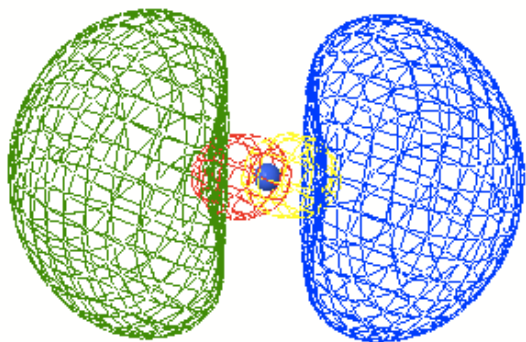
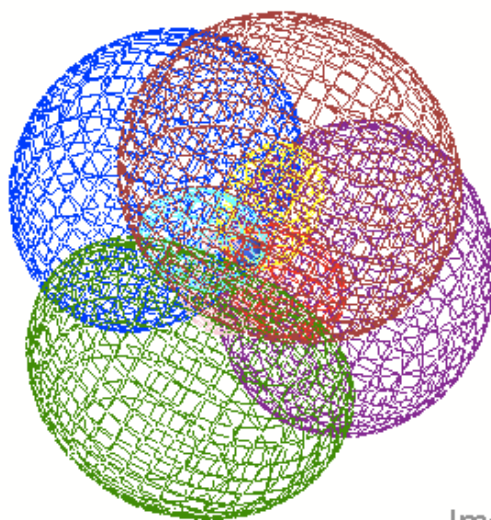


Which represents sp^3 orbitals?



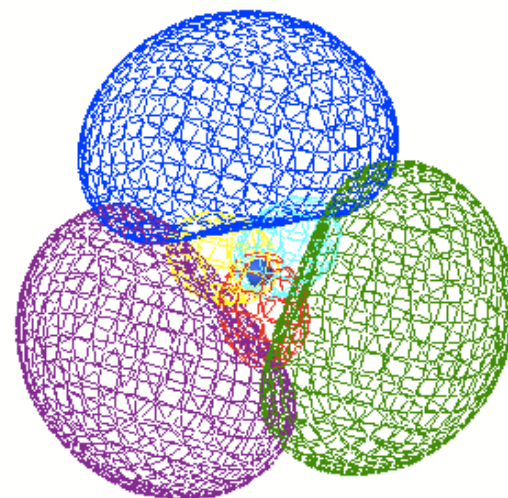
Jmol

(1)



Jmol

(2)



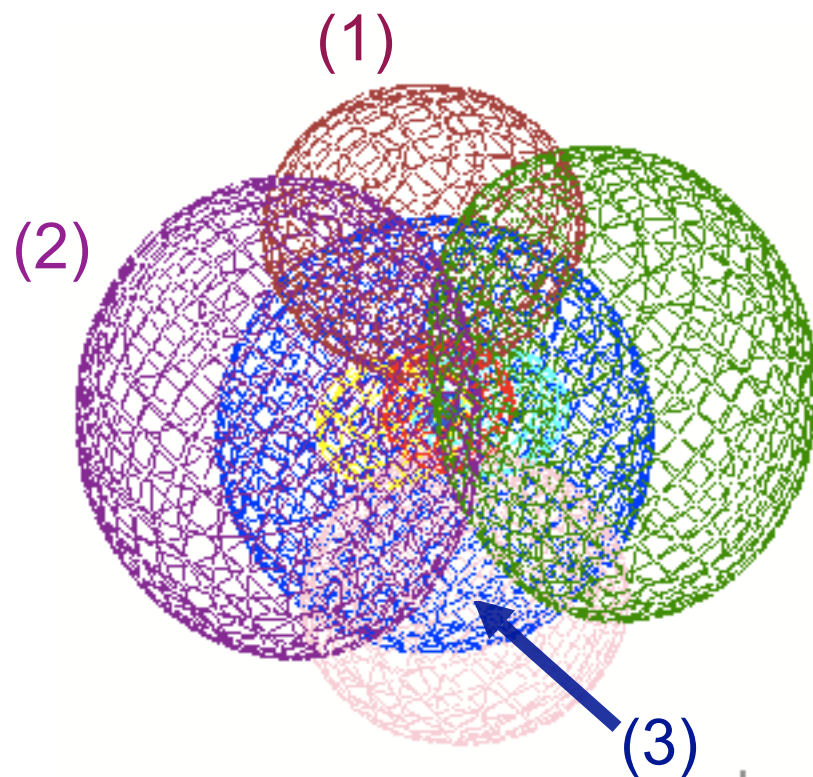
Jmol

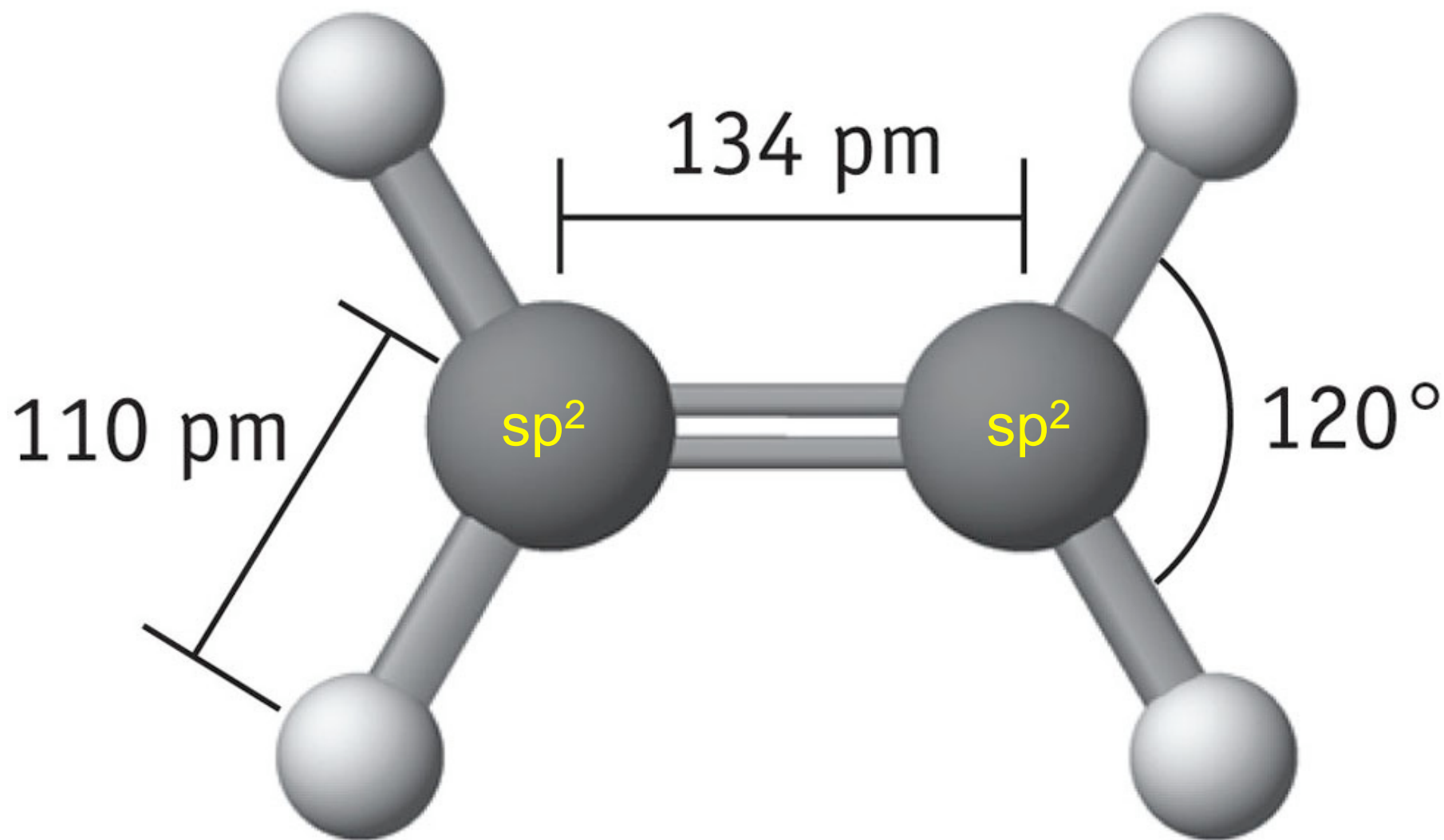
(3)



