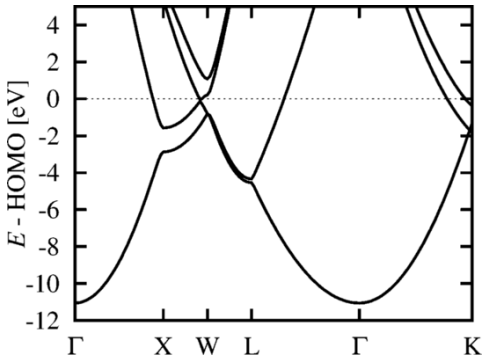
HW5

MTLE-6120: Spring 2023

Due: Feb 17, 2023

1. **Band structure appreciation**

   Given this band structure of an element with single atom/primitive cell:

   (a) Metal or semiconductor?

   (b) How many valence electrons?

   (c) Which group of periodic table?

   (d) Guess which element.

2. **Effective mass**

   For the simplest tight-binding model in 1D, the band structure consists of a single band $E(k) = E_0 - 2t\cos ka$, where E_0 is the isolated energy and t is the coupling strength.

   (a) Calculate the effective mass $m^*(k)$ at any point in the band structure.

   (b) What are the effective masses near the bottom and top of the bands? Explain the dependence of these masses on a and t.

   (c) What is the average value of $(m^*(k))^{-1}$ over the band?

3. **Sketching density of states of real metals**

   For a simple cubic lattice with only nearest neighbour coupling, the density of states of a tight-binding model is $E(\vec{k}) = E_0 - 2t\cos k_x a - 2t\cos k_y a - 2t\cos k_z a$, where $\vec{k}$ is in the Brillouin zone $[-\pi/a, \pi/a]^3$.

   (a) What is band width and total number of states per unit cell for this band?

   (b) It is not easy to calculate the DOS of this dispersion relation, so let us try to approximate it. By Taylor expanding, show that $E \approx E_a + \hbar^2(\vec{k} - \vec{k}_a)^2/(2m_a)$ for some E_a, $\vec{k}_a$ and m_a near the bottom and top of the band. What is the effective mass m_a at each of these band edges?

   (c) Using the above, construct an approximation for the density of states of the form $g(E) = \frac{A}{1+B((E-E_0)/(6t))^2}\sqrt{(E-E_{\min})(E_{\max}-E)}$ for $E_{\min} \le E \le E_{\max}$ and 0 otherwise. Select A and B to produce the correct density of states near the band edges. as well as the correct number of states/cell, and plot the resulting DOS. (You will need to solve for A and B numerically.)

   (d) Assume that the transition metals have tight-binding d electrons with a free-electron like s band. Schematically sketch the density of states, and indicate the Fermi level position for each element in the 3d transition series, Sc ($3d^1 4s^2$) to Zn ($3d^{10} 4s^2$).