**Explain on basis of Band theory, the nature of conductivity of metals, non-metals and insulators.**

**Band Theory and the Nature of Conductivity in Materials**

Band theory explains the electrical conductivity of materials by examining the behavior of electrons in the material's atomic or molecular structure. According to this theory, the energy levels of electrons in a solid form bands, and the behavior of these bands determines the material's electrical conductivity. The key factors to consider are the **valence band**, **conduction band**, and the **band gap**.

**1. Metals:**

* **Structure**: In metals, the valence band and conduction band overlap or are very close to each other, meaning there is little or no band gap.
* **Electron Movement**: Electrons in the valence band can easily move to the conduction band (since the bands overlap), allowing them to flow freely through the material. This is why metals are good conductors of electricity.
* **Resulting Property**: The free electrons in the conduction band can move under an applied electric field, making metals highly conductive.

**Key Point**: Metals have a *partially filled conduction band* or *overlapping valence and conduction bands*, allowing easy electron flow and good electrical conductivity.

**2. Non-metals (Semiconductors and Insulators):**

* **Semiconductors**:
  + In semiconductors, the valence band is completely filled, and there is a small band gap between the valence band and conduction band.
  + Under normal conditions, electrons do not have enough energy to jump from the valence band to the conduction band.
  + However, when energy is supplied (e.g., heat or light), some electrons can acquire enough energy to jump to the conduction band, allowing electrical conduction.
  + The size of the band gap in semiconductors is small enough that thermal or optical energy can excite electrons into the conduction band, making them conduct electricity.

**Key Point**: Semiconductors have a *small band gap*, which allows electrical conduction under certain conditions (e.g., at higher temperatures or with added energy).

* **Insulators**:
  + In insulators, the band gap between the valence band and the conduction band is large.
  + Electrons in the valence band require a significant amount of energy to move to the conduction band, which is not easily supplied under normal conditions.
  + As a result, electrons cannot move freely, and these materials do not conduct electricity under ordinary conditions.

**Key Point**: Insulators have a *large band gap*, which prevents electrons from jumping to the conduction band, making them poor conductors.

**What is band theory:**

**Band Theory** is a concept in solid-state physics that explains the behavior of electrons in solids, particularly in relation to electrical conductivity. It provides a more comprehensive understanding than earlier models, like the free electron model, by considering the energy levels of electrons in a material and how these levels form bands.

**Key Concepts of Band Theory:**

1. **Atomic Orbitals and Energy Levels**: In isolated atoms, electrons occupy discrete energy levels (orbitals). When atoms come together to form a solid, their atomic orbitals combine, leading to the formation of energy bands. These bands represent ranges of energy that electrons in a solid can occupy.
2. **Energy Bands**:
   * When atoms pack together to form a solid, their individual atomic orbitals combine into molecular orbitals that spread over the entire solid. These molecular orbitals form **energy bands**.
   * The **valence band** is the highest energy band that is filled with electrons in a material at absolute zero temperature.
   * The **conduction band** is the next higher band, which is normally empty but can accommodate electrons if they gain enough energy.
3. **Band Gap**:
   * The **band gap** (also called the **energy gap**) is the energy difference between the top of the valence band and the bottom of the conduction band.
   * If the band gap is small, electrons can easily jump from the valence band to the conduction band, enabling electrical conduction.
   * If the band gap is large, electrons cannot move freely to the conduction band, and the material behaves as an insulator.
4. **Free Electrons**:
   * In some materials (especially metals), electrons in the conduction band are free to move throughout the material. These free-moving electrons are responsible for electrical conductivity.
   * In insulators and semiconductors, the electrons in the valence band are tightly bound to atoms and need additional energy to reach the conduction band.

**Band Theory in Different Materials:**

* **Metals**: In metals, the conduction band overlaps the valence band, or the conduction band is partially filled with electrons. This allows for free movement of electrons, making metals good conductors of electricity.
* **Semiconductors**: In semiconductors, there is a small band gap between the valence and conduction bands. At higher temperatures or when energy is applied, electrons can jump to the conduction band, allowing for moderate conductivity.
* **Insulators**: In insulators, the band gap is large, so electrons cannot easily jump from the valence band to the conduction band, making these materials poor conductors of electricity.

