

FIGURE 14.6 Binding and antibinding regions for a heteronuclear diatomic molecule with $Z_b > Z_a$.

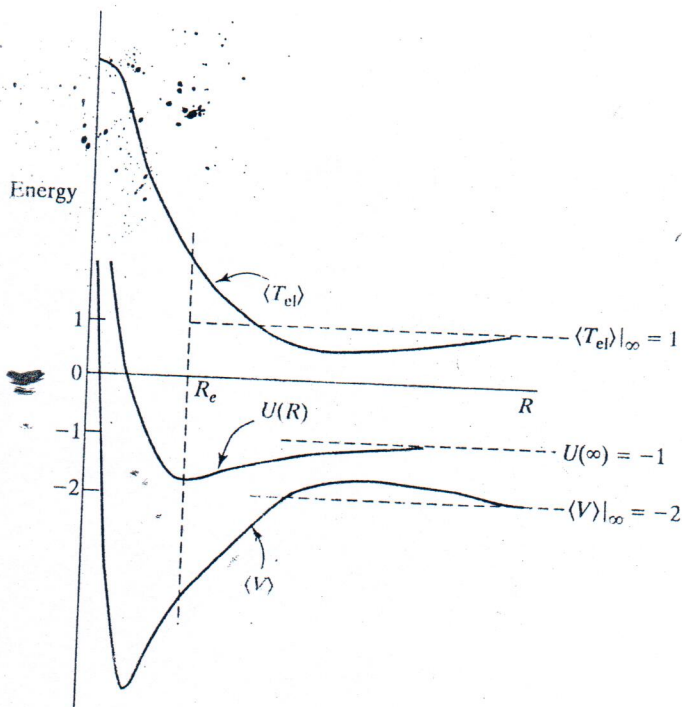
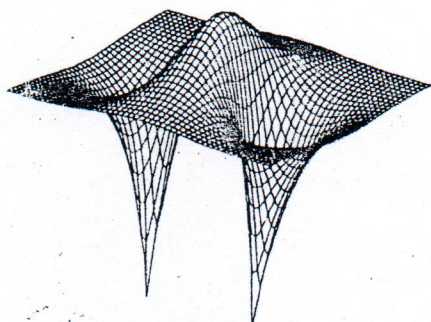
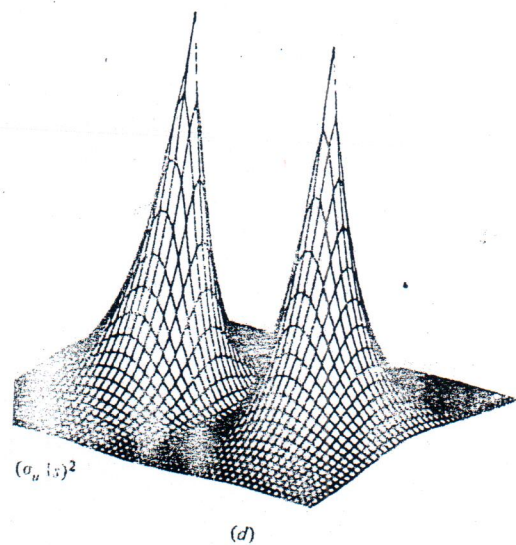
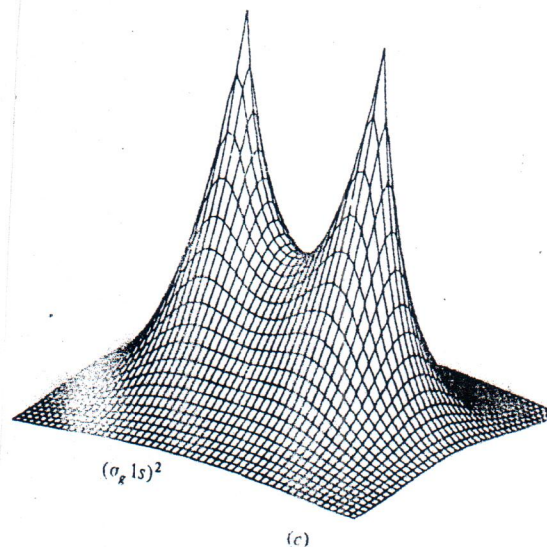
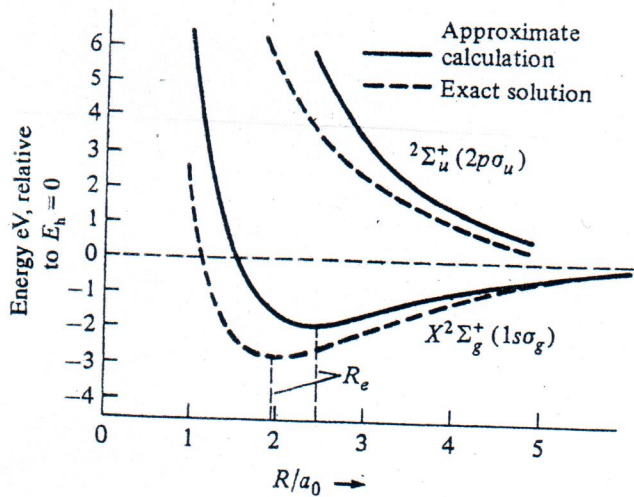


