PH575: Introduction to Solid State Physics SPRING 2019
Homework #4 DUE Friday, 10 May 2019, in class

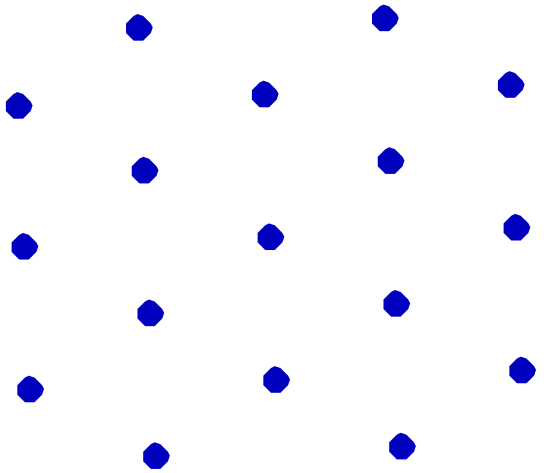
1. Complete the OpenMX mini-project to calculate the band structure for Si. The following elements should be present.
   (a) You should be able to find a cif file for Si from a reputable source (where?) and transfer the information to the OpenMX system and create the appropriate data file. Also, you have to choose the appropriate potentials for Si (what did you choose?). Even if OpenMX has such a file already, make sure you can duplicate the process.
   (b) Draw the structure of one unit cell in XCrysDen or OpenMX viewer or some other program (which one?). Display several unit cells. The important skill is learning to visualize crystal structures.
   (c) Plot the dispersion relation $E(k_x,k_y,k_z)$ for the default fcc k-paths in OpenMX and try adding one or more of your own.
   (d) At which k-point is the maximum of the valence band? At which is the minimum of the conduction band? What is the separation in energy of this "indirect gap" according to your calculation? What is the experimental value? (This problem is well known in the density functional theory literature.)
   (e) What is meant by the terms “indirect gap semiconductor” and “direct gap semiconductor”?
   (f) Plot the *total* and *partial* density of states for Si *s* orbitals, for *p* orbitals. Explain what is meant by “partial density of states”. What states contribute most to the valence band of Si?

2. Look up the band structures $E(k)$ (give a reference & plots) of the four Group 14 elements C to Sn (in the diamond structure). From the band structures,
   (a) Describe and discuss any trends in the band gaps of these materials.
   (b) Are the band gaps direct or indirect, and what is the minimum energy of a photon required to excite an electron across the gap in each material? What is the wavelength of that light?

3. Read the 8-page review article by Marvin Cohen (a well known condensed matter theorist and electronic structure pioneer) posted under "Articles" on the class website.
   (a) When we model silicon by density functional theory (or similar techniques), the “core” of the silicon atom is assumed to be fixed and inert. What is this core and what is the net charge?
   (b) What idea does Cohen quote from Paul Dirac?
   (c) How many orders of magnitude difference between the resistivity of the most resistive and least resistive known solids?
   (d) Which theory was worked out first: the BCS theory of superconductivity or the band structure of silicon?
   (e) In your own words, explain the difference between the empirical pseudopotential method (EPM) and *ab initio* approaches.
   (f) Figure 5 shows $V(r)$ for an electron attracted to the “core” of an atom. Why does $V(r)$ not look like a Coulomb potential?
   (g) The contours in Fig. 7 are labeled 24, 16, 12 *etc*., but no units are given. What unit is being used? Coulombs per cubic meter? Electrons per cubic centimeter? Something else?
   (h) Cohen writes: “Silicon is said to be the basis of geology, and carbon is the basis of life.” How does Cohen explain why silicon and carbon play such different roles?

3. Study the Poster/Paper section of the class web page http://physics.oregonstate.edu/~tatej/COURSES/ph575/doku.php?id=papers and propose a material to study for the term project.
   (a) Give a 1-paragraph motivation for the study.
   (b) Describe the structure (space group, atoms per unit cell, etc.)
   (c) What properties or structure are you interested in investigating with OpenMX?

4. For this triangular lattice where neighboring atoms are separated by the same distance,



   (a) Draw **a** and **b**, the lattice vectors such that $n\mathbf{a} + m\mathbf{b}$ (n,m integers) will take you to any and every lattice point.
   (b) Draw a unit cell that is **not** the Wigner Seitz cell
   (c) Draw the Wigner Seitz cell.
   (d) Comment on the symmetries of the two cells you've drawn
   (e) What are the reciprocal lattice vectors?
   (f) Draw the reciprocal lattice and the first and second Brillouin zones.

5. Look up a Si band structure that is detailed enough to include "spin-orbit coupling". In such a band structure, you will find reference to "heavy holes", "light holes" and "split-off holes".
   (a) Explain what these terms refer to and explain why the "heavy" hole is heavy and the "light" hole is light.
   (b) What the values of the effective masses of the heavy, light and split-off holes and the value of the electron effective mass at the bottom of the conduction band (usually quoted in terms of the free electron mass)?
   Make sure you quote sources for all references.

6. Find a recent article in a journal that investigates (or at least mentions) the sign of the electric charge carriers and the effective mass in an interesting material. Summarize the basic questions addressed and the conclusions.