Bonding in Polyatomics

1. LCAO approach
2. Combine AOs that have good orbital overlap (anything that can overlap, will)
3. and similar energy.
4. Number of AOs = number of MOs
5. MOs should have the same symmetry as the molecule.

Linear Models for Hydrides: BeH$_2$, CH$_2$ (triplet), H$_2$O

\[
\begin{align*}
1s_H - 2s_{Be} + 1s_H \\
1s_H + 2p_{x,Be} - 1s_H \\
-1s_H + 2p_{x,Be} + 1s_H \\
1s_H + 2s_{Be} + 1s_H
\end{align*}
\]

\[
\begin{align*}
\sigma_1 & \quad \sigma_2 & \quad \sigma_3 & \quad \sigma_4 & \quad \sigma_4^* \\
\text{nb } 2p_y & \quad \text{nb } 2p_z & \quad 2p_{z,Be}
\end{align*}
\]