FIGURE 14.1 Variation of the average potential and kinetic energies of a diatomic molecule. The unit of energy is taken as the electronic kinetic energy of the separated atoms.

TABLE 13.2 Properties of Homonuclear Diatomic Molecules in Their Ground Electronic States

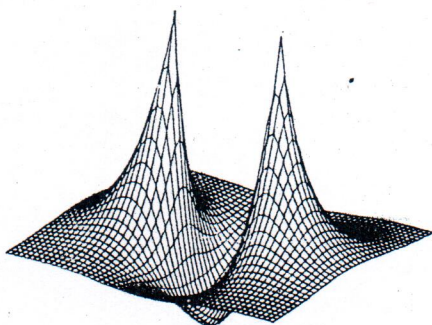
Molecule	Ground Term	Bond Order	D_e /eV	$R_e/\text{\AA}$	$\tilde{\nu}_e/\text{cm}^{-1}$
H_2^+	$2\Sigma_g^+$	$\frac{1}{2}$	2.79	1.06	2322
H_2	$1\Sigma_g^+$	1	4.75	0.741	4403
He_2^+	$2\Sigma_u^+$	$\frac{1}{2}$	2.5	1.08	1698
He_2	$1\Sigma_g^+$	0	0.0009	3.0	
Li_2	$1\Sigma_g^+$	1	1.07	2.67	351.4
Be_2	$1\Sigma_g^+$	0	0.10	2.45	
B_2	$3\Sigma_g^-$	1	3.1	1.59	1051
C_2	$1\Sigma_g^+$	2	6.3	1.24	1855
N_2^+	$2\Sigma_g^+$	$2\frac{1}{2}$	8.85	1.12	2207
N_2	$1\Sigma_g^+$	3	9.91	1.10	2358
O_2^+	$2\Pi_g$	$2\frac{1}{2}$	6.78	1.12	1905
O_2	$3\Sigma_g^-$	2	5.21	1.21	1580
F_2	$1\Sigma_g^+$	1	1.66	1.41	892
Ne_2	$1\Sigma_g^+$	0	0.0036	3.1	14

Data from K. P. Huber and G. Herzberg, *Constants of Diatomic Molecules* (vol. IV of *Molecular Spectra and Molecular Structure*), Van Nostrand Reinhold, 1979; and (for Be_2) V. E. Bondybey, *Chem. Phys. Lett.*, **109**, 463 (1984).



$$\delta_1 = (\sigma_g 1s)^2 - \frac{1}{2}(1s_A^2 + 1s_B^2)$$

(a)



$$\delta_2 = (\sigma_u 1s)^2 - \frac{1}{2}(1s_A^2 + 1s_B^2)$$

(b)

FIGURE 12-8

Differences in probability densities between (a) the bonding $\sigma_g 1s$ function and (b) the antibonding $\sigma_u 1s$ function of H_2^+ according to Eq. (12-34). The two upward-pointing peaks of (b) represent a buildup of probability density *outside* the internuclear region; the sag between these peaks represents a decrease in probability density between the nuclei. Note that this decrease and increase are relative to the density due to two noninteracting $1s^2$ atomic probability densities. The two downward-pointing peaks of (a) represent a decrease of probability density outside the internuclear region, and the mound between these indicates an increase of probability density between the nuclei.

