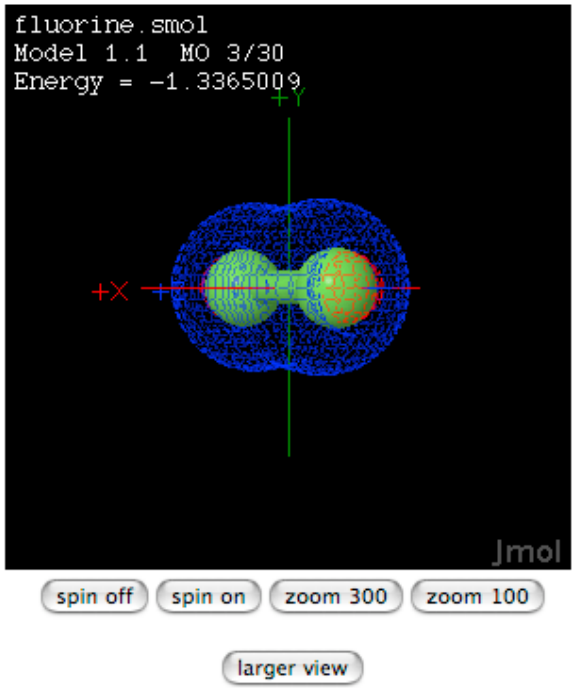
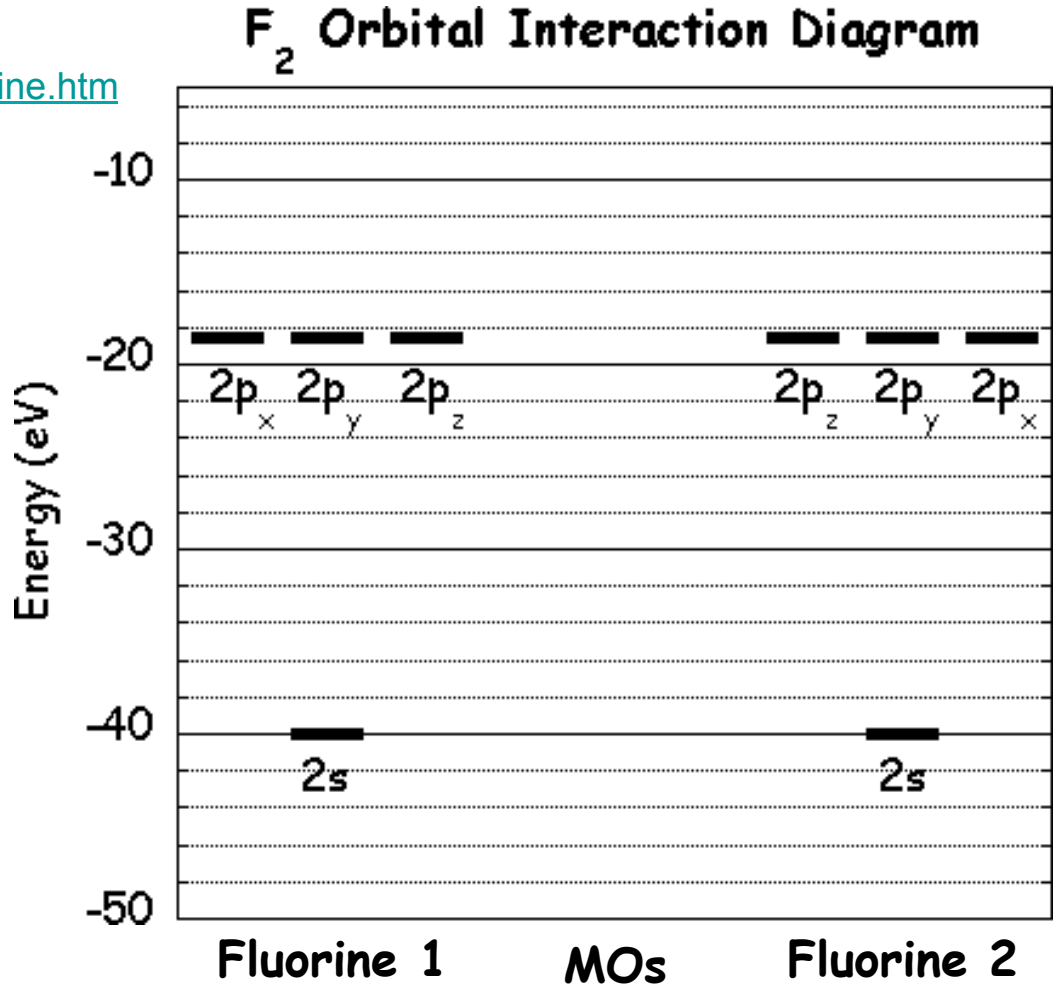
Discussion Problem
Construct the F_2 MO Diagram