sp^2 hybridization

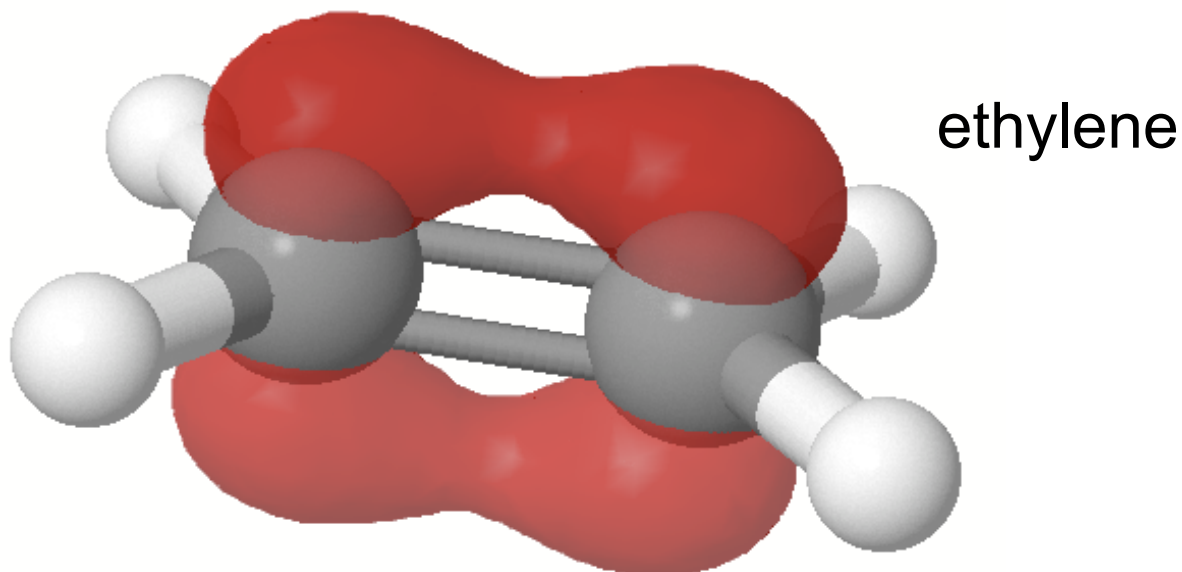
Which is the unused p orbital?





Ethylene, C_2H_4

What is shown in red?

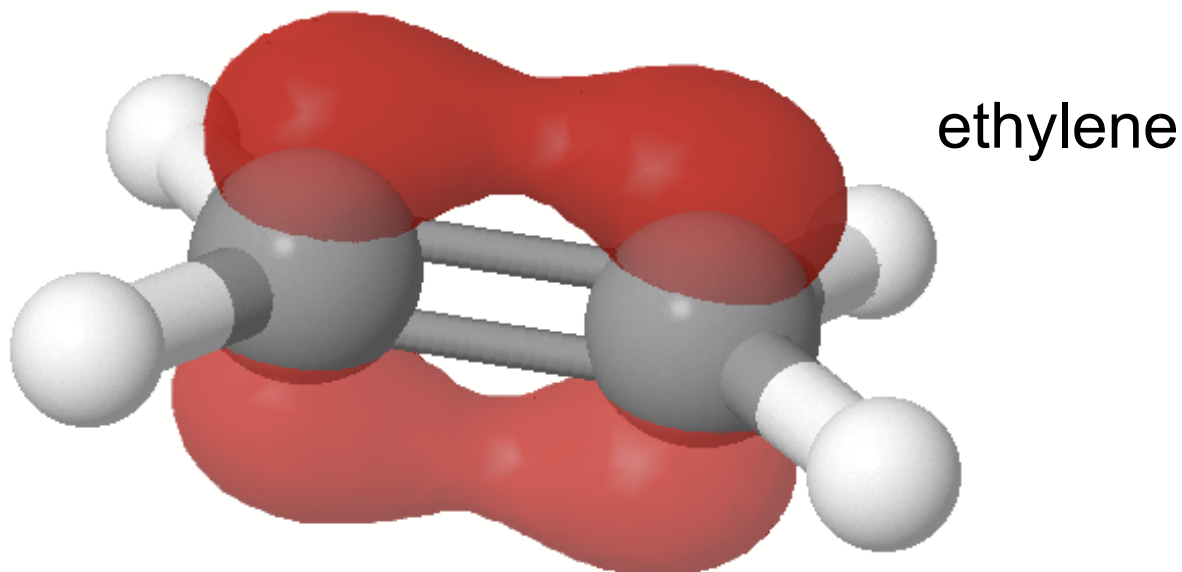


- 1) Two π bonding orbitals
- 2) One π bonding and one p antibonding orbital
- 3) One π bonding orbital
- 4) One π antibonding orbital
- 5) Two p orbitals



See in 3D!

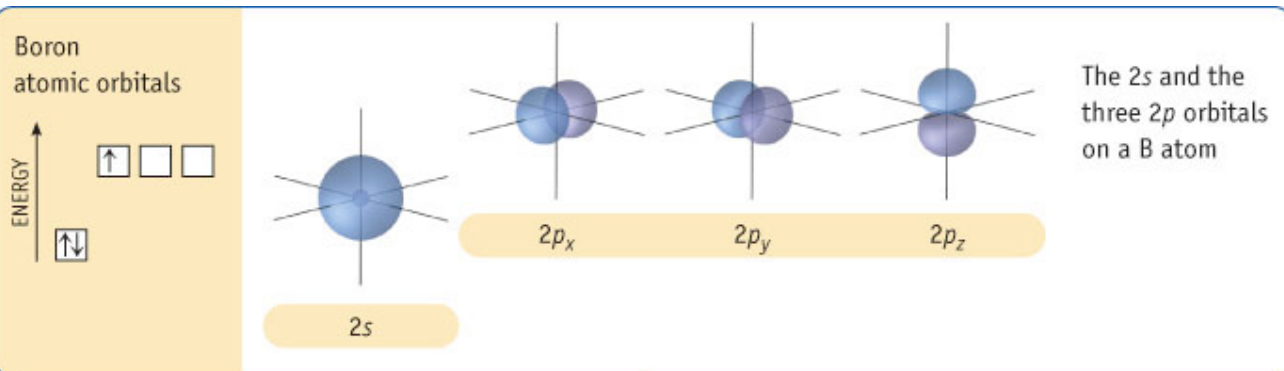
What is shown in red?



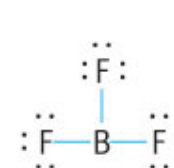
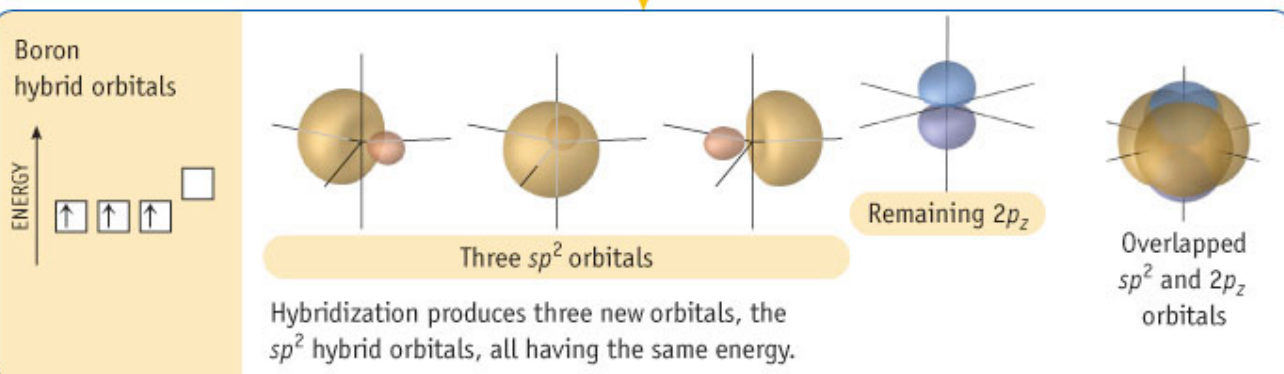
- 1) Two π bonding orbitals
- 2) One π bonding and one p antibonding orbital
- 3) **One π bonding orbital**
- 4) One π antibonding orbital
- 5) Two p orbitals

sp² hybridization

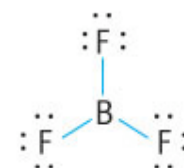
View in 3D!