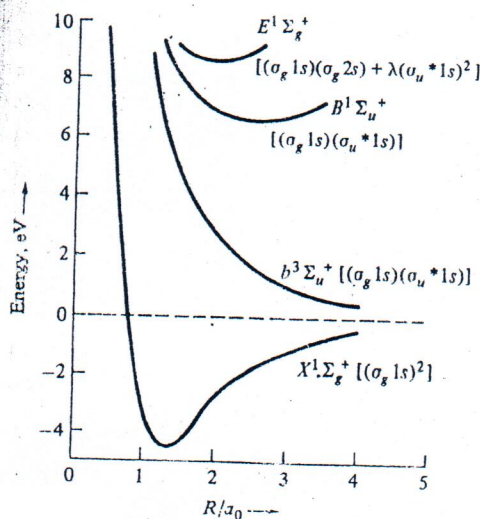
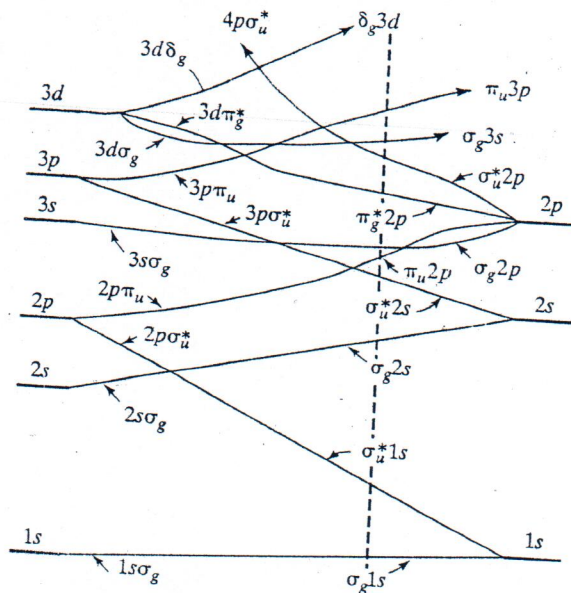


FIGURE 12-12

Potential-energy curves for the ground state and three excited states of dihydrogen. The brackets after each spectroscopic term symbol indicate the MO configuration which serves as a first approximation to these states. [From W. Kolos and C. C. J. Roothaan, *Rev. Mod. Phys.* 32:227 (1960). Reproduced by permission of the authors.]



United-atom state

Separated-atoms state

FIGURE 13.16 Correlation diagram for homonuclear diatomic MOs. (This diagram does not hold for H_2^+ .) The dashed vertical line corresponds to the order in which the MOs fill.

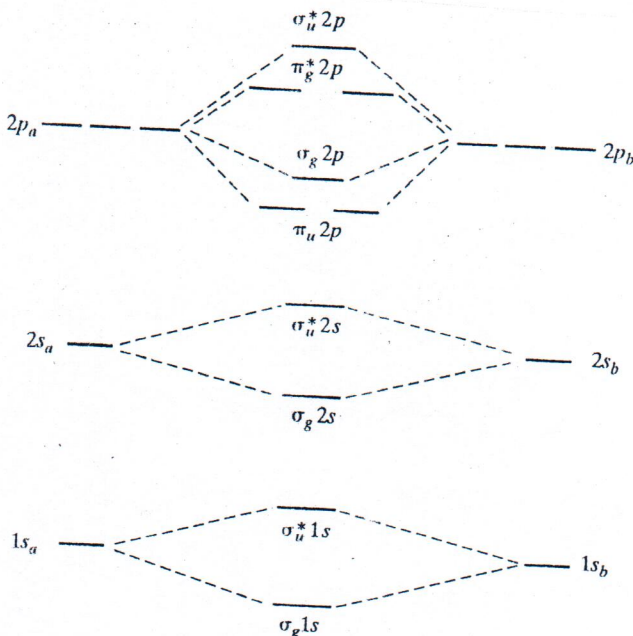


FIGURE 13.17 Homonuclear diatomic MOs formed from 1s, 2s, and 2p AO's.

TABLE 12-2

Molecular orbital electron configurations of the ground states of the homonuclear diatomic molecules of the first full period, including hydrogen

Molecule	MO configuration	Spectroscopic symbol
H_2	$(1\sigma_g)^2$	$1\Sigma_g^+$
He_2	$(1\sigma_g)^2(1\sigma_u)^2$	$1\Sigma_g^+$
Li_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2$	$1\Sigma_g^+$
Be_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2$	$1\Sigma_g^+$
B_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^2$	$3\Sigma_g^-$
C_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^4$	$1\Sigma_g^+$
N_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(3\sigma_g)^2(1\pi_u)^4$	$1\Sigma_g^+$
O_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(3\sigma_g)^2(1\pi_u)^4(1\pi_g)^2$	$3\Sigma_g^-$
F_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^4(3\sigma_g)^2(1\pi_g)^4$	$1\Sigma_g^+$
Ne_2	$(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^4(3\sigma_g)^2(1\pi_g)^4(3\sigma_u)^2$	$1\Sigma_g^+$

Note: The MOs are listed in order of increasing energy. Note that F_2 has $1\pi_u$ and $3\sigma_g$ in the opposite order to O_2 and N_2 .