Start w/ Simpilest "Ionic Bonding"

Principle: Electron transfered from one atom to another, ions attract

eg) $Na + Cl \longrightarrow Na^+ + Cl^- \longrightarrow NaCl$

Way to analyze this reaction is to think about energies associated w/ each step.

$E_{ionization}$ - E to pull e off Na

$$= E_{(Na^+ + e^-)} - E_{Na}$$

$E_{Affinity}$ - E you get back when you put e on Cl to make Cl ion

$$= E_{(Cl + e^-)} - E_{Cl^-}$$

$E_{cohesive}$ Bonding - E you get out from putting ions together.

$$= E_{(Na^+ + Cl^-)} + E_{NaCl}$$

Total Budget for Reaction:

$$\Delta E = E_{ION} - E_{Aff} - E_{coH}$$

If $\Delta E < 0$, then reactions proceeds

(Careful, different ΔE if talking about making 1 NaCl molecule or a bunch of salt. # of atoms bonded to is different)

$E_{Bonding}$ easiest to understand

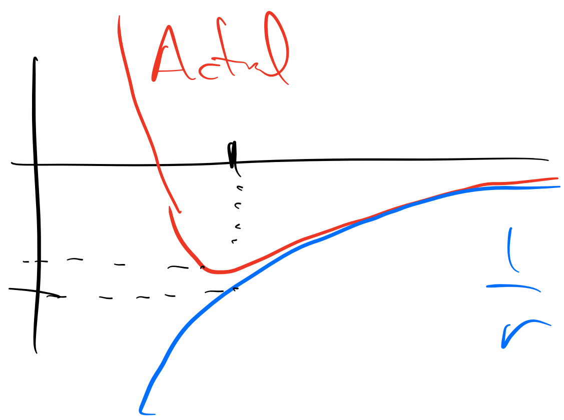
$$= \frac{1}{2}\sum_{i\neq j} \frac{k\,\varepsilon_i \varepsilon_j}{|\vec{r}_{ij}|} \quad \text{(Coulomb Interaction)}$$

Simple picture fairly accurate when you know r_{ij} you get right answer

<u>Problem</u>: goes to $-\infty$ as $r \to 0$ (doesn't make sense)

What's really happening

close →



However also have bonding between two atoms that one the electrons just as much as each other (even same atoms) eg O_2

<u>Covalent Bonding</u> (Purely QM effect)

"Atoms are sharing electrons. This sharing Binds the Atoms together"

— Some other chemist

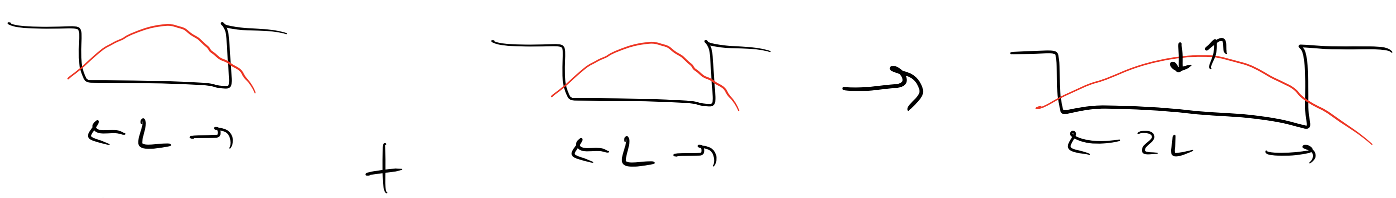
Can we understand better from Physics what we mean by this?

<u>Nice Picture</u> "Particle in Box"

$$H + H \longrightarrow H_2$$

What am I talking about w/ Particle in Box?