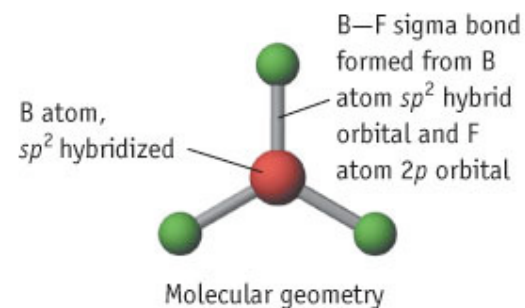
Orbital hybridization



Lewis structure

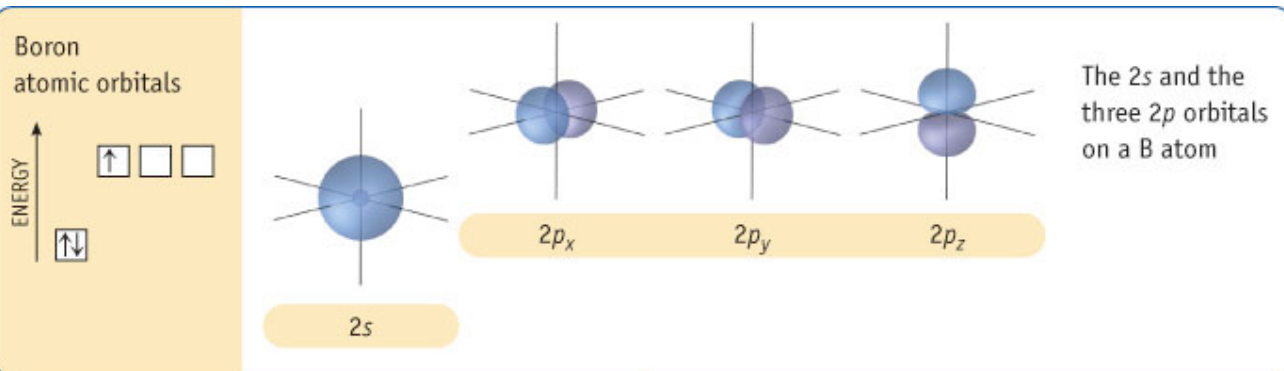


Electron-pair geometry

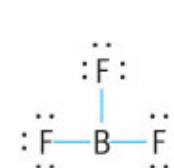
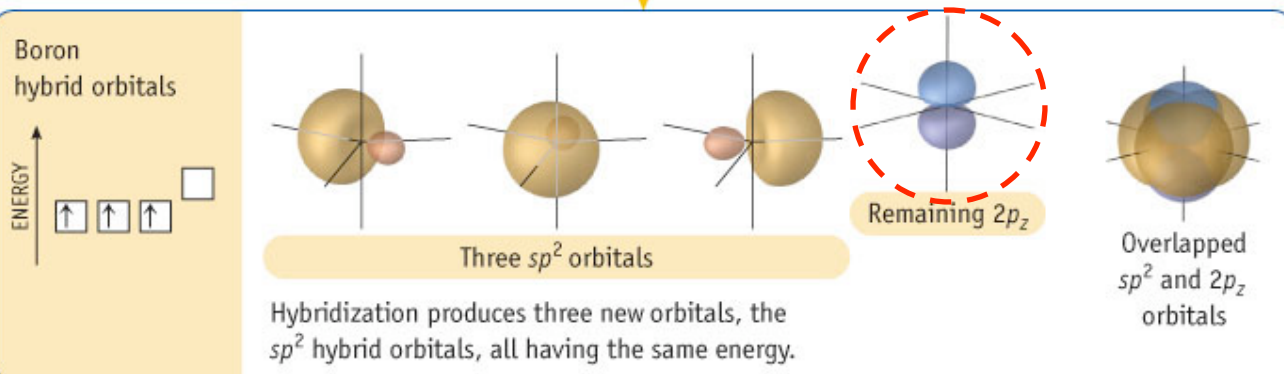


sp² hybridization

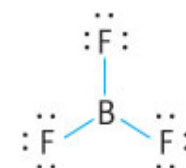
View in 3D!



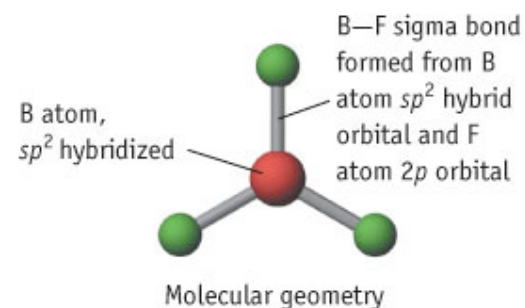
Orbital hybridization



Lewis structure



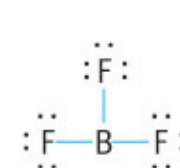
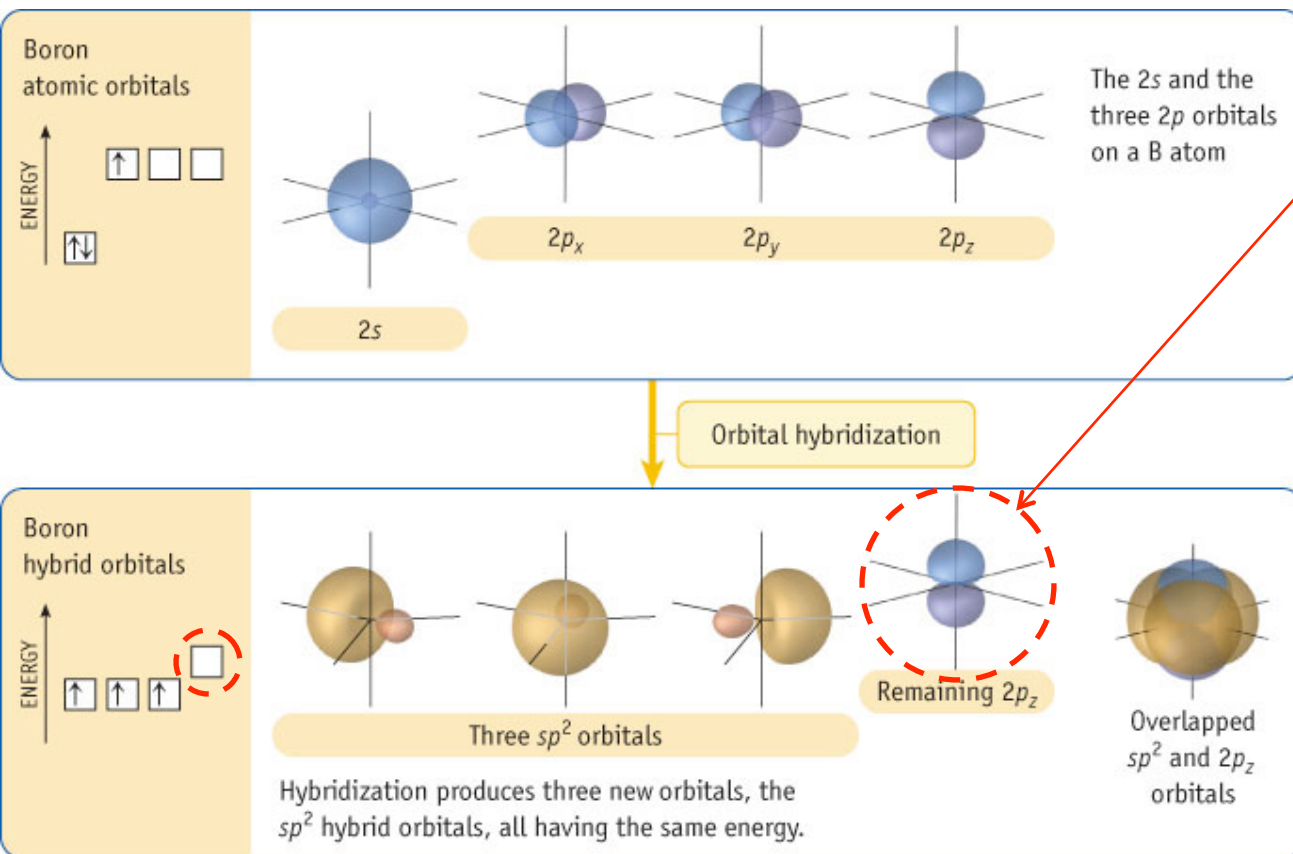
Electron-pair geometry



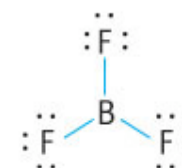
sp^2 hybridization

View in 3D!

Left over (unused)
atomic orbital



Lewis structure



Electron-pair geometry

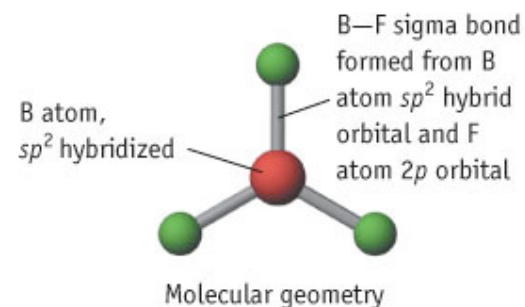


Fig. 9-8, p. 414

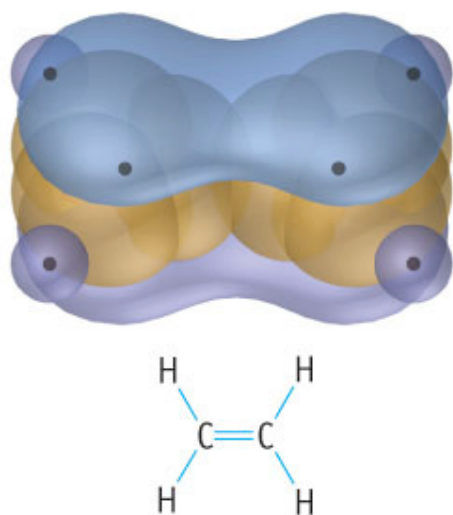


Unhybridized p orbital. Used for π bonding in C_2H_4 .

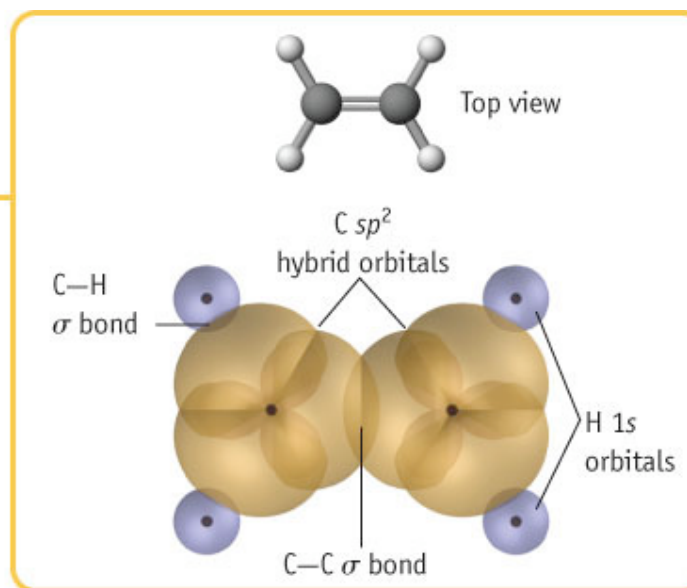


Three sp^2 hybrid orbitals. Used for $\text{C}-\text{H}$ and $\text{C}-\text{C}$ σ bonding in C_2H_4 .

