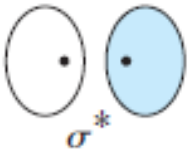
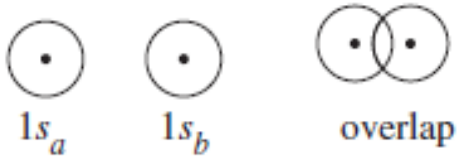
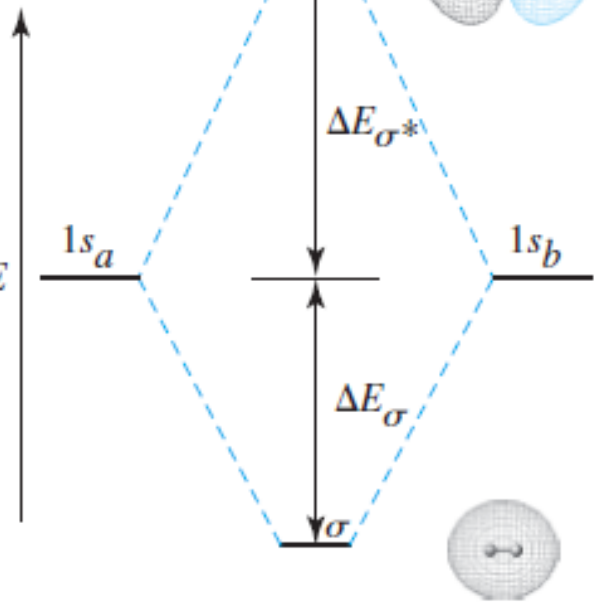
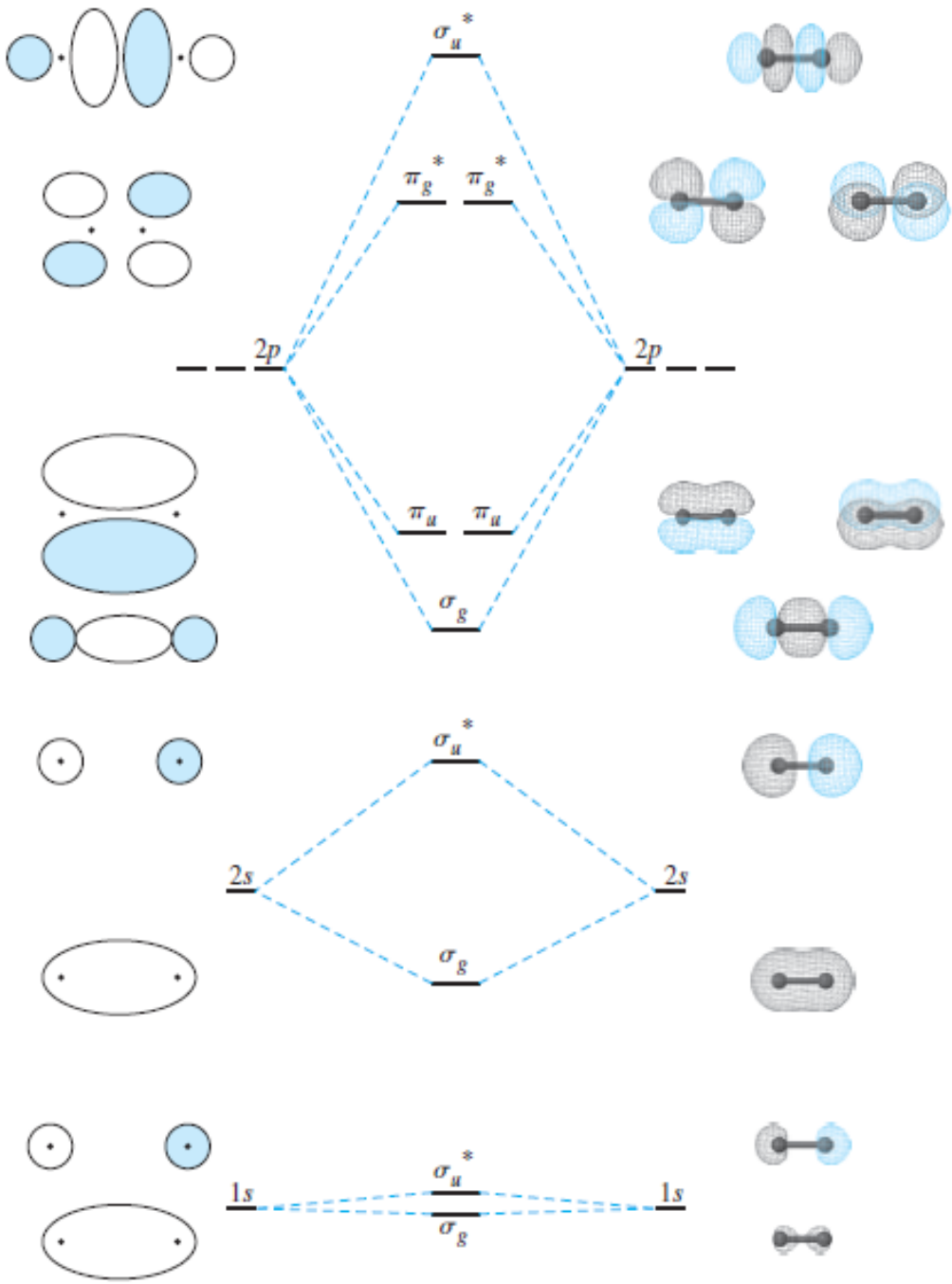
$$\sigma^* = \frac{1}{\sqrt{2}}[\psi(1s_a) - \psi(1s_b)]$$

