Simple Molecules

\[ 2 \text{H} \text{binding energy} = -27.2 \text{eV} \]

\[ 2 \text{nd e} - \text{1st e} = -4.136 - 25 \text{eV} \]

\[ = -54.4 \text{eV} \]

\[ \text{total He} \]

\[ E = -\frac{1}{2} \text{mc}^2 \sum \frac{Z}{r} \]

What keeps H-H from collapsing to He-like structure??

(Gould vs. repulsion nuclei)

\[ E_{\text{Coul}} = \frac{Z_1 Z_2 e^2}{r} \]

\[ 27.2 \text{eV at } r = a_0 \]
Molecule

Quantum Attraction
opposed by
Coulomb Repulsion

Energy

nucleus separate \( R \)

molecule Potential

Quantum binding

1. Molecules will be bound by energy similar to last electron ionic attraction.

2. Nuclei separate \( x_0 \) will be

\[ 1 - 2 \times a_0 \]

\( L + 2 \) \( \implies \) Molecular Vibrations

\( h \nu = \Theta (E_{\text{atom}} \sqrt{\frac{m_e}{m_N}}) \)

Q: Why Noble gases do not form molecules?
**Numeric Example**

$H_2$ : binding $O(5 eV)$

Separation $O(1.2 a_0)$

\[ V = -E_0 + \frac{1}{2} k (x-x_0)^2 \]

\[ k = \text{oscillated const} \]

\[ \hbar \omega = \hbar \sqrt{\frac{k}{M}} \]

\[ m_1 + m_2 \approx M \]

\[ V = E_0 \left( \frac{x}{x_0} - 1 \right)^2 - E_0 \]

\[ k = \frac{2E_0}{x_0^2} \]

*note (isotope dependence) $\Rightarrow \hbar \omega = O(0.1 eV)$*
Beyond Vibration

\[ E_r = \frac{L^2}{2I} = \frac{\hbar^2 \ell (\ell + 1)}{2 \left( m_1 r_1^2 + m_2 r_2^2 \right)} \]

Hydrogen

\[ m_1 = m_2 = 2\mu \]
\[ r_1 = r_2 = \frac{x_0}{2} \]

\[ x_0 \sim 1.2a_0 = \frac{1.2 \frac{\hbar c}{m \alpha c^2}}{2\mu} \]

\[ \frac{E_r}{E_e} = \frac{1}{e} m \alpha^2 \alpha^2 \]

Atomic energy, hydrogen

\[ E_r \sim 10^{-3} eV \cdot \ell (\ell + 1) \]

\[ \text{thermal energy} \]
Material Transparencies

- Why are many liquids transparent?
  Only transparent in the 'visible' spectrum ($\lambda \sim 400 - 700 \text{ nm}$)
  \[ E_y = 3eV \quad 1.77eV \]

- Why are many crystals transparent?
  "No" Absorption in Visible
  a) rotations are 'threomoe'
  b) vibrations are 'infrared'
  c) atomic excitations
    and 'ultraviolet'

  Visibility 'window'

Special cases
- metals: light reflected (boundaries)
- mid-heavy elements with unenclosed shells: ionic or excited, e.g., in visible
\[(T + V) \psi = E \psi\]

\[T = -\frac{\hbar^2}{2me} \nabla_x^2 \frac{\hbar^2 e^2}{2m_z} \frac{1}{\sqrt{x_1^2 - x_3^2}} - \frac{\hbar^2 e^2}{2m_z} \frac{1}{\sqrt{x_2^2 - x_3^2}}\]

*Quantum Chemistry*

\[V = -\frac{Z_1 e^2}{4\pi \varepsilon_0} \frac{1}{\sqrt{x_1^2 - x_3^2}} - \frac{Z_2 e^2}{4\pi \varepsilon_0} \frac{1}{\sqrt{x_2^2 - x_3^2}} + \frac{Z_1 Z_2 e^2}{4\pi \varepsilon_0} \frac{1}{\sqrt{x_1^2 - x_3^2}}\]

**Steps:** Separate CM motion $$\Rightarrow$$ 6 coord.

**Born Oppenheimer:** Freeze nuclei, obtain molecule potential field

Solve for vibrations, rotations