Condensed Matter Physics 2023
Assignment

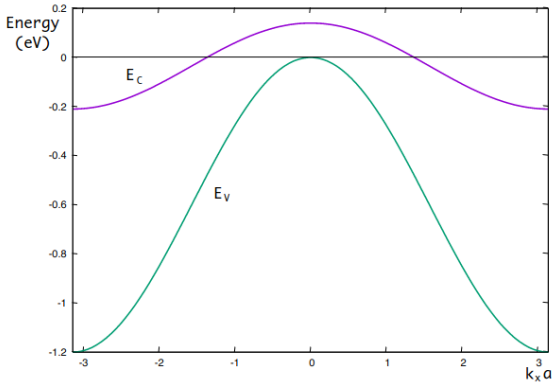
To be submitted by Friday 19th May

1. Let's consider an orthorhombic crystal where the three lattice vectors have a magnitude of $a = 2$, $b = 3$ and $c = 5$ Å.
   (a) Write the direct and reciprocal primitive lattice vectors (include the units).
   (b) What is the wavevector $\mathbf{k}$ at the first Brillouin zone boundary in the [010], [110] and [111] directions?
   (c) Along the [100] direction, the conduction (c) and valence (v) bands are given by:

$$E_c = 0.7\left[\frac{1}{5} - \frac{1}{2}\sin^2\left(\frac{k_x a}{2}\right)\right]$$

$$E_v = 0.6[\cos(k_x a) - 1]$$

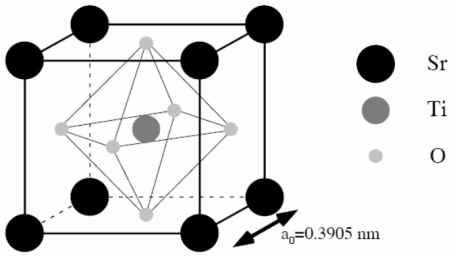
   where the energy is given in eV, and the Fermi level is at $E = 0$. The band dispersion is plotted below. Is the crystal a metal or an insulator?



   (d) Calculate the group velocity of electrons in the conduction band at $k_x = 0$ and $k_x = \pi/(2a)$ (note: be careful about the units).

(5 points)

2. The figure below shows the unit cell of strontium titanate ($SrTiO_3$), which has a so-called perovskite structure. The lattice is simple cubic with lattice constant $a = 3.905$ Å.



   (a) Determine the basis for this structure.[1]
   (b) Calculate the X-ray structure factor.
   (c) Use the calculated structure factor to obtain the ratio of the intensities of the (200) and (100) peaks.
   (d) Calculate the diffraction angles 2θ of the (100), (110) and (200) peaks observed using monochromatic X-rays with $\lambda = 1.55$ Å.

(5 points)

3. (a) Describe the dispersion relation for the phonons of a diatomic linear chain where the atoms have different masses and are equally spaced, assuming the same spring constant. Describe the motion of the atoms at the first Brillouin zone boundary.

[1] Hint: it is a 5 atom basis (as the name of the material, $SrTiO_3$, suggests...).

(b) Explain how the phonon dispersion curves would change if the masses of the atoms were equal.

(c) For the $SrTiO_3$ crystal of Question 2, state how many phonon modes there would be and of what type.

(4 points)

4. Choose one topic from the list below (note: some topics haven't (yet?) been discussed in class; with permission, you may also choose another topic of your interest not from the list, ask via email or Ed). From the perspective of condensed matter physics, explain the essential concepts and principles that underlie our understanding of the topic, and some important applications.

   - Phonons in crystalline materials
   - Semiconductor devices
   - Crystallography
   - Superconductivity
   - Van der Waals heterostructures
   - Density functional theory
   - Defects/impurities in semiconductors
   - Classical and quantum Hall effect

   Additional instructions:

   1. You are limited to a maximum of 2 pages (not counting references), 12 point Times New Roman font or equivalent. You may make use of headings and figures.
   2. While you should mention some of the material from the lectures/textbook (if the topic was discussed), you must go beyond what is covered in class.
   3. This assignment is designed to strengthen your ability to write concisely in a form appropriate for a scientific report or publication; focus on quality, rather than quantity. Note: while I can't prevent you from using some AI tool, you should keep in mind the important learning outcomes mentioned, and come up with your own writing.
   4. Advanced only. You should also describe briefly an example related to the chosen topic from recent research, referencing publications appropriately.

   (10 points)