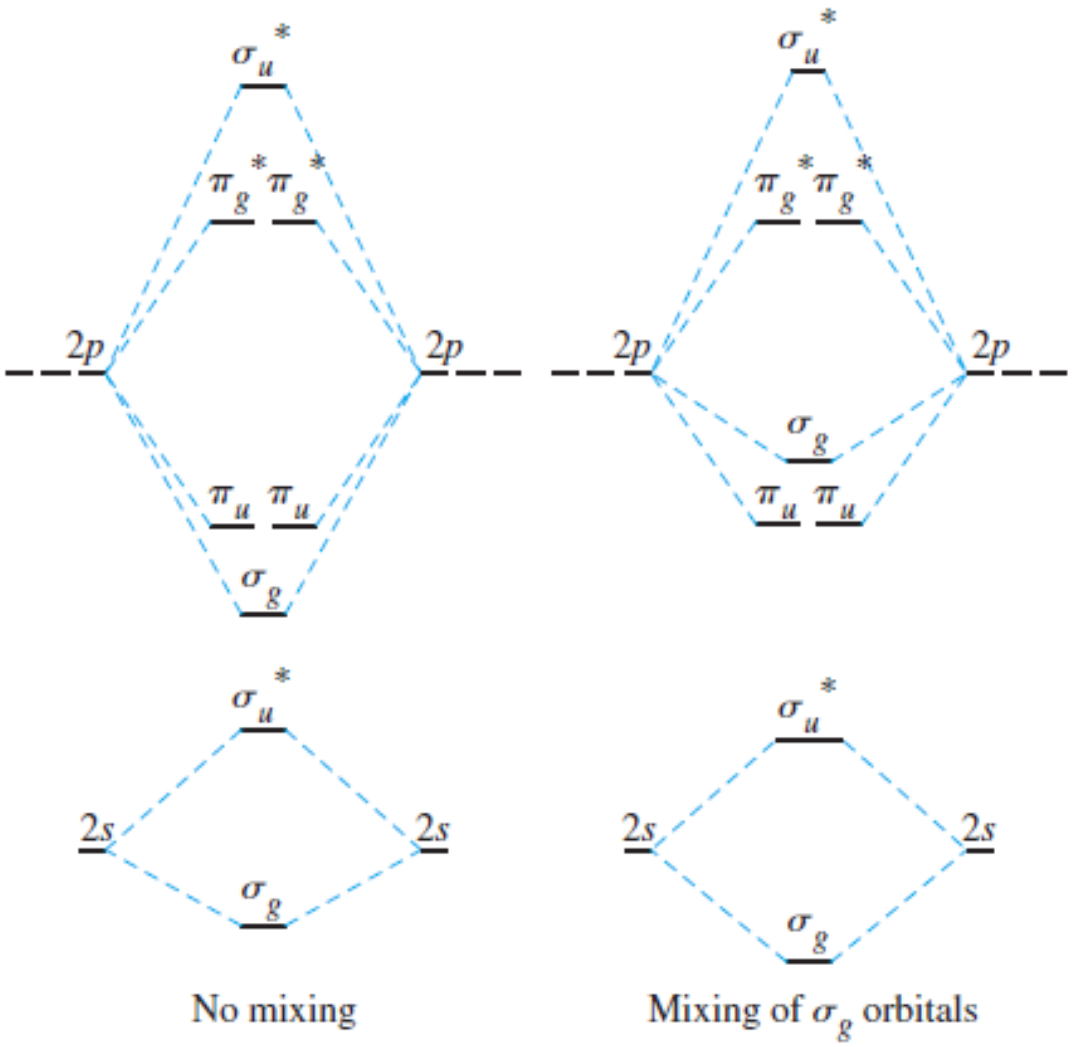


