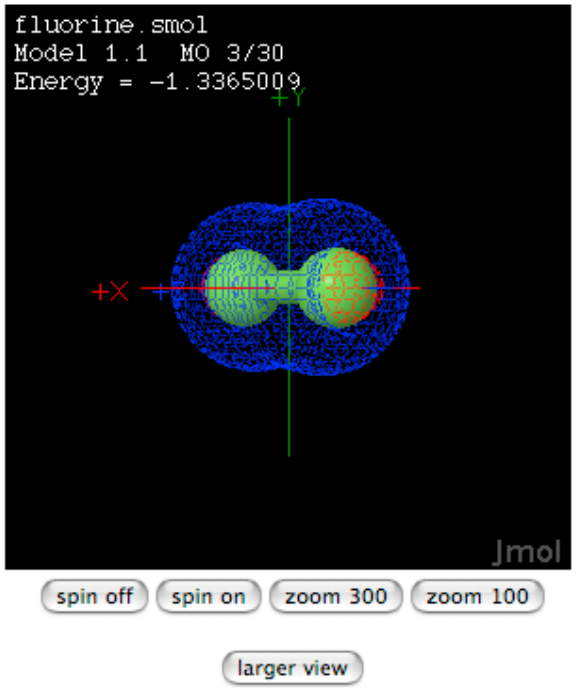
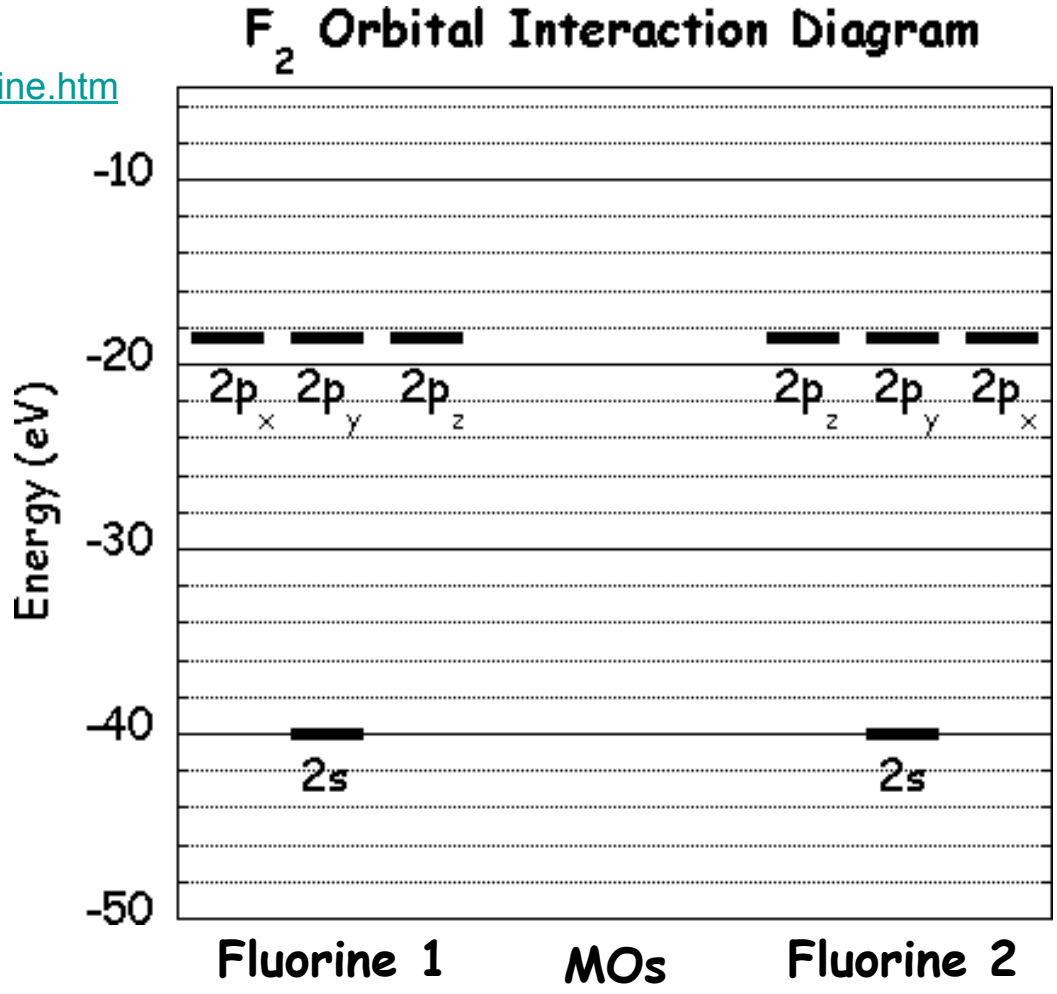
# Discussion Problem
# Construct the $F_2$ MO Diagram

**Instructions**: (Part 2) Complete the $F_2$ orbital interaction diagram below. The 8 MOs should be labeled and ordered correctly relative to one another. Absolute position however is not expected. Draw dashed lines to show which atomic orbitals interact to form the MOs.

