Molecule	orbitals	I_p (eV)
C_2H_4		10.51
	$1b_{3u}$(HOMO)	
C_6H_6		9.25
	$1e_{1g}$(HOMO1)	
	$1e_{1g}$(HOMO2)	
H_3^+		32.33
	$1a_1'$(HOMO)	
H_2O		12.60
	$1b_1$(HOMO)	
SO_2		12.34
	$6a_1$(HOMO)	
	– – –	
N_2O_4		11.50
	$6a_g$(HOMO)	
NH_3		10.20
	$3a_1$(HOMO)	
CH_4		12.60
	$1t_2$(HOMO1)	
	$1t_2$(HOMO2)	
	$1t_2$(HOMO3)	
C_2H_6		11.50
	$1e_g$(HOMO1)	
	$1e_g$(HOMO2)	
C_3H_8		11.00
	$2b_1$(HOMO)	
CH_3Cl		11.30
	2e(HOMO1)	
	2e(HOMO2)	

Taken from Zhao et al J Phys B 2011

Molecule	orbitals	I_p (eV)
C_4H_{10} (butane)		10.60
	$7a_g$(HOMO)	
	– – –	
C_4H_{10} (isobutane)		11.13
	$6a_1$(HOMO)	
	– – –	
	– – –	
CH_2Cl_2		11.33
	$3b_1$(HOMO)	
	– – –	
$CHCl_3$		11.37
	$2a_2$(HOMO)	
CCl_4		11.47
	$2t_1$(HOMO1)	
	$2t_1$(HOMO2)	
	– – –	
	$2t_1$(HOMO3)	
	– – –	

Molecule	orbitals	I_p (eV)
SF_6		15.69
	$1t_{1g}$(HOMO1)	

TABLE II. Equilibrium distances, ionization energies calculated in the exchange-only LDA + LB model and experimental vertical ionization potentials for several linear molecules.

Molecule	R (Å)	LDA + LB (eV)	I_p (eV)
H_2^+	1.058	29.99	29.99
D_2/H_2	0.742	13.65	15.47
N_2	1.098	14.99	15.58
O_2	1.208	10.62	12.03
F_2	1.412	16.03	15.70
S_2	1.889	10.36	9.36
CO	1.128	13.22	14.01
NO	1.151	9.14	9.26
SO	1.481	9.37	10.29
CO_2	1.163	14.63	13.78
C_2H_2	1.203 (R_{CC})	11.19	11.41
	1.058 (R_{CH})		
HF	0.917	15.03	15.77
HCl	1.275	11.41	12.75
HCN	1.067 (R_{CH})	13.46	13.80
	1.159 (R_{CN})		

From Zhao et al PRA81, 033423 (2010)

Molecule	Spin orbital	LDA + LB	LBα	I_p
N_2	$3\sigma_g$(HOMO)	15.0	15.5[a]	15.6[b]
	$1\pi_u$(HOMO-1)	16.5	16.9[a]	17.2[b]
	$2\sigma_u$(HOMO-2)	17.8	18.5[a]	18.7[b]
O_2	$1\pi_g$(HOMO)	10.6	12.8[a]	12.3[c]
	$1\pi_u$(HOMO-1)	17.3	17.4[a]	16.7[c]
	$3\sigma_g$(HOMO-2)	17.1	18.3[a]	18.2[c]
CO_2	$1\pi_g$(HOMO)	14.6	13.9[d]	13.8[e]
	$1\pi_u$(HOMO-1)	18.3	17.5[d]	17.6[e]
	$3\sigma_u$(HOMO-2)	16.8	17.2[d]	18.1[e]
CO	5σ(HOMO)	13.2		14.0[e]
	1π(HOMO-1)	16.6		16.9[e]
HCl	2π(HOMO)	11.4		12.8[f]
	5σ(HOMO-1)	15.0		16.3[f]
C_2H_2	$1\pi_u$(HOMO)	11.2		11.4[e]
	$3\sigma_g$(HOMO-1)	15.7		16.4[e]