$1s - 1s = \text{exclusion}$

$1s + 1s = \text{intersection}$

$\sigma^*$

$\sigma$

internuclear distance $0.74 \text{ Å}$

$104.2 \text{ kcal/mol}$

$e^-$ not between nuclei if populated

$e^-$ between nuclei $= \text{bonding interaction}$

$= \text{antibonding interaction}$
If the idea of LCAO is

\[ H \ 1s^1 + H \ 1s^1 = \ \frac{H_2 \sigma^*}{H_2 \sigma^2} \]

Can this approach be extended to methane, CH\(_4\)?

Yes, but the mathematics is very challenging!

\[ C \ 1s^2 + C \ 2s^2 + C \ 2p_x^1 + C \ 2p_y^1 + C \ 2p_z + H \ 1s^1 + H \ 1s^1 + H \ 1s^1 + H \ 1s^1 = ? \]
So, to model how atomic orbitals overlap to provide valance bonds, we will

- choose to combine only 2 orbitals at a time
- invent hybrid atomic orbitals to reconcile LCAO with VSEPR