**Instructions**: (Part 3) Complete the electron occupancy for both sets of AOs and the MOs (use ↓↑ to represent electrons of opposite spin). Compute the bond order. _____

http://osxs.ch.liv.ac.uk/~ng/external/orbitalsfluorine.htm

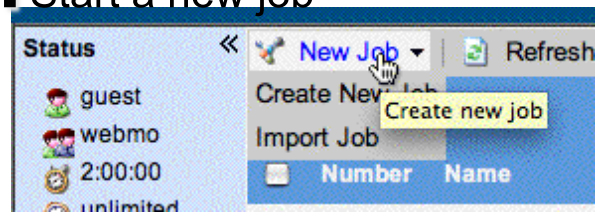


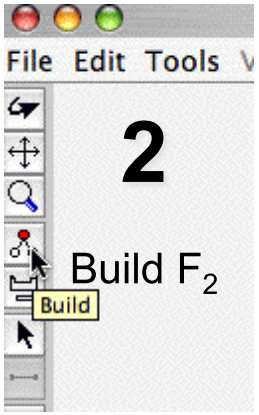



# Discussion Problem: Calculate the MOs for $F_2$

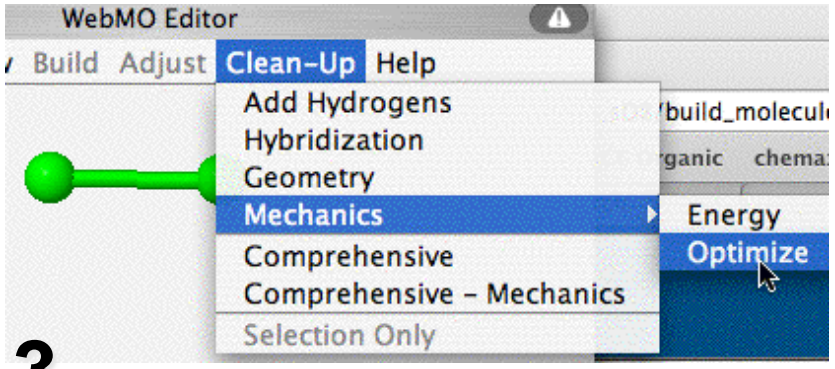
## (Use WebMO: first optimize the geometry)

**1** Start a new job



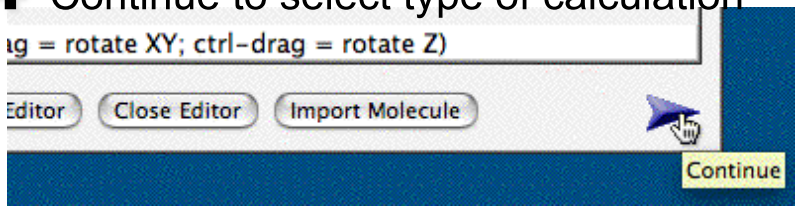



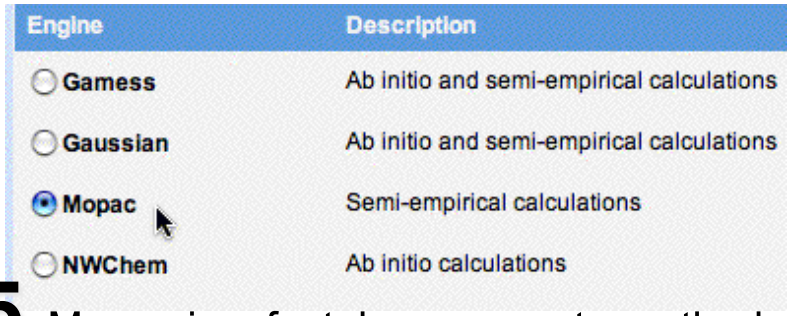

**2** Build $F_2$




**3** Perform a crude optimization

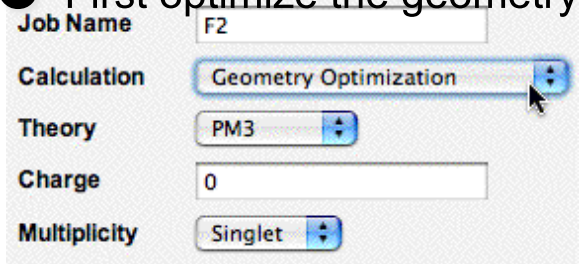
**4** Continue to select type of calculation



