Molecules (cont)

Covalent bond: two atoms (often identical) are bound by attraction via shared electrons.

Simplest example: $H_2$ molecule

\[ \phi_0 (r) \propto e^{-r/a_0} \]

Single $H$ atom in ground electronic state

Single potential well

\[ P_{\text{tr}} = 4\pi r^2 |\psi_0 (r)|^2 \propto r^2 e^{-2r/a} \]

Probability density distribution

Molecule = double potential well

\[ X_{\text{em}} = \frac{x_2 + x_1}{2} \]

\[ R = x_2 - x_1 \]

\[ X_1 = X_{\text{em}} - \frac{R}{2} \]

\[ X_2 = X_{\text{em}} + \frac{R}{2} \]
Electrons can tunnel from one atom to another \( \Rightarrow \) joint wave function

Symmetric potential (w/respect to the center of mass)

\[ \Psi \]

Joint wave function must be either symmetric or antisymmetric.

Symmetric: \( \Psi_+ (\vec{r}_1, \vec{r}_2) = \Psi_1 (\vec{r}_1) + \Psi_2 (\vec{r}_2) \)

Anti-symmetric: \( \Psi_- (\vec{r}_1, \vec{r}_2) = \Psi_1 (\vec{r}_1) - \Psi_2 (\vec{r}_2) \)

We can use a form of a single atom electron wave function to roughly estimate the electron wavefunction contributions for a molecular states.

Two atoms very far away

\[ x_{cm} - R/2 \quad x_{cm} \quad x_{cm} + R/2 \]

Each electron is centered around each proton.
Two atoms close by

**Symmetric case**

\[ \psi_0(r_1) \]

\[ \phi_0(r_2) \]

Highest electron density b/w two protons

\[ \bar{e} + \bar{e} \]

\[ p \rightarrow p \]

Protons are effectively attracted

**Anti-symmetric case**

\[ -\psi_0(r_2) \]

Electrons are mostly outside

\[ \bar{e} \rightarrow \bar{e} \]

\[ p \rightarrow p \]

Protons are effectively repulsed

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\[ E \]

\[ R_0 \]

\[ R \]

**anti-symmetric case**

**anti-bound orbital**

(spin of two electrons are ↑↓)

**symmetric case**

**bound orbital**

(spins of two electrons are ↑↑)

\[ B = 4.5 \text{ eV} \]

To break this molecule it is enough to flip the spin of one of the electrons, and move from bound to anti-bound state (photo dissociation)