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

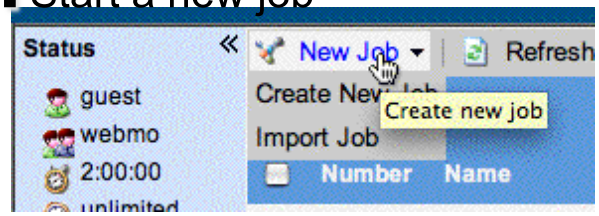


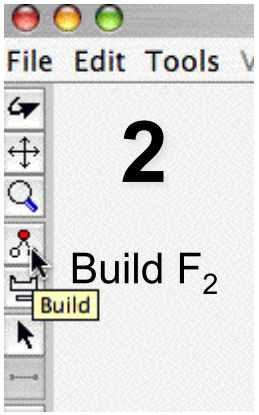


Discussion Problem: Calculate the MOs for F_2

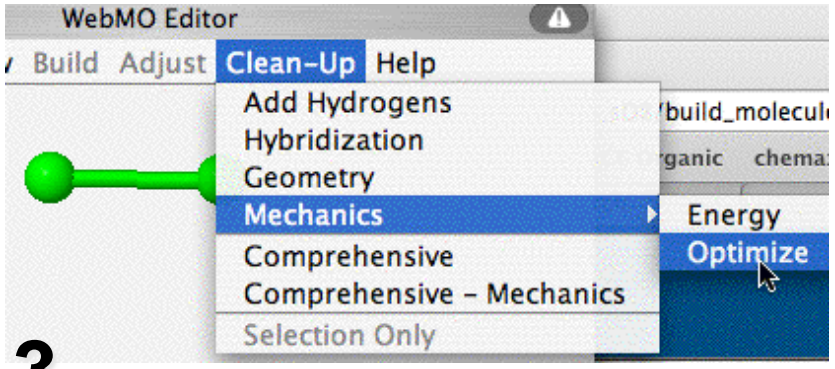
(Use WebMO: first optimize the geometry)

1 Start a new job



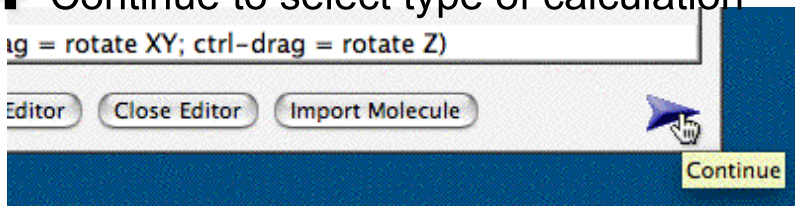


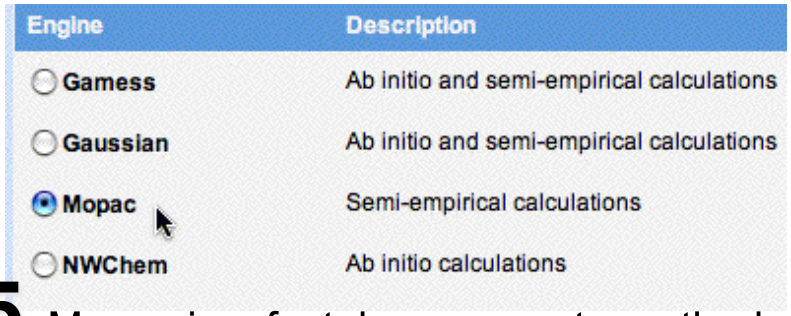
2 Build F_2



3 Perform a crude optimization

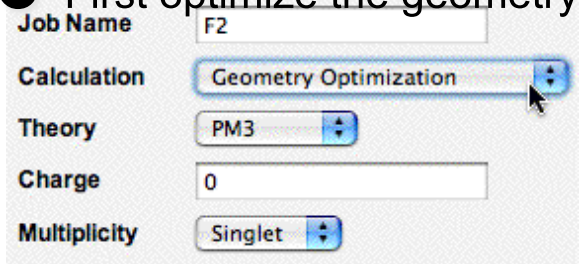
4 Continue to select type of calculation





5 Mopac is a fast, less accurate method

6 First optimize the geometry



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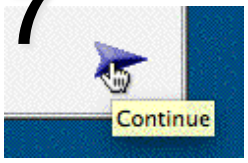
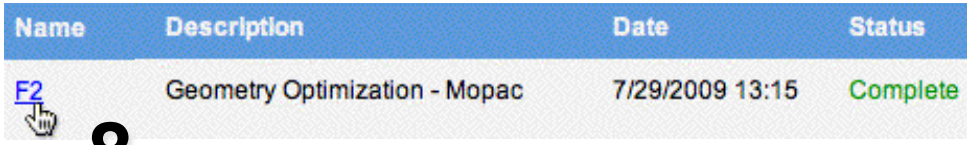
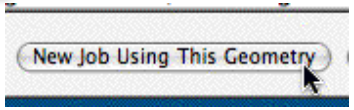




8 View the results

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

9 Onward…



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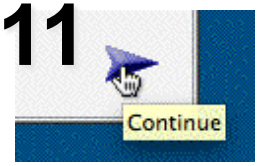
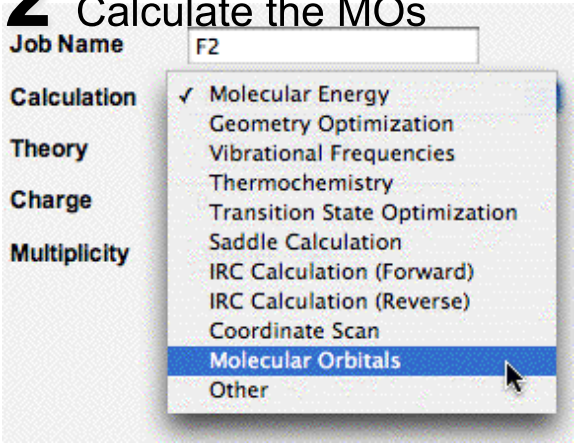


12 Calculate the MOs



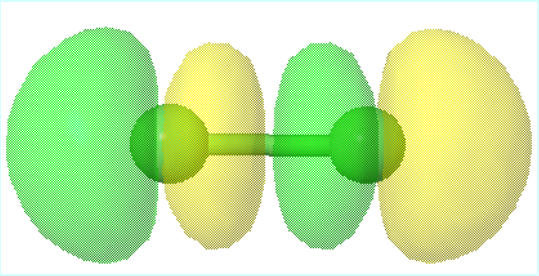
13 View results

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