

Energy Bands in Solids—An Alternate Approach

In an alternate approach to finding the energy levels of electrons in solids, we consider the energy levels of the individual atoms as they are brought together to form a solid. In Section 9-2 we saw that when two H atoms are brought together, the two 1s levels (one for each atom) are split into two molecular levels having different energies depending on the space symmetry of the wave functions. The symmetric total wave function ψ_S resulted in the lower potential energy and a stable molecule, while the antisymmetric function ψ_A did not lead to a stable molecule (see Figures 9-6 and 9-8).

Now let's see what happens when we bring more than two atoms together. Figure 10-25 shows sketches of one-dimensional *s*-state wave functions for six atoms. These might represent, for example, six sodium atoms each with a 3*s* electron. In Figure 10-25*a*, the wave function is symmetric between each pair of atoms. The charge concentration between two atoms is roughly the same as that for the symmetric state of two atoms as illustrated on the left of Figure 9-6*b*. In Figure 10-25*f*, the wave function is antisymmetric between any two adjacent atoms and is similar to that for the antisymmetric state of two atoms shown on the right of Figure 9-6*b*. The six energy levels (12, counting spin states), which are all the same when the atoms are

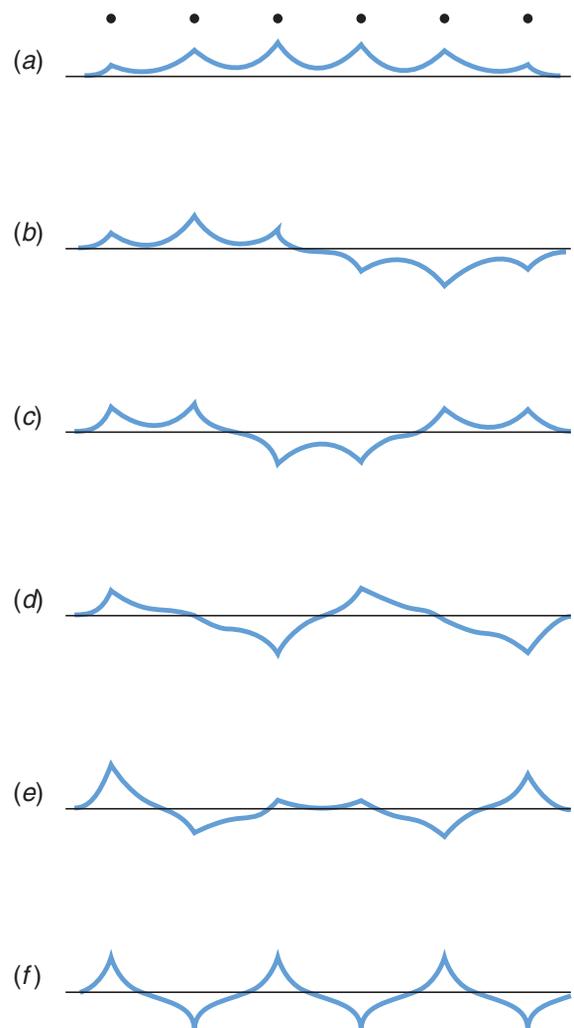


FIGURE 10-25 Wave functions with different symmetries of six atoms in one dimension. The perfectly symmetric function (a) has the lowest energy, whereas the perfectly antisymmetric function (f) has the highest energy. The energy increases as the curvature of the total wave functions increases.

far apart, split into six different energies when they are close. The lowest energy corresponds to Figure 10-25*a* and the highest to 10-25*f*. Recall from our discussion in Section 6-3 that wave functions with the lower curvature correspond to the lower energy. The difference in these two energies depends on the spacing of the atoms, as in Figure 9-8*b*, but not on the number of atoms since the concentration of charge for these extreme cases (perfectly symmetric and perfectly antisymmetric) does not change when more atoms are added. Figure 10-26 shows the splitting of the $1s$ states and $2s$ states for six atoms as a function of lattice separation. For N atoms, there are N states in a band, so these bands are nearly continuous in the case of macroscopic solids where $N \sim 10^{23}$. The bands may be widely separated in energy, or they may be close together, or they may even overlap, depending on the kind of atom, the type of bonding, and the crystal structure.

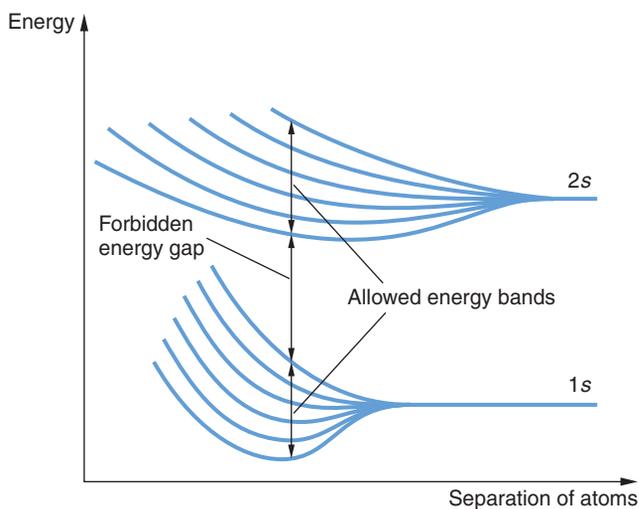


FIGURE 10-26 Energy splitting of the $1s$ and $2s$ states for six atoms as a function of separation of the atoms.