



FIGURE 5.5 Molecular Orbitals for the First 10 Elements, Assuming Interactions Only Between Atomic Orbitals of Identical Energy.

EXAMPLE

Add a *g* or *u* label to each of the molecular orbitals in the energy-level diagram in Figure 5.2.

From top to bottom, the orbitals are σ_u^* , π_g^* , π_u , and σ_g .

► **Exercise 5.2** Add a *g* or *u* label to each of the molecular orbitals in Figure 5.3(a).

5.2.2 Orbital Mixing

So far, we have primarily considered interactions between orbitals of identical energy. However, orbitals with similar, but not equal, energies interact if they have appropriate symmetries. We will outline two approaches to analyzing this interaction, one in which the molecular orbitals interact and one in which the atomic orbitals interact directly.

When two molecular orbitals of the same symmetry have similar energies, they interact to lower the energy of the lower orbital and raise the energy of the higher orbital. For example, in the homonuclear diatomics, the $\sigma_g(2s)$ and $\sigma_g(2p)$ orbitals