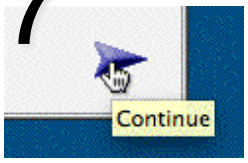



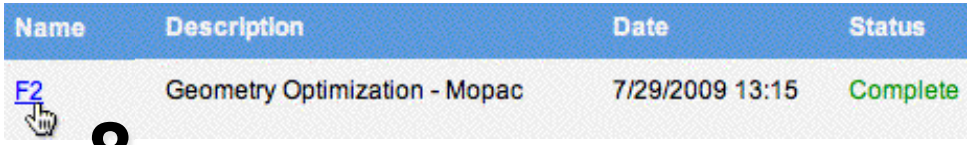

**5** Mopac is a fast, less accurate method

**6** First optimize the geometry




**7**

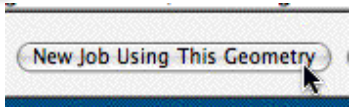



**8** View the results

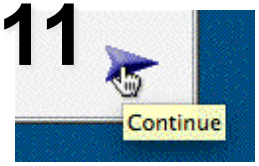
# Discussion Problem (Continued)
# Now Calculate MOs for the Optimized Geometry

**9** Onward…

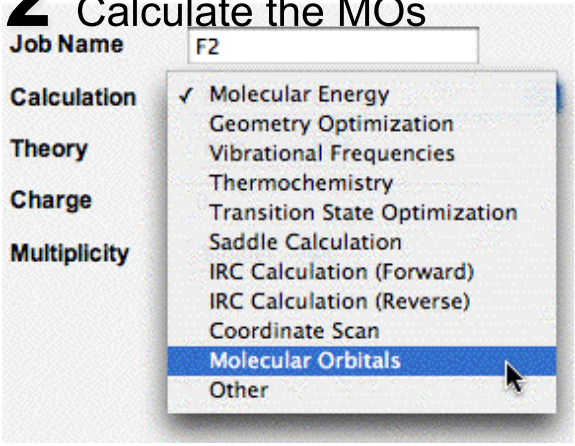



**10**


**11**




**12** Calculate the MOs



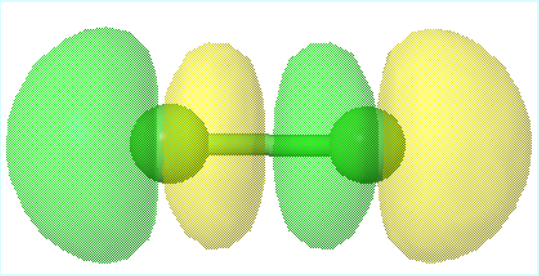

**13** View results

| Name | Description | Date | Status |
|---|---|---|---|
| F2 | Molecular Orbitals - Mopac | 7/29/2009 13:23 | Complete |
| F2 | Geometry Optimization - Mopac | 7/29/2009 13:15 | Complete |

**14** Check out MO #8

| Orbital | Symmetry | Occupancy | Energy | Actions |
|---|---|---|---|---|
| 1 | sig | 2 | -24.417 eV | |
| 2 | siu | 2 | -22.363 eV | |
| 3 | piu | 2 | -19.338 eV | |
| 4 | piu | 2 | -19.338 eV | |
| 5 | sig | 2 | -18.926 eV | |
| 6 | pig | 2 | -15.350 eV | |
| 7 | pig | 2 | -15.350 eV | |
| 8 | siu | 0 | 0.183 eV | |
| Electron density | | | | View |

**Which LCAO resulted in this MO?**



# Interpretation of the $F_2$ MO Diagram

- A large energy difference exists between 2p and 2s (>20 eV).
- Thus, 2p + 2s interactions are not important.
- We can ignore $\sigma_{s/p}$ and $\sigma^*_{s/p}$

- Each atom brings 7 valence electrons
- $F_2$ MO has a total of 14 e-

- One bonding electron pair (a sigma bond)

- 6 nonbonding electron pairs