H_2 molecule: the electronic wavefunction is a function of 6 electron coordinates + two spin coordinates
The wavefunction can be approximately written as a product of two 1-electron wavefunctions. This neglects correlation of the electron motion due to Coulomb repulsion and Pauli exclusion.

Hamiltonian:

e-e repulsion

nuclear repulsion

$$\hat{H} = \hat{h}_1 + \hat{h}_2 + \frac{e^2}{4\pi\varepsilon_0 r_{12}} + \frac{e^2}{4\pi\varepsilon_0 R}$$

$$\hat{h}_i = \frac{1}{2m_e}\hat{\vec{p}}_i^{\,2} - \frac{e^2}{4\pi\varepsilon_0 r_{iA}} - \frac{e^2}{4\pi\varepsilon_0 r_{iB}}$$

Molecular orbitals:
Instead of using an atomic basis of $1s_A$ and $1s_B$, use what we learned from H_2^+ and start with the basis set of σ and σ^* functions that are $\pm$ combinations of $1s_A$ and $1s_B$