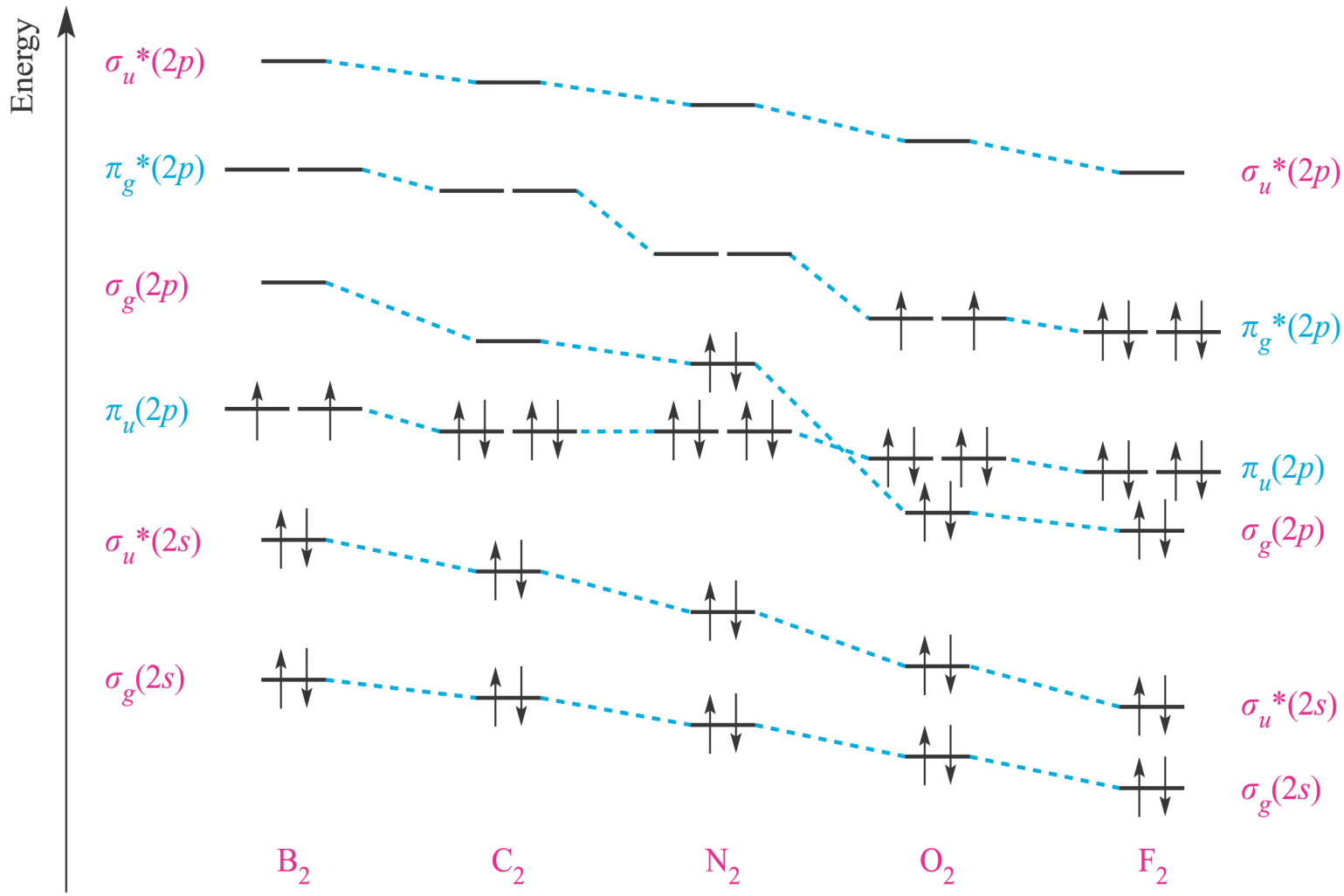


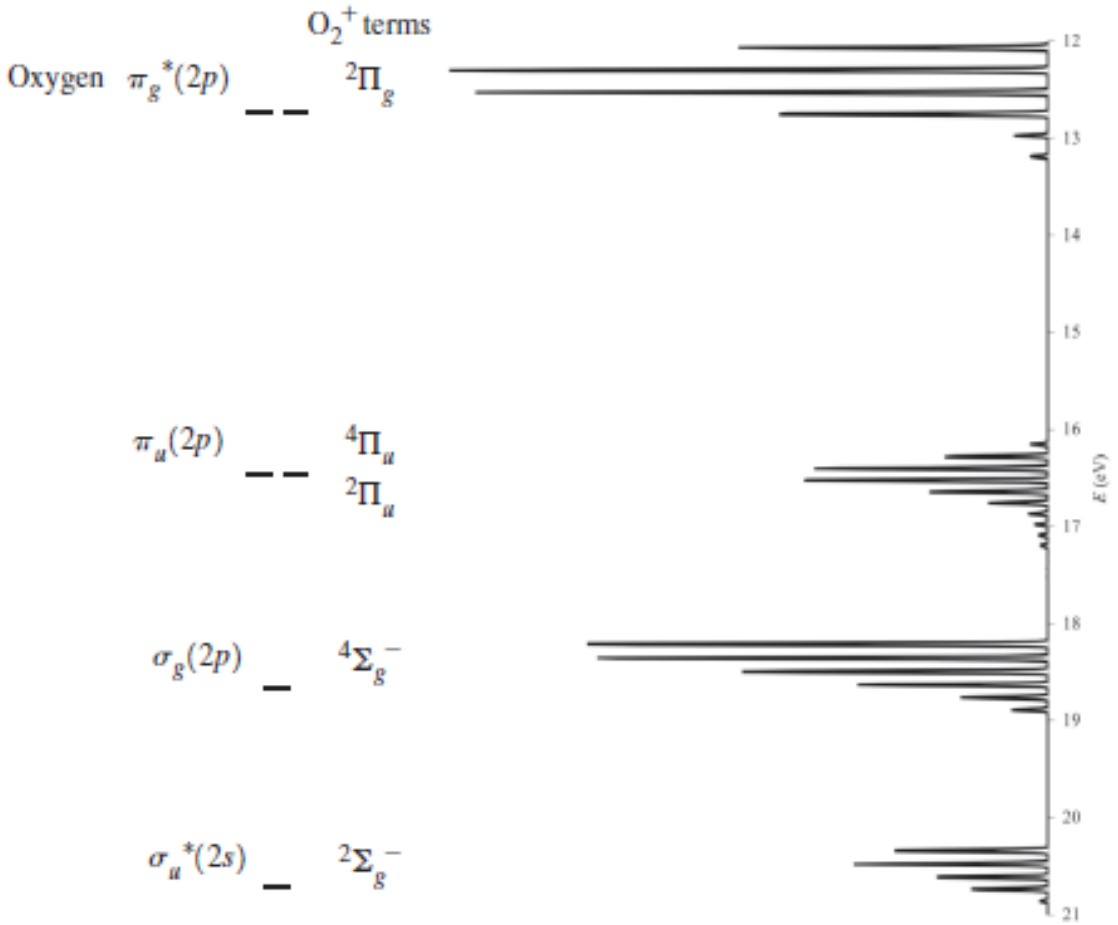
$$\sigma = \frac{1}{\sqrt{2}}[\psi(1s_a) + \psi(1s_b)]$$

