0. Midterm exam on Friday May 2 covers all material up and including material in class on Monday April 28. You will not be required to repeat any of the detailed calculations in this set on the test, but you should understand the concepts. We will discuss the heteronuclear chain in class a bit more.

1. Further explore the Wien program using Si as an example.
   (a) Calculate the partial density of states for Si $s$ orbitals, for $p$ orbitals and for “interstitial” states. You will have to use the manual to understand how to edit the case.int file under Tasks/DOS to calculate more than 1 density of states. Explain what is meant by “partial density of states”. What states contribute most to the valence band of Si?
   (b) Plot the dispersion relation $E(k_x,k_y,k_z)$ for the default fcc k-paths in Wien. At which $k$-point is the maximum of the valence band? At which is the minimum of the conduction band? What is meant by the terms “indirect gap semiconductor” and “direct gap semiconductor”? What is the smallest direct gap in Si according to your calculation? According to well-established results in literature? (This problem is well known in the density functional theory literature.)
   (c) Try to get XCrysDen working to visualize the structure, and to plot the dispersion relation for different $k$-paths. (not graded, but you’ll need this skill for the project).

2. Propose a material to study for the Wien MT2 project.
   (i) Give a 1-paragraph motivation for the study.
   (ii) Describe the structure (space group, atoms per unit cell, etc.)
   (iii) Would you like to use the Flair/Gem program in addition to (or instead of) the Wien program? If so, please email Dr. Tate and Dr. Schneider (tate@physics.oregonstate.edu; Guenter.Schneider@physics.oregonstate.edu). The Flair/gem webpage is http://www.physics.oregonstate.edu/~schneidg/ph575project-flair-gem/. Number of people is limited to about 10 on a first-come basis.

3. Consider an infinite linear chain of A and B atoms in which there are nearest neighbor interactions only with matrix element $\beta$ and where the on-site Hamiltonian matrix elements on A and B atoms are $E_A$ and $E_B$, respectively. The A-B bond length is $a$.
   Calculate and sketch the band structure and show that there are two bands and that the Brillouin zone may be defined to lie between $-\pi/2a$ and $+\pi/2a$.
   Examine the corresponding eigenstates and show that the states in the lower band are bonding and those in the upper band are antibonding.
   (After Sutton, problem #15, and also related to the problem on hwk #3.)

4. Group velocity in a crystal.
   (a) Sutton #13. In this problem you are to show that $v_k = \frac{1}{h} \frac{dE(k)}{dk}$. We rationalized this in class, but did not show it rigorously. Use Sutton's hint to substitute the most general form a Bloch wave function $|\psi_k\rangle = e^{ikx}|u_k\rangle$ into the definition of the group
velocity \( v_k = \frac{\mathbf{p}}{m^*} \langle \psi_k | \hat{\mathbf{p}} | \psi_k \rangle \). It will be useful to convert to wave function form.

Also substitute the Bloch wave function into Schrödinger's equation. You have to connect the two to derive the desired result.

(b) Apply this expression for \( v_k \) to the 1-d dispersion relation given and do the required calculation.

(c) Explain what it means to have the group velocity be zero at the zone boundary.

5. Look up the band structures \( E(k) \) (give a reference to where you find them) of the five Group IV elements C to Sn (in the diamond structure). From the band structures,

(a) Describe and discuss the trend in the band gaps of these semiconductors.

(b) Are the band gaps direct or indirect, and what wavelength of light is required to excite an electron across the gap?

(d) Discuss the effective mass of electrons close to the bottom of the conduction band and of holes close to the top of valence band.