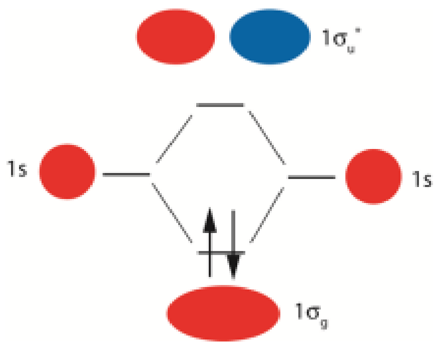

To discuss electronic transitions, we first need an efficient way to describe these states. First, we will use our MO diagrams to construct electron configurations. For H_2, the MO diagram leads to the electron configuration $(1\sigma_g)^2$. Now, we can use these configurations to define molecular term symbols which describe the electronic state of the molecule. Begin by adding the angular momentum and spin for each electron together:

$$M_L = \sum_{i=1}^{n} m_{\ell_i}, \quad M_S = \sum_{i=1}^{n} m_{s_i}$$

Electron in σ orbital: m = 0. Electron in π orbital: m = 1.

Then, we calculate the allowed values of the total angular momentum (L) and spin (S) from:

$$-L \le M_L \le L, \quad -S \le M_S \le S$$

With L and S, molecular term symbols are constructed as follows:

$$^{2S+1}\Lambda_{g/u}, \quad \Lambda = |M_L|$$

We have a shorthand to keep track of ∧ values:

Λ	0	1	2	3
	Σ	Π	Δ	Φ

Finally, g or u subscript is determined using the following symmetry relationships:

$$g \times g = u \times u = g, \quad u \times g = g \times u = u$$

Let’s apply these rules to H_2:

$$(1\sigma_g)^2$$

$$M_L = 0+0=0, \quad M_S = \frac{1}{2}+\left(-\frac{1}{2}\right)=0$$

$$L=0, \quad S=0$$

$$g \times g = g$$

$$^{2S+1}\Lambda_{g/u} \Rightarrow {}^1\Sigma_g$$

Excited state of H2: $(1\sigma_g)\,(1\sigma_u^*)$

Now the electrons do not have to be spin paired; therefore, we have the possibility of both singlet and triplet states!

$$M_L = 0+0=0, \quad M_S = -1,0,1$$

$$L=0, \quad S=0,1$$

$$g \times u = u$$

$$^{2S+1}\Lambda_{g/u} \Rightarrow {}^1\Sigma_u, {}^3\Sigma_u$$

Hund’s Rule: State with greatest spin multiplicity is lowest in energy.