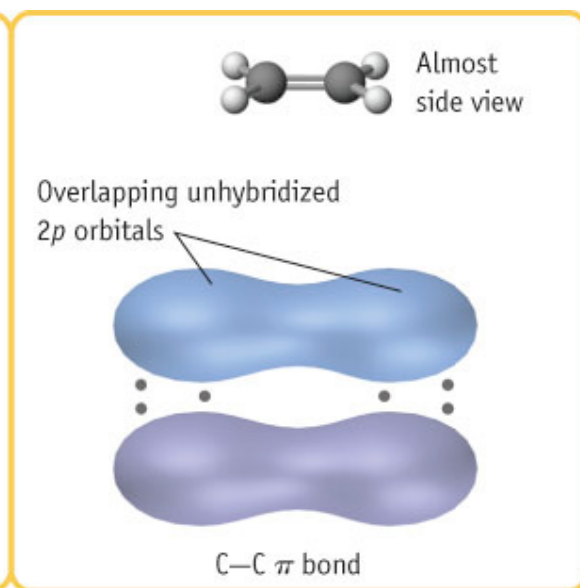
See in 3D!



(a) Lewis structure and bonding of ethylene, C_2H_4 .



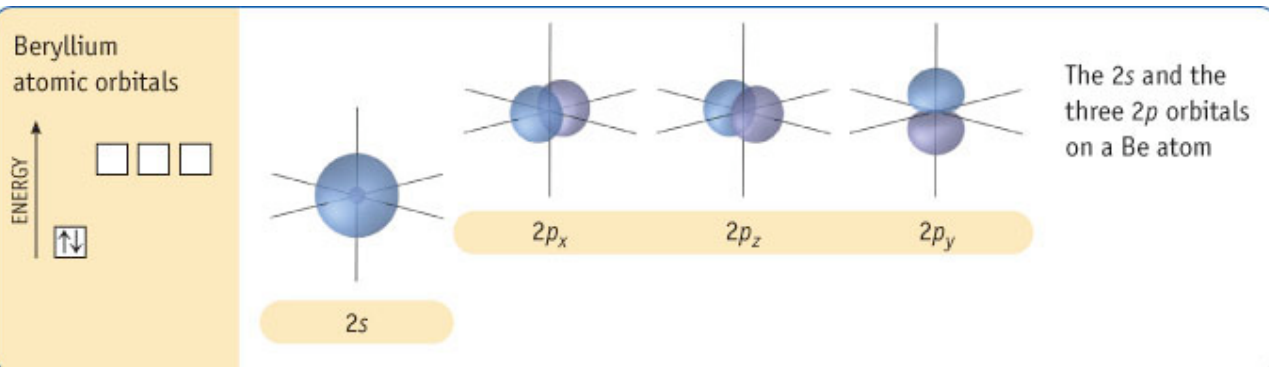
(b) The C—H σ bonds are formed by overlap of C atom sp^2 hybrid orbitals with H atom $1s$ orbitals. The σ bond between C atoms arises from overlap of sp^2 orbitals.



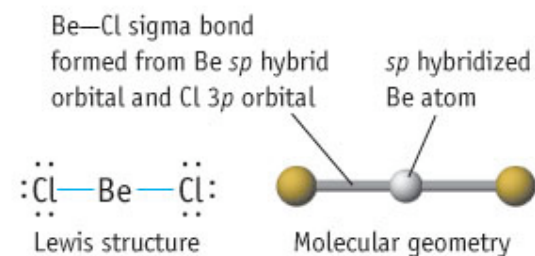
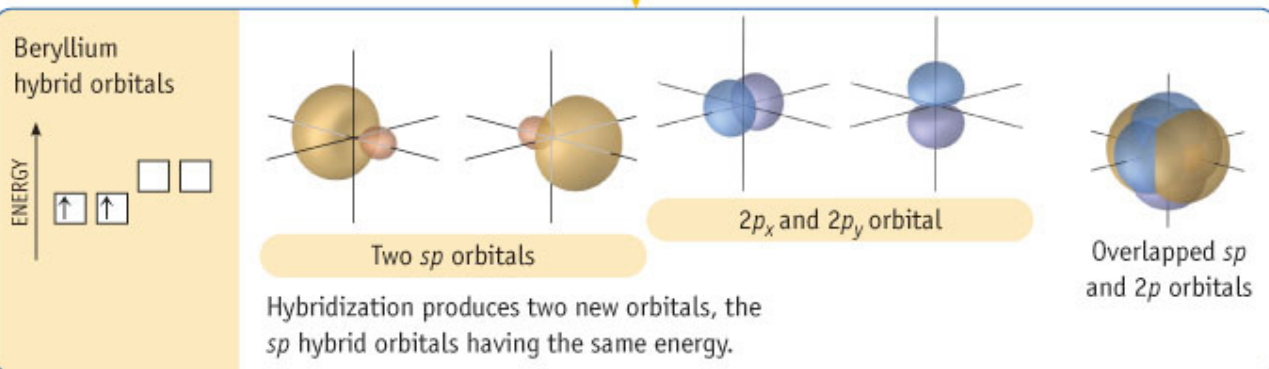
(c) The carbon-carbon π bond is formed by overlap of an unhybridized $2p$ orbital on each atom. Note the lack of electron density along the C—C bond axis from this bond.

sp hybridization

See in 3D!

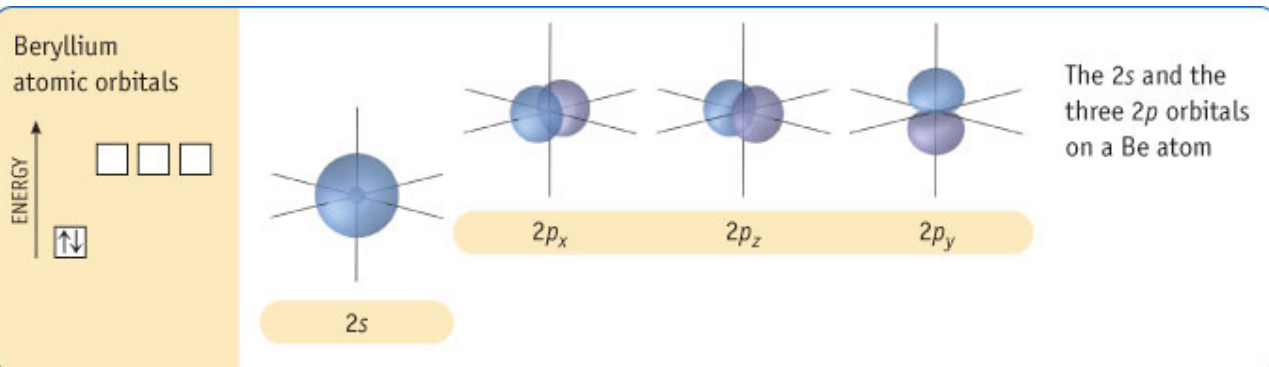


Orbital hybridization

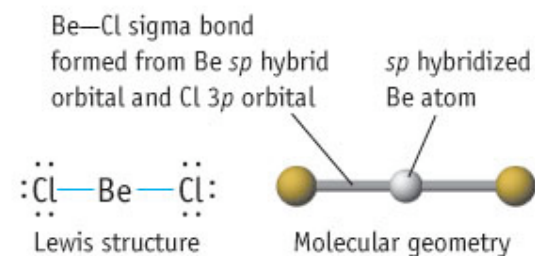
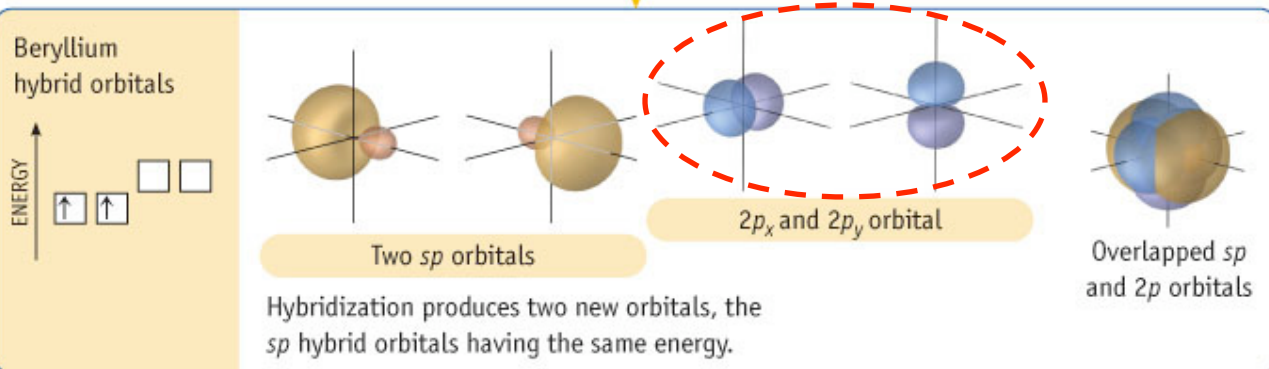


sp hybridization

See in 3D!