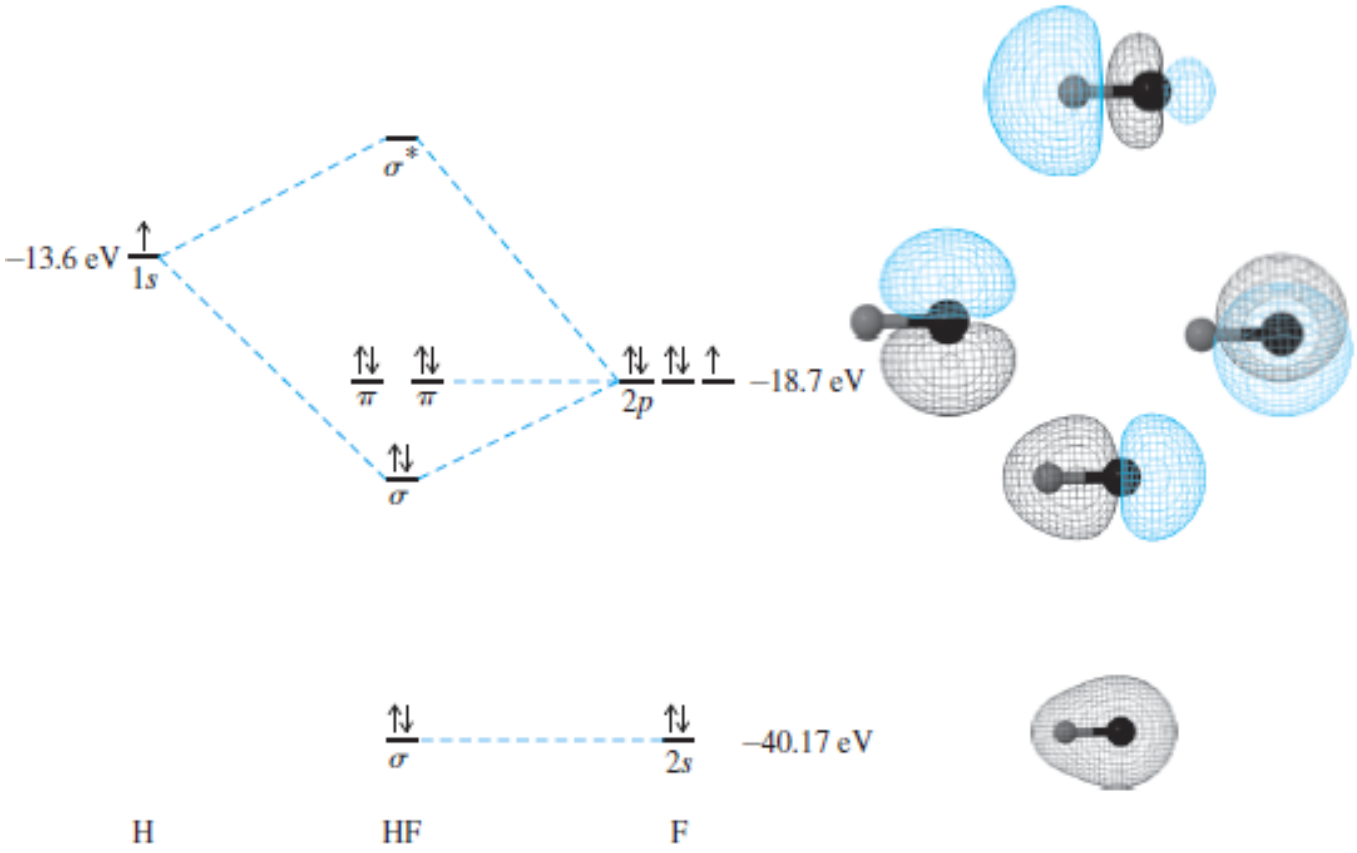


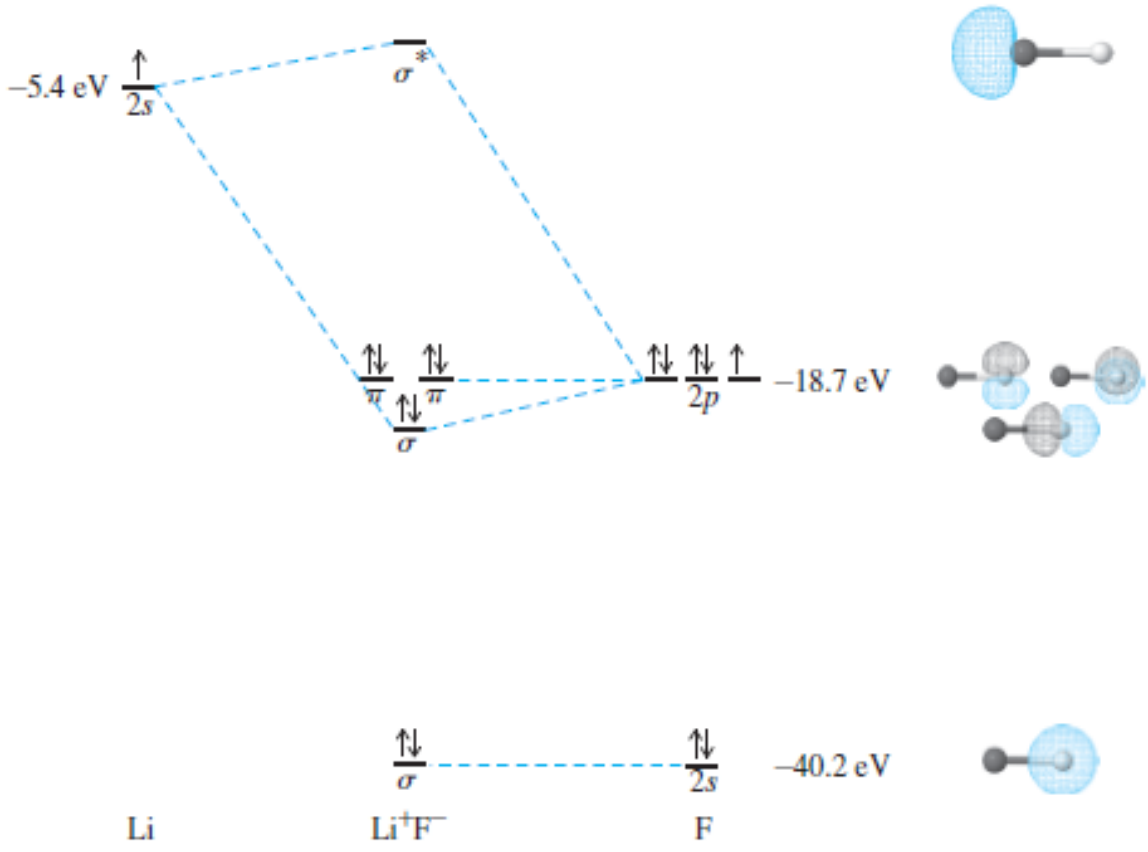

σ_u^*
π_g^* π_g^*
2p
2p
π_u π_u
σ_g
σ_u^*
2s
2s
σ_g
σ_u^*
1s
1s
σ_g


σ_u^*
$\pi_g^* \pi_g^*$
2p
2p
π_u π_u
σ_g
σ_u^*
2s
2s
σ_g
No mixing
(a)
σ_u^*
$\pi_g^* \pi_g^*$
2p
2p
σ_g
π_u π_u
σ_u^*
2s
2s
σ_g
Mixing of σ_g orbitals
(b)


Energy
$\sigma_u^*(2p)$
$\pi_g^*(2p)$
$\sigma_g(2p)$
$\pi_u(2p)$
$\sigma_u^*(2s)$
$\sigma_g(2s)$
$\sigma_u^*(2p)$
$\pi_g^*(2p)$
$\pi_u(2p)$
$\sigma_g(2p)$
$\sigma_u^*(2s)$
$\sigma_g(2s)$
B_2
C_2
N_2
O_2
F_2


O_2^+ terms
Oxygen $\pi_g^*(2p)$
$^2\Pi_g$
$\pi_u(2p)$
$^4\Pi_u$
$^2\Pi_u$
$\sigma_g(2p)$
$^4\Sigma_g^-$
$\sigma_u^*(2s)$
$^2\Sigma_g^-$
12
13
14
15
16
17
18
19
20
21
$\mathcal{E}$ (eV)


σ*
–13.6 eV
1s
π
π
2p
–18.7 eV
σ
σ
2s
–40.17 eV
H
HF
F


–5.4 eV
2s
σ*
π
π
σ
2p
–18.7 eV
σ
2s
–40.2 eV
Li
Li+F–
F

Elementary Step	Chemical/Physical Change	$\Delta H°$(kJ/mol)*
$Li(s) \longrightarrow Li(g)$	Sublimation	161
$Li(g) \longrightarrow Li^+(g) + e^-$	Ionization	520
$\frac{1}{2}F_2(g) \longrightarrow F(g)$	Bond dissociation	79
$F(g) + e^- \longrightarrow F^-(g)$	–Electron affinity	–328
$Li(s) + \frac{1}{2}F_2(g) \longrightarrow Li^+(g) + F^-(g)$	Formation of gas-phase ions from the elements in their standard states	432

Elementary Step	Chemical Change	ΔH°(kJ/mol)
$Li^+(g) + F^-(g) \longrightarrow LiF(g)$	Formation of gaseous ion pairs	–755
$Li^+(g) + F^-(g) \longrightarrow LiF(s)$	Formation of crystalline solid	–1050