Big Idea:

MO diagrams can predict properties.

Li₂ has 6 e⁻

BO = 1
$O_2$, $F_2$, $[Ne_2]$

for these elements, 2s is much lower in E than 2p:

2p $\sigma_u$

2p $\Pi_g$

2p $\Pi_u$

2s $\sigma_u$

$\sigma$ overlap greater than $\Pi$ overlap
For $B_2, C_2, N_2$

$2s$ is close in energy to $2p$ level; $s-p$ mixing switches order of $2p \Pi_0$ and $2p \Sigma^-$.

\[ <\text{use for hetero nucleus, too}> \]
Note correlation:

<table>
<thead>
<tr>
<th>Molecule</th>
<th>BO</th>
<th>( k ) (( \text{m}^{-1} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_2 )</td>
<td>1</td>
<td>450</td>
</tr>
<tr>
<td>( O_2 )</td>
<td>2</td>
<td>1200</td>
</tr>
<tr>
<td>( N_2 )</td>
<td>3</td>
<td>2300</td>
</tr>
</tbody>
</table>

In general,

\( \text{BO} \uparrow \) then \( \text{BE} \uparrow \)
Molecular Term Symbols

- for $e^{-}$ in $\Sigma$ orbitals, $m_l = 0$
- for $e^{-}$ in $\Pi$ orbitals, $m_l = \pm 1$

- parity: for homonuclear molecules, (or any centrosymmetric), we must specify $g$ or $u$

- Symbols for total orbital moment, $M_l$
  \[
  \begin{array}{c|cccc}
  M_l & 0 & 1 & 2 & 3 \\
  \hline
  \text{symbol} & \Sigma & \Pi & \Delta & \Phi \\
  \end{array}
  \]

- reflection: for $\Sigma$ terms, we must specify whether sign changes (−) on reflection, or not (+)
$[E \times \frac{1}{2}]$

$\text{He}_2^+$

$(1s\sigma_5)^2(1s\sigma_u)^1$

parity $= U$

spin $= \frac{1}{2}$

$M_L = 0$

$^2\Sigma_u^+$
configuration

\[(2s\sigma_g)^2 (2s\sigma_u)^2 (2p\pi_u)^6 (2p\pi_u)^2\]

Several terms are consistent with configuration:

\[
\begin{array}{ccc}
1 & 1 & M_s \\
1 & 1 & -1 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
\end{array}
\]

\[
\begin{array}{ccc}
1 & 1 & M_L \\
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
\end{array}
\]

\[
\begin{array}{ccc}
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
\end{array}
\]

- since \( M_L = \pm 2 \), we must have a \( L = 2 \) (\( \Delta \)) term. It occurs only if \( S = 0 \).

- A term with \( L = 0 \) (\( \Sigma \)) and \( S = 1 \) accounts for 3 \( \Sigma^g \) states.

- The leftover state is just \( M_s = 0 \), so \( S \) must be 0:

\[
\begin{array}{ccc}
1 & 1 & 0 \\
\end{array}
\]

- State: high \( S \), low \( M_L \)