10.3 Electronic structure of diatomic molecules 38 493

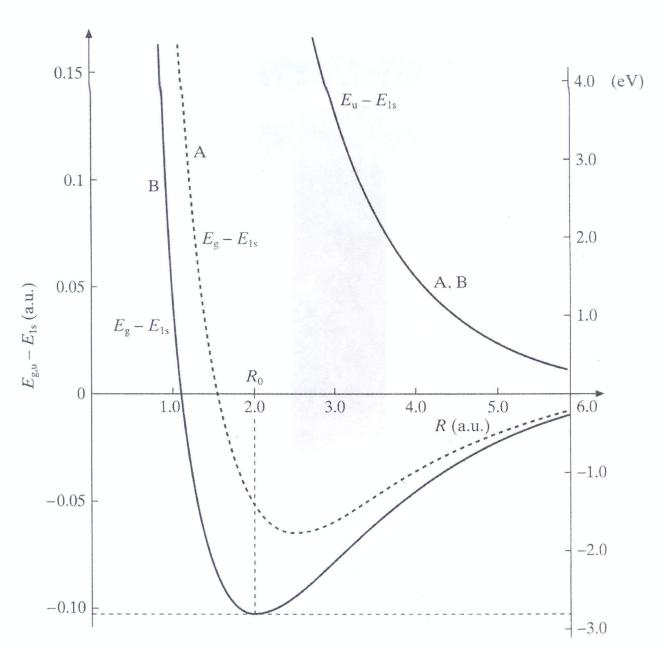


Figure 10.8 The lowest electronic potential energy curves of  $H_2^+$ . The curves labelled A show  $E_g(R) - E_{1s}$  and  $E_u(R) - E_{1s}$  calculated using the simple LCAO wave functions of (10.33) while the curves labelled B show the exact values of the same quantities calculated from equations (10.49) and (10.50).