CHM 3411, Dr. Chatfield, Spring 2018
Problem Set 9

This is not to be turned in. However, the material will be on Exam 2, so you are strongly encouraged to do this problem set. Solutions will be posted on Friday, March 23.

Suggested "warmups" (not to turn in): Discussion Questions 10.C1-3; Exercises [all (b)] 10B.1,2,4(a),4(b) 10C.4-6

This problem set explores Molecular Orbital Theory applied to diatomic molecules.

2. Atkins Exercises 10C.1(a), 10C.1(b) (together because they cover the same concept, with different twists)

3. Atkins Exercises 10C.2(b), 10C.3(b) (together because they cover the same concept, with different twists)

4. We saw in class that a molecular orbital can be constructed as a linear combination of atomic orbitals (LCAO-MO). Below are unnormalized MOs expressed in this way. For a homonuclear diatomic molecule with the z axis coincident with the internuclear axis, characterize the MOs as σ, π, or δ (see note below regarding δ orbitals); bonding or antibonding; and g (gerade) or u (ungerade). Sketch the AOs and resulting MO in each case. Notes: (1) Follow the convention that $2p_{zA} + 2p_{zB}$ represents an orientation with constructive interference. (2) Although we did not discuss δ MOs in class, they are analogous to d AOs; observed from along the z axis, δ MOs look like d AOs.

a) $2p_{yA} + 2p_{yB}$ b) $2p_{zA} - 2p_{zB}$ c) $3d_{xyA} + 3d_{xyB}$

5. Atkins Problem 10C.1