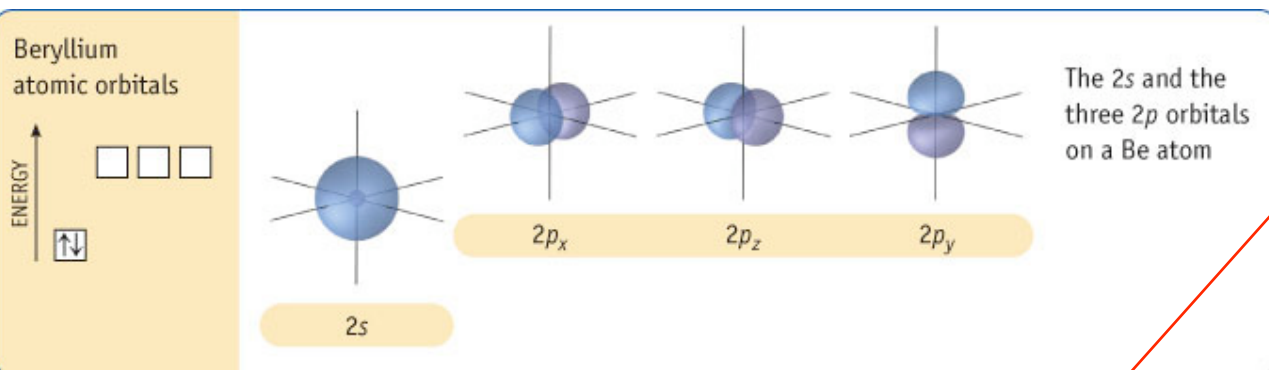
Orbital hybridization



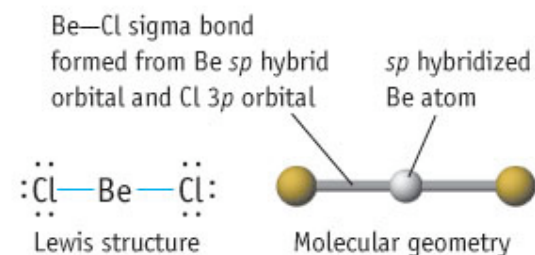
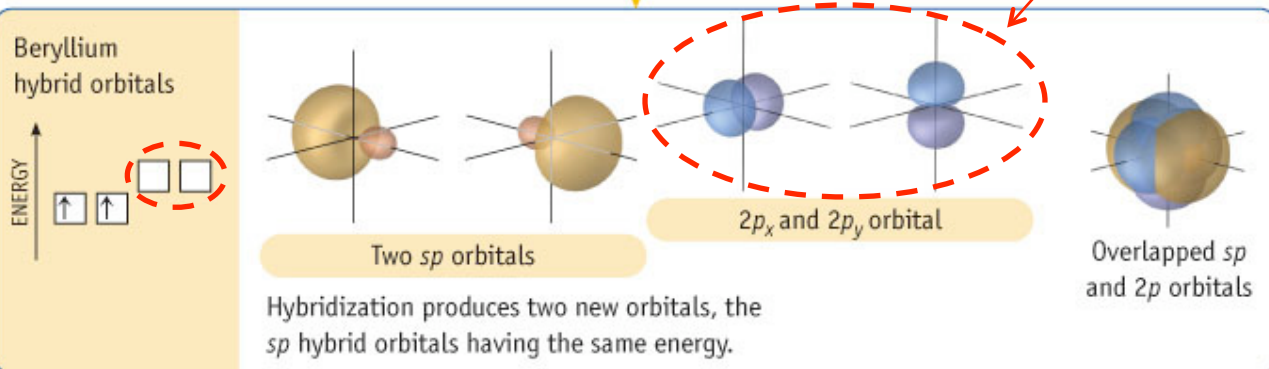
sp hybridization

See in 3D!

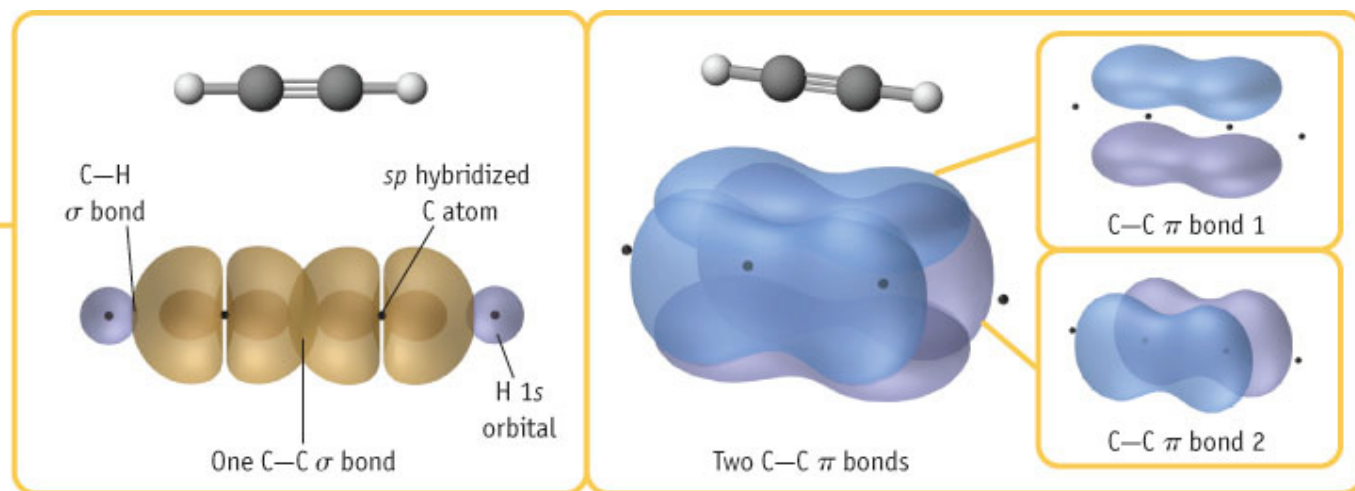
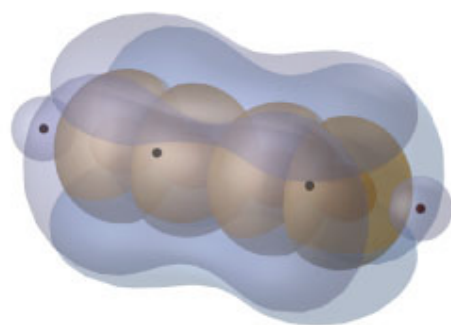
Left over (unused)
atomic orbitals



Orbital hybridization

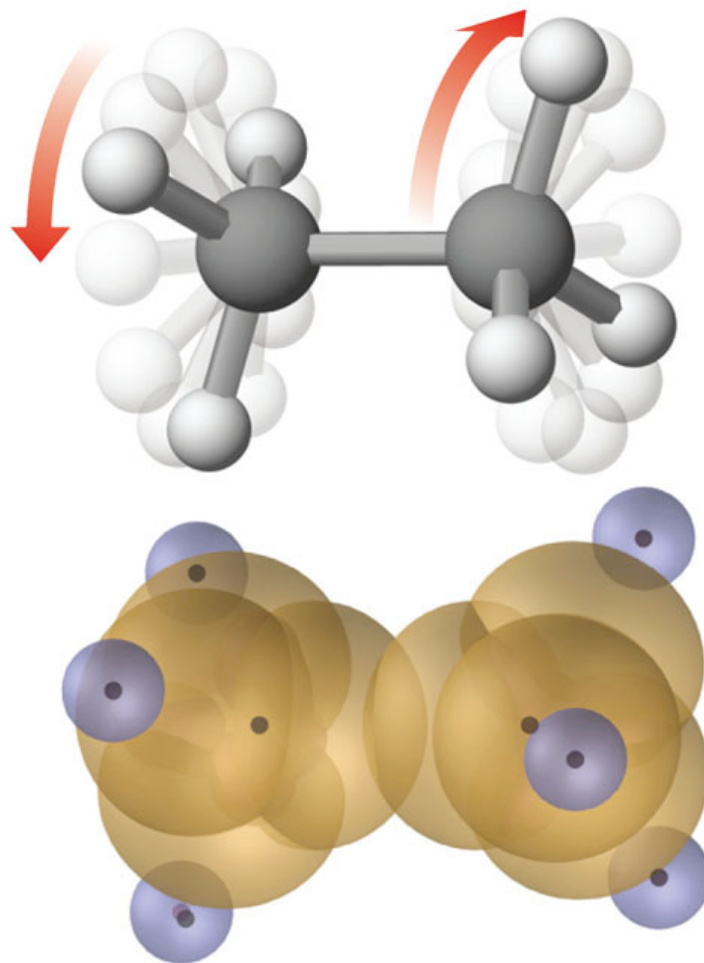


See in 3D!



