* Summary

Quantum mechanics explains the bonding together of atoms to form **molecules**. In a **covalent bond**, the atoms share electrons. The electron clouds of two or more atoms overlap because of constructive interference between the electron waves. The positive nuclei are attracted to this concentration of negative charge between them, forming the bond.

An **ionic bond** is an extreme case of a covalent bond in which one or more electrons from one atom spend much more time around the other atom than around their own. The atoms then act as oppositely charged ions that attract each other, forming the bond.

These **strong bonds** hold molecules together, and also hold atoms and molecules together in solids. Also important are **weak bonds** (or **van der Waals bonds**), which are generally dipole attractions between molecules.

When atoms combine to form molecules, the energy levels of the outer electrons are altered because they now interact with each other. Additional energy levels also become possible because the atoms can vibrate with respect to each other, and the molecule as a whole can rotate. The energy levels for both vibrational and rotational motion are quantized, and are very close together (typically, 10^{-1} eV to 10^{-3} eV apart). Each atomic energy level thus becomes a set of closely spaced levels corresponding to the vibrational and rotational motions. Transitions from one level to another appear as many very closely spaced lines. The resulting spectra are called **band spectra**.

The quantized rotational energy levels are given by

$$E_{\text{rot}} = \ell(\ell + 1)\frac{\hbar^2}{2I}, \qquad \ell = 0, 1, 2, \cdots, \tag{29–1}$$

where I is the moment of inertia of the molecule.

The energy levels for vibrational motion are given by

$$E_{\text{vib}} = \left(\nu + \tfrac{1}{2}\right)hf, \qquad \nu = 0, 1, 2, \cdots, \tag{29–3}$$

where f is the classical natural frequency of vibration for the molecule. Transitions between energy levels are subject to the selection rules $\Delta\ell = \pm 1$ and $\Delta\nu = \pm 1$.

Some **solids** are bound together by covalent and ionic bonds, just as molecules are. In metals, the electrostatic force between free electrons and positive ions helps form the **metallic bond**.

In the free-electron theory of metals, electrons occupy the possible energy states according to the exclusion principle. At $T = 0$ K, all possible states are filled up to a maximum energy level called the **Fermi energy**, E_{F}, the magnitude of which is typically a few eV. All states above E_{F} are vacant at $T = 0$ K.

In a crystalline solid, the possible energy states for electrons are arranged in **bands**. Within each band the levels are very close together, but between the bands there may be forbidden **energy gaps**. Good conductors are characterized by the highest occupied band (the **conduction band**) being only partially full, so lots of states are available to electrons to move about and accelerate when a voltage is applied. In a good insulator, the highest occupied energy band (the **valence band**) is completely full, and there is a large energy gap (5 to 10 eV) to the next highest band, the *conduction band*. At room temperature, molecular kinetic energy (thermal energy) available due to collisions is only about 0.04 eV, so almost no electrons can jump from the valence to the conduction band in an insulator. In a **semiconductor**, the gap between valence and conduction bands is much smaller, on the order of 1 eV, so a few electrons can make the transition from the essentially full valence band to the nearly empty conduction band, allowing a small amount of conductivity.

In a **doped** semiconductor, a small percentage of impurity atoms with five or three valence electrons replace a few of the normal silicon atoms with their four valence electrons. A five-electron impurity produces an ***n*-type** semiconductor with negative electrons as carriers of current. A three-electron impurity produces a ***p*-type** semiconductor in which positive **holes** carry the current. The energy level of impurity atoms lies slightly below the conduction band in an *n*-type semiconductor, and acts as a **donor** from which electrons readily pass into the conduction band. The energy level of impurity atoms in a *p*-type semiconductor lies slightly above the valence band and acts as an **acceptor** level, since electrons from the valence band easily reach it, leaving holes behind to act as charge carriers.

A semiconductor **diode** consists of a ***pn* junction** and allows current to flow in one direction only; *pn* junction diodes are used as **rectifiers** to change ac to dc, as photovoltaic cells to produce electricity from sunlight, and as lasers. **Light-emitting diodes** (**LED**) use compound semiconductors which can emit light when a forward-bias voltage is applied; uses include readouts, infrared remote controls, visible lighting (flashlights, street lights), and very large TV screens. LEDs using organic molecules or polymers (**OLED**) are used as screens on cell phones and other displays. Common **transistors** consist of three semiconductor sections, either as ***pnp*** or ***npn***. Transistors can amplify electrical signals and in computers serve as switches or **gates** for the 1s and 0s of digital bits. An integrated circuit consists of a tiny semiconductor crystal or **chip** on which many transistors, diodes, resistors, and other circuit elements are constructed by placement of impurities.

Questions

1. What type of bond would you expect for (*a*) the N_2 molecule, (*b*) the HCl molecule, (*c*) Fe atoms in a solid?
2. Describe how the molecule $CaCl_2$ could be formed.
3. Does the H_2 molecule have a permanent dipole moment? Does O_2? Does H_2O? Explain.
4. Although the molecule H_3 is not stable, the ion H_3^+ is. Explain, using the Pauli exclusion principle.
5. Would you expect the molecule H_2^+ to be stable? If so, where would the single electron spend most of its time?
6. Explain why the carbon atom $(Z = 6)$ usually forms four bonds with hydrogen-like atoms.
7. The energy of a molecule can be divided into four categories. What are they?
8. If conduction electrons are free to roam about in a metal, why don't they leave the metal entirely?
9. Explain why the resistivity of metals increases with increasing temperature whereas the resistivity of semiconductors may decrease with increasing temperature.
10. Compare the resistance of a *pn* junction diode connected in forward bias to its resistance when connected in reverse bias.
11. Explain how a transistor can be used as a switch.