Problem Set 4
Questions for discussion

These are questions submitted by your classmates, Clyde, and Prof. Kandel. You should look over these questions before the problem session at 3:30 on Wednesday, September 23, and you should come to the session ready to discuss them. You do not necessarily need to have answers for all of these questions (some may be so open-ended that there is no one simple answer), but you should think about them and have something to say.

1. I’m still a little confused about curvature and its relation to energy. I know that an orbital that has more curvature has more energy, but why is this? And what exactly is curvature?

2. Can we please discuss how the relationship of atomic orbital energies affects molecular orbitals?

3. When a certain amount of energy is added to $H^+_2$, its electron goes from a $1s_A + 1s_B$ orbital to a $1s_A - 1s_B$ in which the electron interferes with itself. Is the bond always broken in this case? And if so, is the energy it takes to do this the bond energy? Also, how does this compare to the energy it takes to form the ground state orbital to a higher level positive interference orbital?

4. If an anti-bonding orbital is more anti-bonding than a bonding orbital is bonding, could an electron in a $\sigma^*_1s$ orbital move to a $\sigma_{2p_z}$ orbital in order to prevent the bond from being broken?

5. Is the bond length of a molecule in an excited state shorter or longer than the bond length in the ground state? Why?

6. Why is constructive interference for the $\sigma_{2p_z}$ orbital a subtraction of the two atoms’ $p_z$ orbitals, rather than an addition like other sigma orbitals?

7. When filling orbitals such as the $\sigma/\sigma^*$ and $\pi/\pi^*$, does the filling order change for those elements whose orbitals fill out of order as well? If so, for which elements is this true?

8. Why does bond energy not change the sigma orbitals’ energy?