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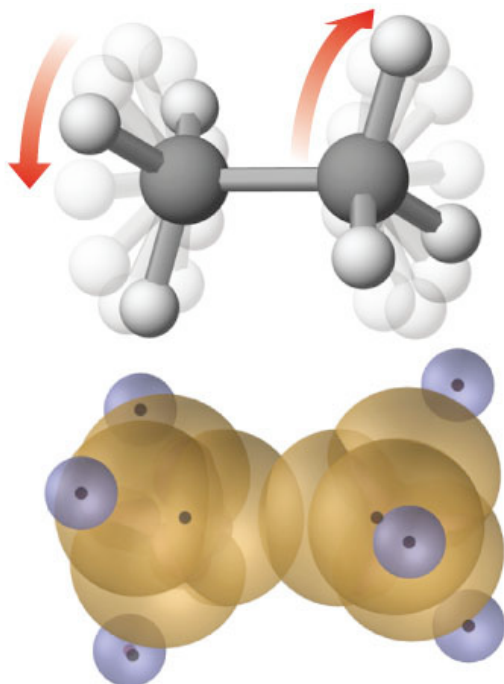
Free Rotation



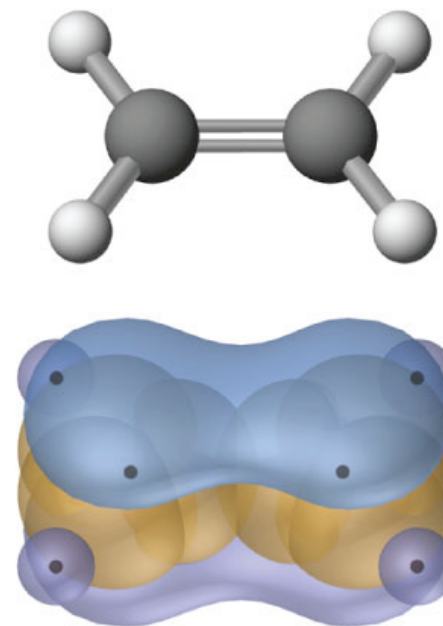
(a) In ethane nearly free rotation can occur around the axis of a single (σ) bond.

Restricted Rotation

Formation of pi bonds requires good overlap



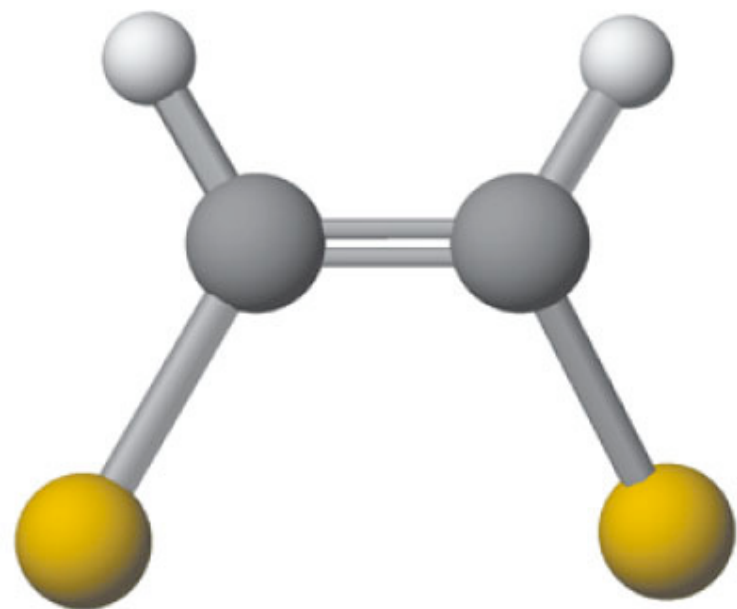
(a) In ethane nearly free rotation can occur around the axis of a single (σ) bond.



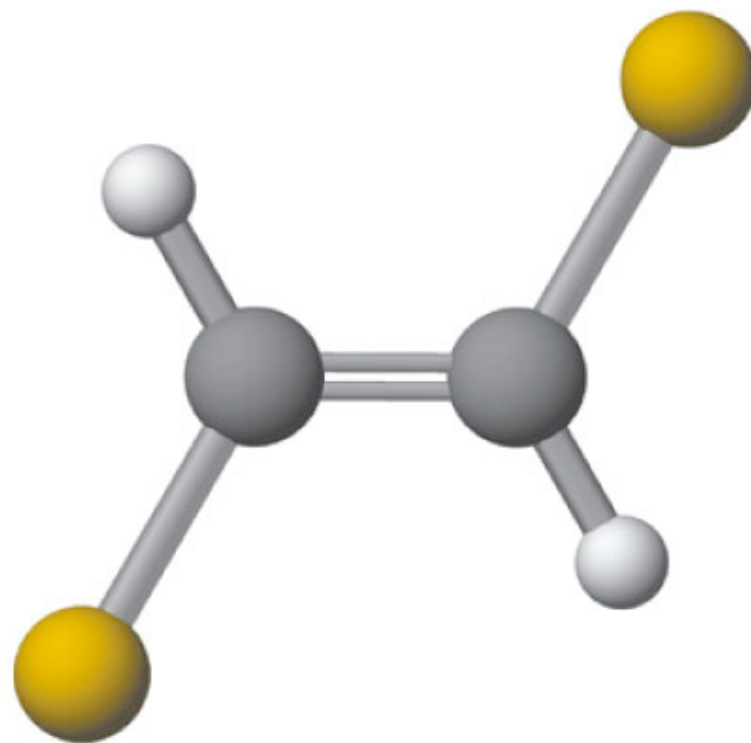
(b) Ethylene rotation is severely restricted around double bonds because doing so would break the π bond, a process generally requiring a great deal of energy.

Restricted Rotation

cis-trans isomers do not interconvert readily



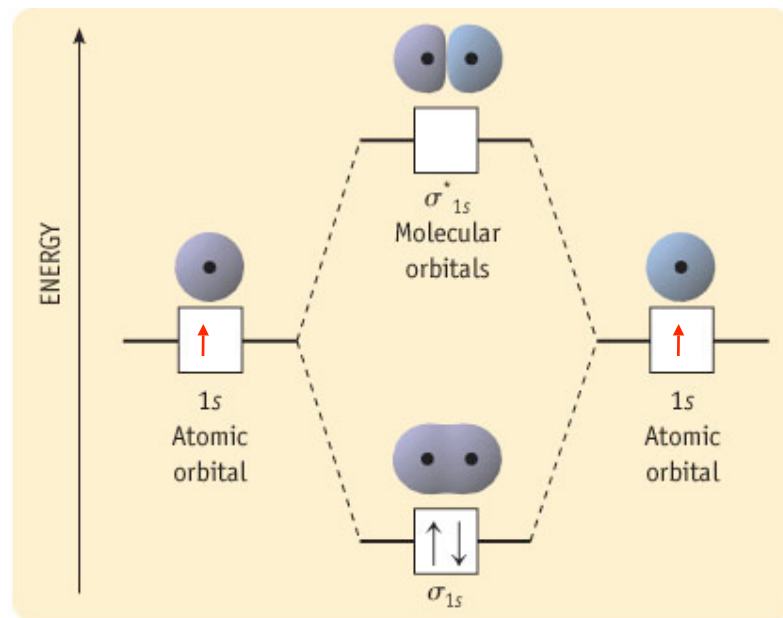
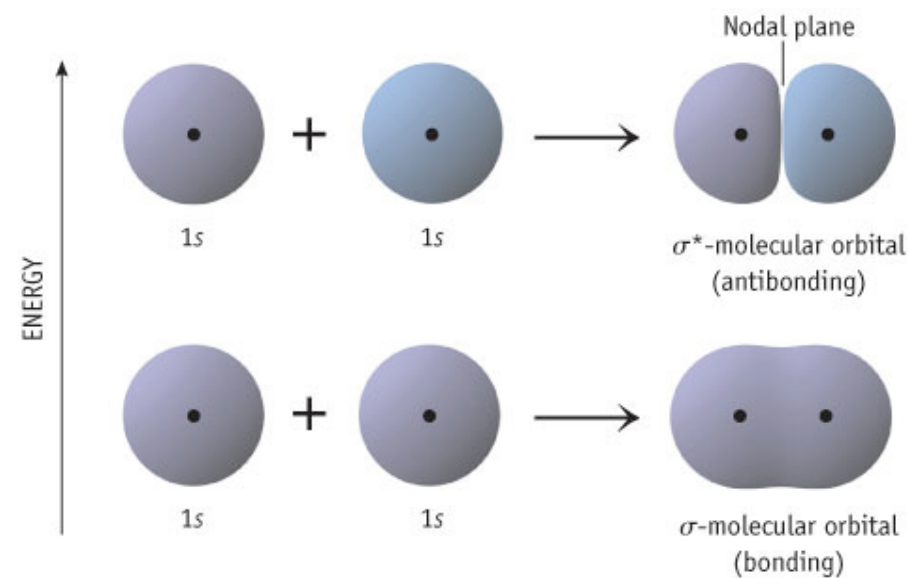
cis-1,2-dichloroethylene



