Reading: Chapter 4. Emphasize 4.7, 4.8, 4.11- 4.14.

Problem Assignment (for practice only; not ever due!!!!!!!!!!)

Exam II: Tuesday, October 26, 5:40-7:40 pm.


7. Overlap of atomic orbitals. In each example, you are given two orbitals, one centered on atom A and the other centered on atom B. Determine whether the overlap between the two orbitals is positive, negative, or zero by symmetry. Use the coordinate system shown below, and make a sketch showing the orbitals and the signs of key regions. Hint: Your book provides the signs of the different lobes of the d orbitals by color coding in Fig. 1.32. All d orbitals have even parity, which means the wavefunction has the property \( \psi(-x, -y, -z) = \psi(x, y, z) \). Thus “opposite” lobes in space have the same sign. All s orbitals also have even parity. In contrast, p orbitals and f orbitals have odd parity: \( \psi(-x, -y, -z) = -\psi(x, y, z) \). Yes, the parity is determined by the evenness or oddness of the quantum number \( \ell \).

A. 4s on A, 4s on B.  
B. 4s on A, 3d\(_z^2\) on B.  
C. 3d\(_{xy}\) on A, 3d\(_{xz}\) on B.  
D. 3d\(_{yz}\) on A, 3d\(_{yz}\) on B.

8. Use the MO picture to describe the chemical bonding in Sc\(_2\). Give the electron configuration and sketch an orbital energy diagram for the valence electrons only. Hint: The promotion energy from 4s to 3d is inexpensive, so Sc\(_2\) is able to make a triple bond. There is one \( \sigma \) bond and two \( \pi \) bonds. Make the approximation that the 4s orbitals on each atom interact strongly to form the \( \sigma \) bond, because they are larger and overlap better. Occupy the \( d \) orbitals on each atom in a way that enables making the two \( \pi \) bonds.