**Origin of Band Theory:**

* Band theory developed to explain the electrical properties of solids, particularly why some materials conduct electricity and others do not. Earlier models, like Drude's free electron theory (1900) and Sommerfeld's quantum mechanical approach (1928), couldn't fully explain these differences.
* A key breakthrough came from **Felix Bloch** in 1928, who showed that in a solid's periodic lattice, electron wavefunctions form **energy bands**. In the 1930s, scientists like **Ralph H. Fowler** and **Nevill Mott** expanded on this, explaining that atomic energy levels combine into bands in solids, with the key concept of the **band gap** separating the valence band (filled with electrons) and conduction band (where electrons can move freely).
* This theory helped explain why metals conduct electricity (overlapping bands), why semiconductors conduct under certain conditions (small band gap), and why insulators do not (large band gap). Band theory laid the foundation for modern **solid-state physics** and the development of electronic devices like transistors.

**Metal Conductivity Based on Band Theory:**

In metals, electrical conductivity is explained by the behavior of electrons within the **energy bands**.

1. **Energy Bands in Metals**:
   * Metals have **overlapping** or **very close** **valence** and **conduction bands**, meaning there is no significant band gap separating them.
   * The **valence band** contains electrons that are bound to atoms, while the **conduction band** is where electrons are free to move and contribute to electrical conduction.
2. **Electron Movement**:
   * In metals, because the valence and conduction bands overlap or are very close together, **electrons in the valence band** can easily move into the conduction band without needing extra energy.
   * This allows the electrons to be free to move throughout the material under an applied electric field.
3. **Electrical Conductivity**:
   * Since there are many free electrons in the conduction band, metals can conduct electricity very well.
   * These free electrons act as charge carriers, and when an electric field is applied, they move through the metal, allowing current to flow.

**Special cases:**

In the context of band theory, there are a few special cases of materials that deviate from the standard behavior of metals, semiconductors, and insulators. These cases involve unique conditions or phenomena that influence conductivity. Here are a few examples:

**1. Superconductors:**

* **Behavior**: Superconductors are materials that, below a critical temperature, exhibit **zero electrical resistance**. This means they conduct electricity without any energy loss.
* **Band Theory Explanation**: In superconductors, at low temperatures, electrons pair up to form **Cooper pairs**. These pairs move through the lattice without scattering, leading to zero resistance. While band theory explains the general behavior of electrons, the phenomenon of superconductivity involves **quantum mechanical effects** that go beyond classical band theory.

**2. Semimetals:**

* **Behavior**: Semimetals have **overlapping valence and conduction bands**, but their electron and hole concentrations are low compared to metals.
* **Example**: **Graphite** and **bismuth** are semimetals. While they conduct electricity, their conductivity is lower than that of metals.
* **Band Theory Explanation**: In semimetals, the **valence band** and **conduction band** overlap slightly, allowing some electrons to move freely, but the overall density of free electrons is not as high as in metals, leading to lower conductivity.

**3. Mott Insulators:**

* **Behavior**: Mott insulators are materials that should, according to traditional band theory, be conductors (based on their band structure), but they act as insulators due to **strong electron-electron interactions**.
* **Example**: **Vanadium oxide** (V₂O₃) is a Mott insulator.
* **Band Theory Explanation**: According to traditional band theory, a material with a small band gap should be a conductor. However, in Mott insulators, the **strong Coulomb repulsion** between electrons causes them to localize, preventing conductivity. This phenomenon requires a more sophisticated theory that includes electron correlations.

**4. Topological Insulators:**

* **Behavior**: Topological insulators are materials that are **insulating in the bulk** but have **conducting surface states** that are protected by the material's topology.
* **Example**: **Bismuth telluride** (Bi₂Te₃) is a topological insulator.
* **Band Theory Explanation**: In topological insulators, the bulk is an insulator (with a large band gap), but due to the material’s unique electronic structure and symmetry, **surface states** exist that allow electrical conduction. These surface states are protected from scattering by impurities and disorder, leading to unique conducting properties at the surface.