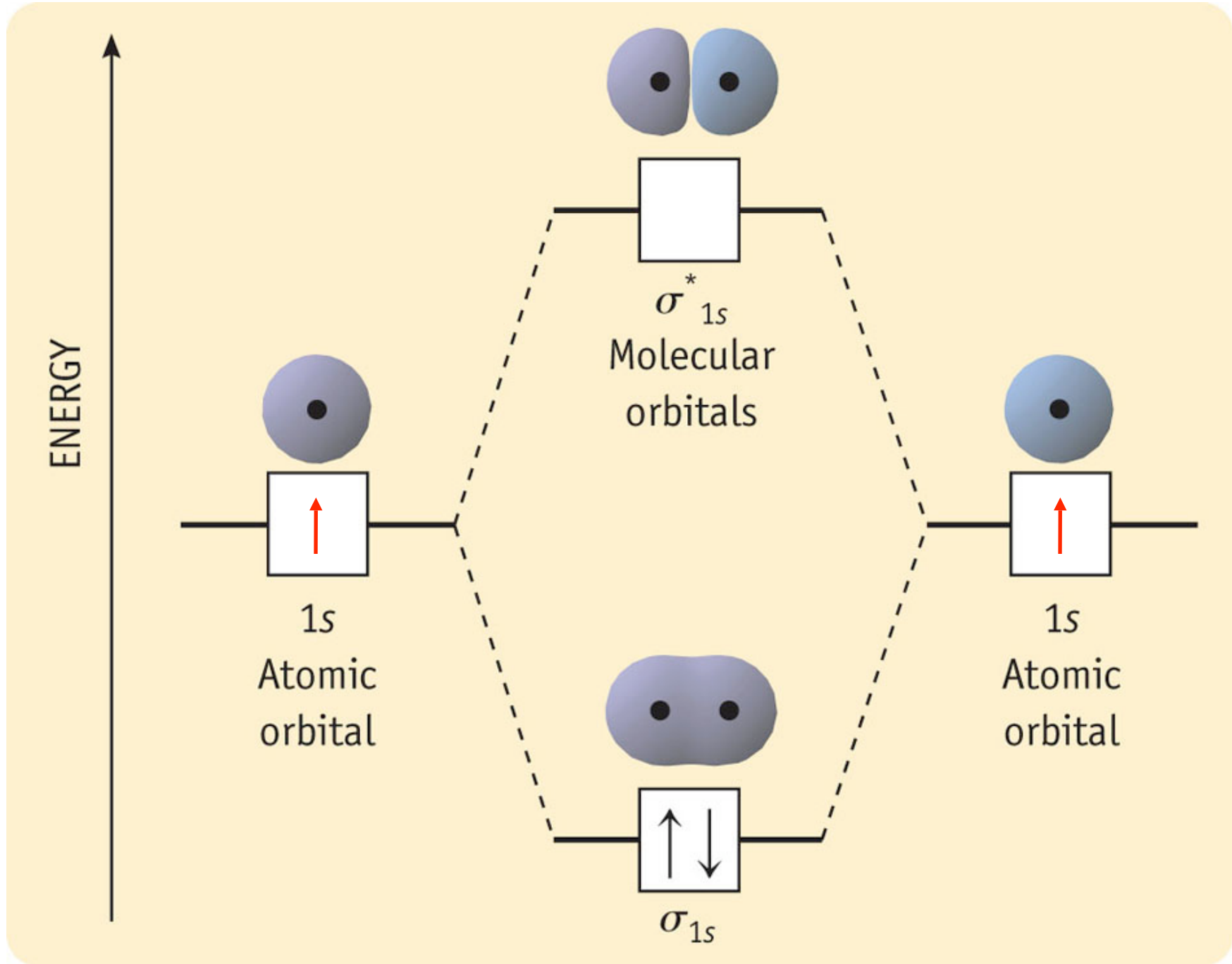
trans-1,2-dichloroethylene

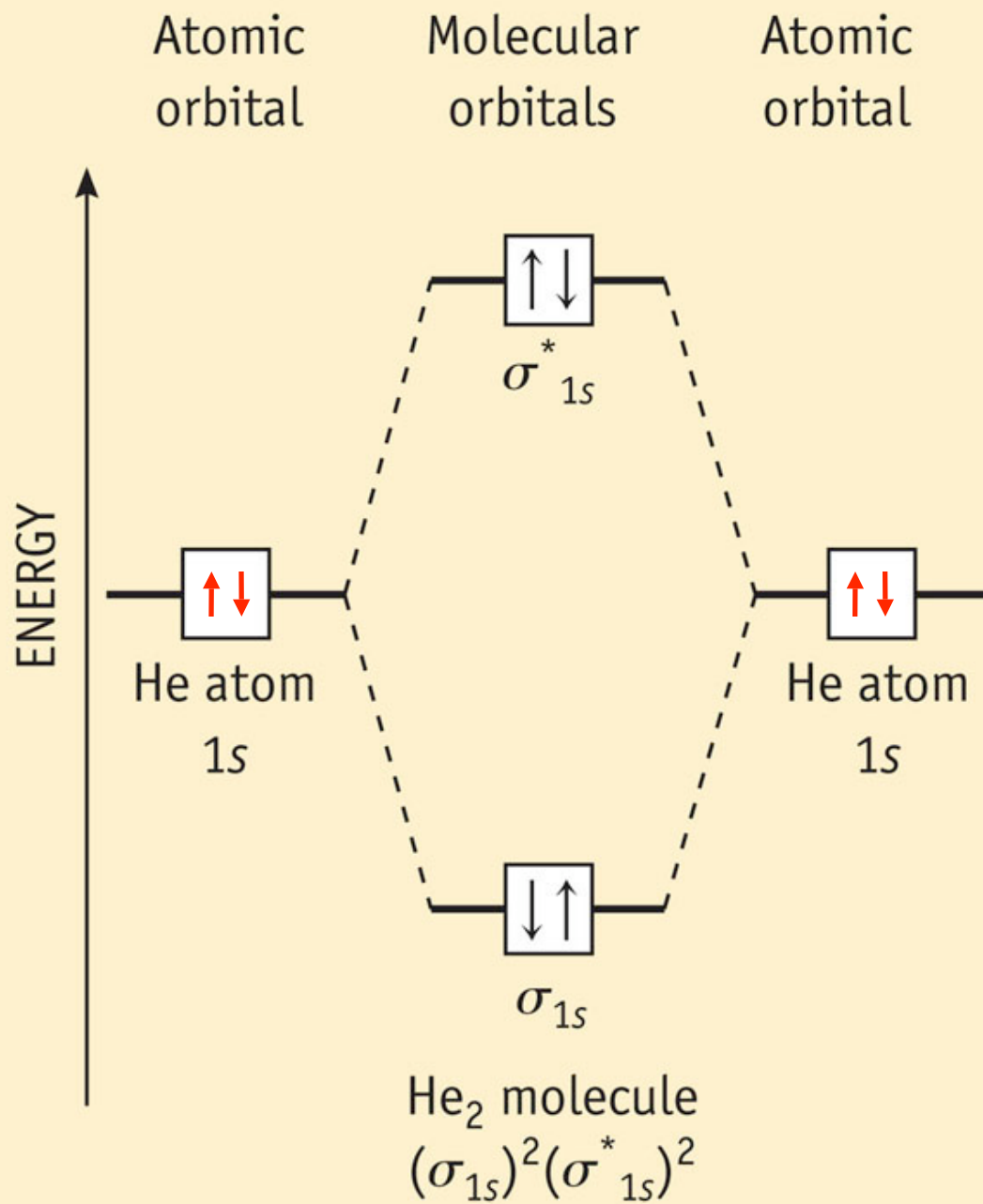
Back to H₂

Conserve energy when “mixing” orbitals



