}$ $2p$ overlap of p_z orbitals

$\frac{1\downarrow}{2s}$

$\frac{1\downarrow}{1s}$



Hybridization

For each class of hybridization, give the linear combination that forms one of the hybrid orbitals

- sp $\psi_{h1} = \frac{1}{\sqrt{2}}(\psi_s + \psi_{p_z})$ -or- $\psi_{h_1} = \psi_s + \psi_{p_z}$
- sp^2 $\psi_{h2} = \psi_s + \sqrt{\frac{3}{2}}\,\psi_{p_x} - \sqrt{\frac{1}{2}}\,\psi_{p_y}$
- sp^3 $\psi_{h_4} = \psi_s + \psi_{p_x} - \psi_{p_y} - \psi_{p_z}$

Variational Theory

For a particle in a box with length $L = 1$, the ground state wavefunction is $\Psi = \sqrt{2}\sin(\pi x)$ and the ground state energy is $\frac{h^2}{8m}$ $= 0.125\,\frac{h^2}{m}$

The normalized trial function $\phi = \sqrt{30}\,(-x^2 + x)$ has a similar shape and obeys the same boundary conditions. Demonstrate the variational theory by finding the energy expectation value $\left\langle \phi \middle| \hat{H} \middle| \phi \right\rangle$ and comparing it to the true ground state energy.

$$\langle \hat{H} \rangle = \int_0^1 \sqrt{30}(-x^2 + x)\,\frac{-\hbar^2}{2m}\,\frac{d^2}{dx^2}\left[\sqrt{30}(-x^2+x)\right]dx$$

$$\langle \hat{H} \rangle = 30\int_0^1 (-x^2+x)\,\frac{-\hbar^2}{2m}(-2)\,dx = \frac{30\hbar^2}{m}\left[-\frac{1}{3}x^3 + \frac{1}{2}x^2\right]_0^1 = \frac{30\hbar^2}{m}\cdot\frac{1}{6}$$

$$\langle \hat{H} \rangle = \frac{15\hbar^2}{3m} = \frac{15h^2}{3m(2\pi)^2} = \frac{15h^2}{12\pi^2 m} = 0.12665\,\frac{h^2}{m} > \frac{h^2}{8m}$$