**5. Photoconductors:**

* **Behavior**: Photoconductors are materials that **increase their electrical conductivity when exposed to light**.
* **Example**: **Silicon** and **selenium** are common photoconductors.
* **Band Theory Explanation**: In photoconductors, light provides energy to excite electrons from the **valence band** to the **conduction band**. The absorbed photons excite electrons across the band gap, increasing the number of free electrons in the conduction band and enhancing the material’s conductivity.

**Limitations:**

While **band theory** is an effective and powerful tool for explaining the electrical properties of materials, it does have several limitations. These limitations arise when trying to describe more complex or specific phenomena in solids. Below are the main limitations of band theory:

**1. Does Not Account for Strong Electron-Electron Interactions:**

* **Limitation**: Band theory assumes that electrons in a material behave as independent particles, but this does not always reflect reality. In materials where **electron-electron interactions** are strong (like in **Mott insulators** or some **high-temperature superconductors**), band theory fails to explain the observed behavior.
* **Example**: Mott insulators, which should theoretically conduct electricity based on band theory, act as insulators due to strong electron correlation effects that band theory does not fully incorporate.

**2. Simplification of Complex Interactions:**

* **Limitation**: Band theory largely ignores other complex interactions in solids, such as **spin-orbit coupling** (interaction between electron spin and its motion), **magnetic interactions**, and **phonon-electron interactions** (vibrations of the crystal lattice affecting electron movement).
* **Example**: Topological insulators involve intricate spin-orbit coupling and surface states that band theory cannot completely describe without extending into more advanced models.

**3. Limited Applicability to Non-Crystalline Materials:**

* **Limitation**: Band theory is primarily designed for **crystalline solids**, where atoms are arranged in a regular, periodic structure. It is not well-suited to describe **amorphous materials** or materials without a clear periodic structure.
* **Example**: Amorphous semiconductors (like amorphous silicon) don’t have a long-range periodic lattice, making the application of band theory to these materials more challenging.

**4. Does Not Explain Superconductivity Fully:**

* **Limitation**: While band theory can explain electrical conduction in metals and semiconductors, it cannot explain the phenomenon of **superconductivity**, where materials exhibit **zero electrical resistance** below a certain temperature.
* **Example**: In superconductors, electrons form **Cooper pairs** that move without resistance, a phenomenon that band theory alone cannot account for. This requires quantum mechanical theories like **BCS theory**.

**5. Failure to Predict Magnetism in Some Materials:**

* **Limitation**: Band theory is inadequate in explaining the **magnetic properties** of materials like ferromagnets and antiferromagnets. It does not take into account the collective behavior of electron spins that results in magnetism.
* **Example**: Band theory cannot fully explain the ferromagnetism in iron, where electron spins align in a way that leads to a macroscopic magnetic field.

**6. Neglects Temperature and External Conditions:**

* **Limitation**: Band theory generally assumes a material is in a **ground state** (at absolute zero temperature) and does not always consider the effects of temperature, pressure, or external fields on the material's properties.
* **Example**: At higher temperatures or under extreme conditions, electron behavior can change significantly (e.g., in **high-temperature superconductors**), and band theory does not fully account for these temperature-dependent effects.

**7. Inability to Describe Quantum Phenomena in Some Materials:**

* **Limitation**: Band theory is a **classical model** and does not always incorporate the full range of **quantum mechanical effects** observed in certain materials, especially those exhibiting **quantum confinement** (e.g., **quantum dots** or **nanomaterials**).
* **Example**: Quantum dots, with their discrete energy levels due to their small size, show behaviors not fully explainable by band theory.

**Conclusion:**

While band theory is foundational for understanding the electrical properties of many materials, its limitations in dealing with strong electron interactions, non-crystalline materials, and complex quantum effects highlight the need for more advanced models, such as **many-body theory**, **quantum field theory**, and **tight-binding models**. These extended theories address the shortcomings of basic band theory and provide a more comprehensive understanding of material properties under various conditions.

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