<u>H</u>  Box represents attraction to N



$$\frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 + \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 > 2\,\frac{\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2$$

Need to put 2 electrons in Bigger Box

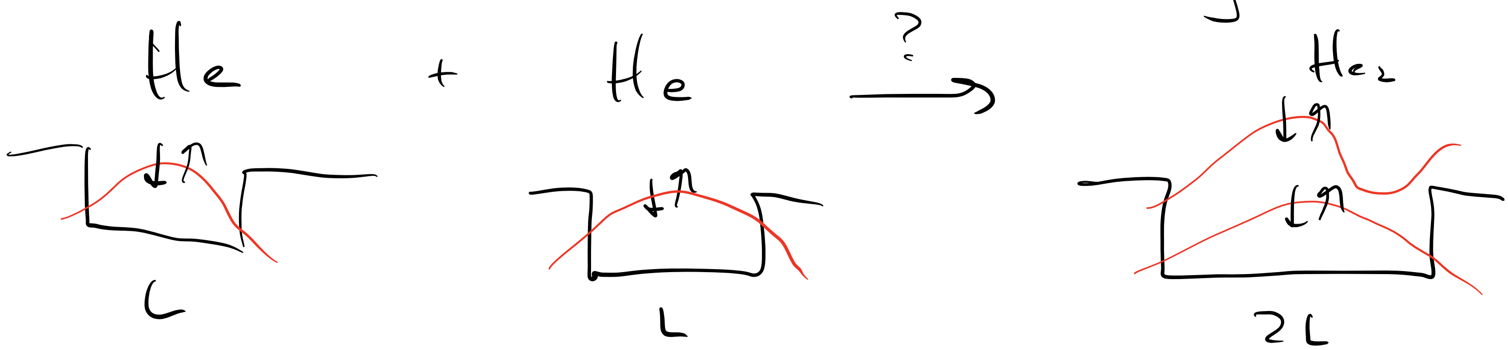
Both can fit in ground state (2 spins)

<u>Whats going?</u>

- Allowing ψ_e to spread out $L \to 2L$
- Smaller $\frac{\partial \psi}{\partial x}$ $\Rightarrow$ Smaller p_e $\Rightarrow$ Smaller E
- Uncertainty Principle Δx Bigger Δp smaller

  Smaller Δp, Smaller $\langle p^2 \rangle$, Smaller KE

Same thing w/ He, and see something different



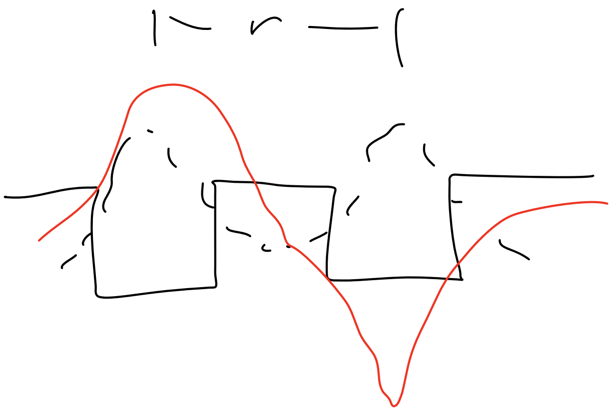
Now we are not going to Bond

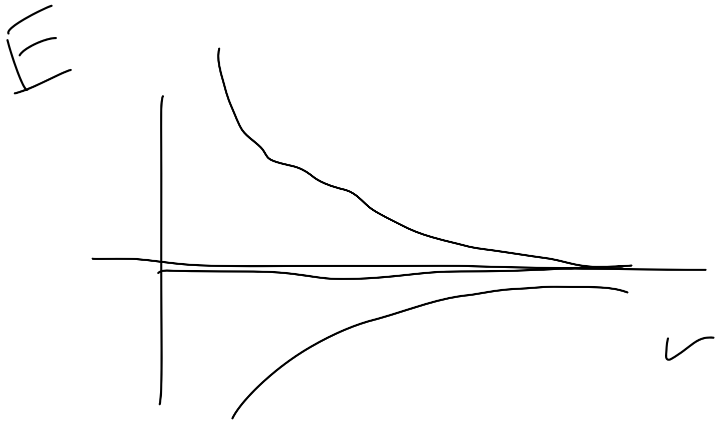
But need to fill excited ψ's to fit more e^-'s

Lower E state "Bonding" Orbital

Higher E State "Anti-Bonding" Orbital

This is why H Bonds to form H_2 but He doesn't





E_{Asym}

E_{free}

E_{sym}