Topic 9-3: Band Structures of Metals and Insulators

**Summary:** We begin this video by introducing four types of materials: metals, insulators, semimetals, and semiconductors. We then show their band structure in two varieties to gain an understanding of the differences between them. We follow this by going through several examples of different compounds as well as their band structures to gain a better understanding of how to classify these four different materials.

- Have been talking about the dispersion a lot
  - Just the bucket we pour electrons into
- Need to figure out which states are actually occupied and how our electrons fill our bands
- Plot band structures from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$ and the line is only semi continuous
  - The dispersion is made up of discrete k points separated by $\frac{2\pi}{L}$
- This means that the number of modes in the band is $\frac{2\pi/a}{2\pi/L} = \frac{L}{a}$ which is the number of unit cells in a particular direction, N
- The band can then hold 2N electrons because we can put a spin up and a spin down electron in each mode
- Depending on how filled the bands are and how they are arranged we can get four different types of materials
- We have metals and insulators on the extremes and semimetals and semiconductors in the middle
  - Shading indicated occupied states
- Can also show this in terms of the density of states
• Example: Carbon and the diamond structure
  o 4 electrons in carbon so we have an even number of electrons no matter if we consider the primitive or conventional cell
  o Diamond is transparent so there is a big gap between a filled band and the next unoccupied band
  o Diamond is an insulator

• Example: GaAs
  o Total of 8 valence electrons, again we have an even number
  o Turns out to be a semiconductor
  o Can think of this as a diamond like structure with sp³ bonding
• Example: Lithium
  o Body centered cubic conventional cell
  o Primitive cell has one atom
  o Group 1 with 3 electrons total
    ▪ 2 core electrons
    ▪ 1 electron in outer band
  o Valence band is half filled
  o Metal
  o Perhaps surprising to invoke atomic orbitals when we’ve been using a traveling wave description. The suggestion is that the modulation term on the traveling wave will lead to s-like atomic orbitals around each atom.

• Example: Beryllium
  o 2 electrons in outer band, should be a filled band
  o 2p orbital has dropped down and mixed with the 2s orbital which leaves multiple bands at the Fermi level
  o Classified as a metal
  o Crystal structure of Be is hexagonally close packed
- 2 atoms per primitive cell
- 4 electrons poured into these bands
  - Might hypothesize this should fill the first two bands and give the highest energy electron back at the gamma point
  - In that case the next lowest energy state would also be at the gamma point
  - So when the unoccupied band drops down into the occupied band the overlap starts at gamma
    - Can see this in the calculated dispersion
  - This is a really clean example of a metal

![Graph showing band structure](image)

- Example: Zinc
  - Far right of transition metals
  - Structure is hexagonally close packed
  - Even number of electrons
  - Calculated dispersion is a mess, many bands at the Fermi level

![Graph showing band structure](image)

- In real systems we need to be careful about predicting how we fill our bands!
- Example of a semimetal is CdO
• Fermi level splits between 2 bands
  o No crossing of the two bands at the Fermi level which makes it a semimetal

• As we alloy CdO with CaO, we can see the two bands pull apart, leading to an insulator

• In short, it is easy to classify the material if you know the dispersion. If you don’t, you’re either looking at optical properties (color), chemical intuition, or calculate the dispersion.
Questions to ponder

1. Connect the use of ZnO as a sunblock material, protecting up from UV light, to its band structure.

2. What type of material is Bi₂Te₃? How many maxima does the valence band edge have in the first brillouin zone?

3. What are aluminum and copper metals? Why do their dispersions look so different?