

* 29-6 Band Theory of Solids

We saw in Section 29-1 that when two hydrogen atoms approach each other, the wave functions overlap, and the two $1s$ states (one for each atom) divide into two states of different energy. (As we saw, only one of these states, $S = 0$, has low enough energy to give a bound H_2 molecule.) Figure 29-21a shows this situation for $1s$ and $2s$ states for two atoms: as the two atoms get closer (toward the left on the graph), the $1s$ and $2s$ states split into two levels. If six atoms come together, as in Fig. 29-21b, each of the states splits into six levels. If a large number of atoms come together to form a solid, then each of the original atomic levels becomes a **band** as shown in Fig. 29-21c. The energy levels are so close together in each band that they seem essentially continuous. This is why the spectrum of heated solids (Section 27-2) appears continuous.

Energy bands

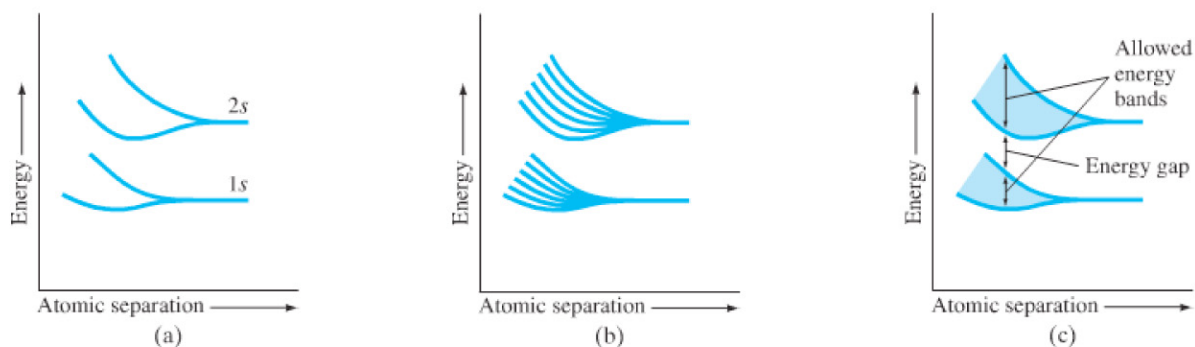


FIGURE 29-21 The splitting of $1s$ and $2s$ atomic energy levels as (a) two atoms approach each other (the atomic separation decreases toward the left on the graph); (b) the same for six atoms, and (c) for many atoms when they come together to form a solid.

The crucial aspect of a good **conductor** is that the highest energy band containing electrons is only partially filled. Consider sodium, for example, whose energy bands are shown in Fig. 29-22. The $1s$, $2s$, and $2p$ bands are full (just as in a Na atom) and don't concern us. The $3s$ band, however, is only half full. To see why, recall that the exclusion principle stipulates that in an atom, only two electrons can be in the $3s$ state, one with spin up and one with spin down. These two states have slightly different energy. For a solid consisting of N atoms, the $3s$ band will contain $2N$ possible energy states. A sodium atom has a single $3s$ electron, so in a sample of sodium metal containing N atoms, there are N electrons in the $3s$ band, and N unoccupied states. When a potential difference is applied across the metal, electrons can respond by accelerating and increasing their energy, since there are plenty of unoccupied states of slightly higher energy available. Hence, a current flows readily and sodium is a good conductor. The characteristic of all good conductors is that the highest energy band is only partially filled, or two bands overlap so that unoccupied states are available. An example of the latter is magnesium, which has two $3s$ electrons, so its $3s$ band is filled. But the unfilled $3p$ band overlaps the $3s$ band in energy, so there are lots of available states for the electrons to move into. Thus magnesium, too, is a good conductor.

Conductors

FIGURE 29-22 Energy bands for sodium.



In a material that is a good **insulator**, on the other hand, the highest band containing electrons, called the **valence band**, is completely filled. The next highest energy band, called the **conduction band**, is separated from the valence band by a “forbidden” **energy gap** (or **band gap**), E_g , of typically 5 to 10 eV. So at room temperature (300 K), where thermal energies (that is, average kinetic energy—see Chapter 13) are on the order of $\frac{3}{2}kT \approx 0.04$ eV, almost no electrons can acquire the 5 eV needed to reach the conduction band. When a potential difference is applied across the material, no available states are accessible to the electrons, and no current flows. Hence, the material is a good insulator.

Insulators

Valence and conduction bands

Energy gap