1. Sutton, problem #9. This problem deals with the issue of what happens if the atomic orbitals used in the diatomic molecule discussion are not strictly orthogonal. Write two paragraphs that interpret the results you obtain for the molecular energy levels and for the molecular orbitals that correspond to them. Also plot $E_a$ and $E_b$ as a function of $S$.

2. Carbon dioxide (CO$_2$) is a symmetric linear molecule that looks like this:

\[ \text{O}_1 \quad \text{C} \quad \text{O}_2 \]

Let $|O_1\rangle$, $|C\rangle$ and $|O_2\rangle$ be atomic states (assumed to be mutually orthogonal) associated with the respective oxygen and carbon atoms. Let $E_O$ and $E_C$ be, respectively, the “on-site” energies of electrons on the isolated oxygen and carbon atoms, and let $\beta$ be the near-neighbor hopping matrix element. Assume only near neighbor interactions.

(i) Following the procedure used in class, obtain the secular equation (the one that involves the determinant) and solve for the energy eigenvalues of this molecule. Identify the energies of the bonding and antibonding states.

3. Discuss qualitatively the bonding between 2 atoms in the following cases:
   (i) sigma bonding between two equivalent $p_z$ orbitals
   (ii) pi bonding between two equivalent $p_z$ orbitals
   (iii) sigma bonding between two equivalent $d_{z^2}$ orbitals
   (iv) pi bonding between two equivalent $d_{yz}$ orbitals

In each case, sketch qualitatively the approximate electron distribution on the isolated atoms and then the distributions corresponding to the molecular orbitals $|\Psi\rangle = |1\rangle + |2\rangle$ and to $|\Psi\rangle = |1\rangle - |2\rangle$ and say which is the bonding combination, which the antibonding and why.

4. The heteronuclear diatomic molecule: Fill in the algebra that leads to Sutton Eq. 2.45 and Eq. 2.46 (explain the physics as you go along) and make a plot like Fig 2.4 based on your results (Sutton's Fig 2.4 is slightly inaccurate). Do a little research to find some parameters for NaCl that indicate where NaCl falls on this plot, i.e. the degree of ionicity of the bond indicated by Eq. 2.48.

5. In preparation to use the band structure computation programs, find the crystal structure of Si.
   (i) The crystal structure of Si is based on a cubic arrangement of atoms. Where, exactly, are these atoms located, in units of the lattice parameter? What are the Si-Si bond lengths and angles? Draw a sketch. (It will be very helpful to find a program that does this for you. There are several available on line.)
   (ii) What is the lattice parameter of Si?
   (iii) What is the space group of Si?