Computer Lab Report Form #7:
SOE: Symmetry, Overlap, Energy

Student's Name: ____

BU ID____

Lab Section Day/Time/TF____________________________________

Molecular Orbitals Investigation 1: Bonding Between Hydrogen Atoms

Activity 1: Ground State Distance Between H-Atoms in H_2

1. Vary the distance between the atomic nuclei and complete column 2 from your observations of the Energy Meter. Then compute column 3 directly (page 66):

Distance Between Nuclei (Å)	Electrostatic Energy from Meter (eV)	$V_{nucleus1,\,nucleus2} = \frac{kZ_1Z_2}{R}$ (eV)
0.20		
0.40		
0.60		
0.80		
1.00		
1.20		
1.40		
1.60		
1.80		
2.00		
2.20		
2.40		
2.60		
2.80		

2. Why are the values measured by the Energy Meter for the electrostatic energy of the molecule smaller than the values computed directly from the formula for the Coulomb potential (page 66)?

3. Why can the occupancy of an orbital never exceed 2 (page 67)?

4. Complete the following table for ground state distance between H-atoms (page 68).

Distance (Å)	$AO_1\ Energy \times Occupancy_1 + AO_2\ Energy \times Occupancy_2$ (eV)	$MO\ Energy \times Occupancy$ (eV)	ΔEnergy = $MO\ Energy \times Occupancy$ $- AO_1\ Energy \times Occupancy_1$ $- AO_2\ Energy \times Occupancy_2$ (eV)
4.0	-27.202	-27.202	0
3.0			
2.5			
2.0			
1.5			
1.0			
0.5			

5. Please, complete the following table for the H_2 molecule (page 70).

Distance Between Nuclei (Å)	**Electrostatic Energy (eV)**	**Electron Energy (“Delta”) (eV)**	**Bond Energy (eV)**
0.20 (0.197)			
0.40 (0.405)			
0.60 (0.603)			
0.80 (0.800)			
1.00 (0.997)			
1.20 (1.205)			
1.40 (1.403)			
1.60 (1.600)			
1.80 (1.797)			
2.00 (1.995)			
2.20 (2.203)			
2.40 (2.400)			
2.60 (2.597)			
2.80 (2.805)			
3.00 (3.003)			

6. Graph the results of the above table for the H_2 molecule on the graph paper on the following page. Add to this graph the values for the Electrostatic, Electron, and Bond Energies for the distance at which you find the minimum Bond Energy (page 70 -71):

Molecular Orbitals Investigation 2: Multi-Electron Atoms Bonding

1. ***What are the occupancies of AO_1, AO_2, MO_1 and MO_2 (page 79)?***

2. Complete the following table for the ground state distance between He atoms (page 79).

Distance (Angstroms)	$AO_1\ Energy \times Occupancy$ $AO_2\ Energy \times Occupancy$ (eV)	$MO_1\ Energy \times Occupancy$ $+MO_2\ Energy \times Occupancy$ (eV)	ΔEnergy = $MO_1\ Energy \times Occupancy$ $+MO_2\ Energy \times Occupancy$ $-AO_1\ Energy \times Occupancy$ $-AO_2\ Energy \times Occupancy$ (eV)
4.0	-98.392	-98.390	+0.002
3.0 (3.003)			
2.5 (2.504)			
2.0 (2.005)			
1.5 (1.496)			
1.0 (0.997)			
0.5 (0.499)			

3. Can two He atoms ever bond to form a He_2 molecule? If not, why not? If yes, then how (page 79)?

Activity2: What About Period Two Elements?

Li_2

4. Find the bond length for Li_2 by minimizing the Bond Energy. What is the value of the electrostatic repulsion of the Li nuclei at this distance? What is the reduction of the energy of the electrons for the molecule compared to when the two atoms are separated by a very large (infinite) distanc (page 83)?

The Bond Energy for Li_2 is minimized at a distance of______Å.
At this distance:

Electrostatic Energy =_______ eV;

Electron Energy =________ eV

Bond Energy = _______ eV;

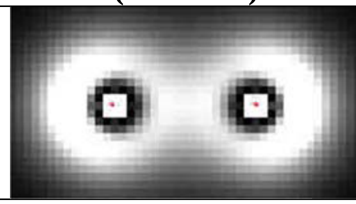
The reduction of energy for the molecule compared to when the atoms are very far apart is the Bond Energy which is __________ eV.

Be_2

5. What happens to the electron cloud density as the two Be atoms approach each other? Where is it greatest? If you were relating the 2s AOs of Be to this higher energy MO for Be_2, what would you say the relationship is (page 85)?

6. Can you find a bond length for Be_2? If yes, what is it? If no, why not? Do you see a relationship to the case of He_2 (page 85)?

7. Complete the following table for B_2 (page 88).

MO	**Energy (eV) and Occupancy**	**Appearance (Sketch It)**	**Description**
sigma$_1$	**-17.769 eV Occupancy = 2**		**Looks like the sum of the two 2s AO orbitals.**
sigma$_2$			.
pi$_1$			
pi$_1$			
sigma$_3$			
pi$_2$			
pi$_2$			
sigma$_4$			