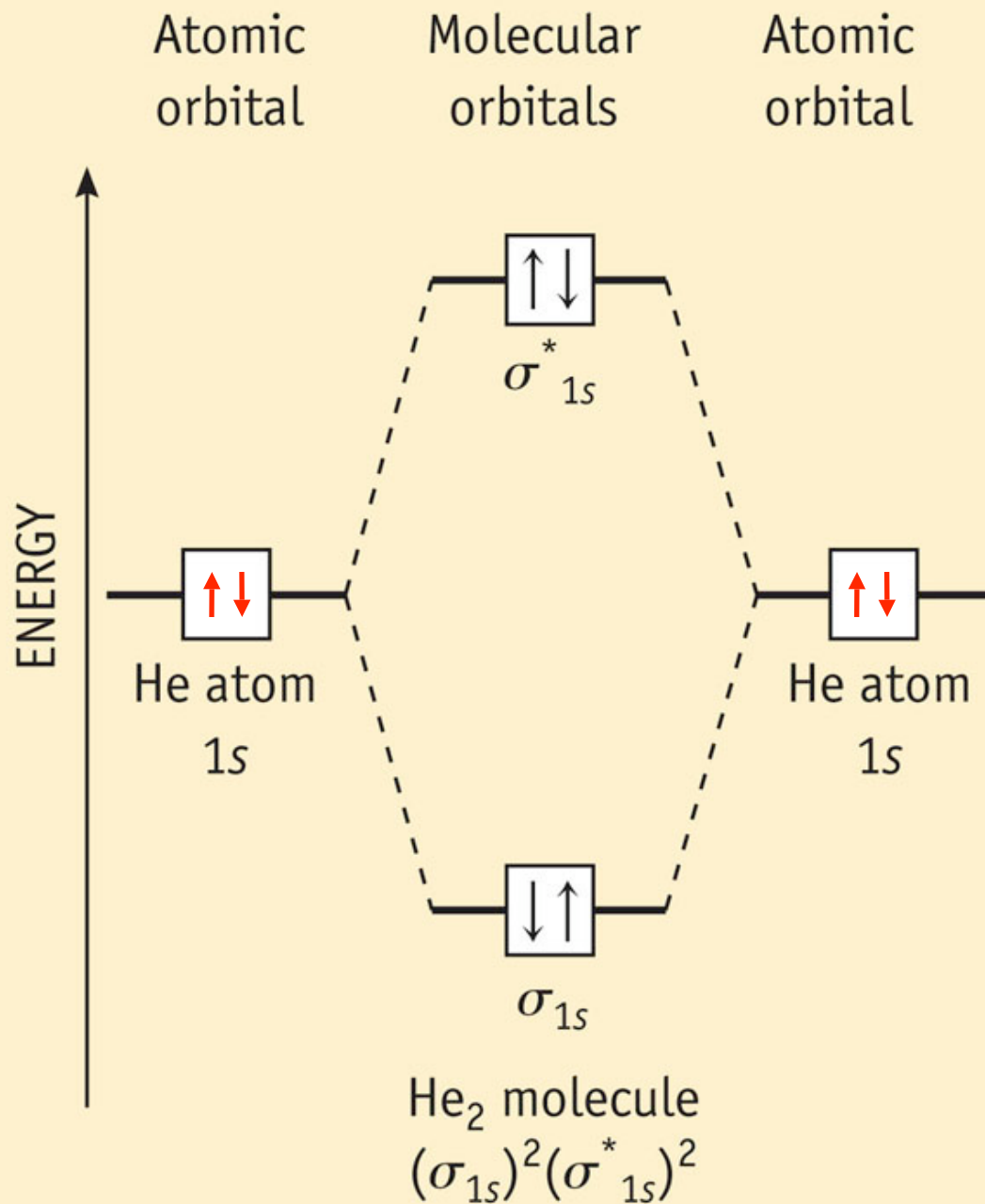
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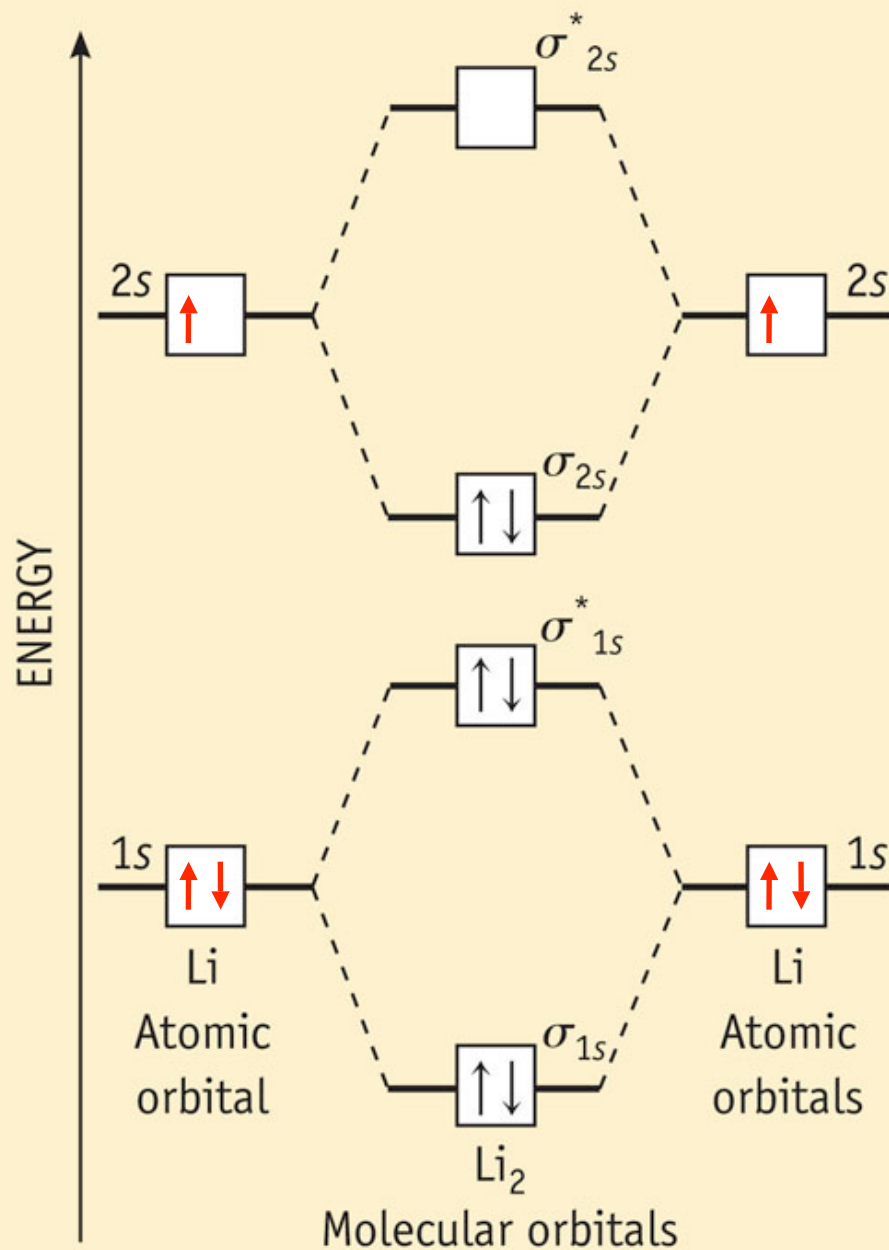




He₂

Doesn't
exist

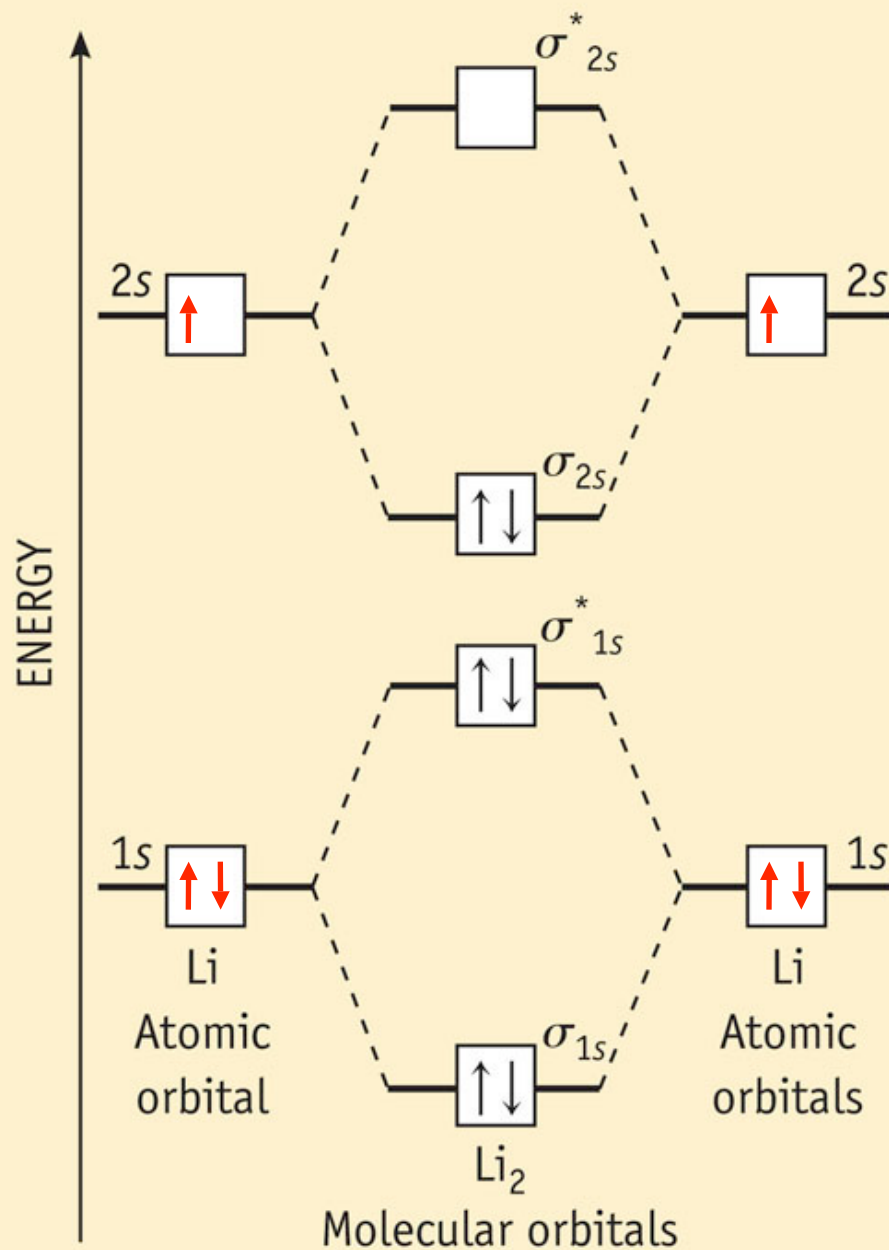


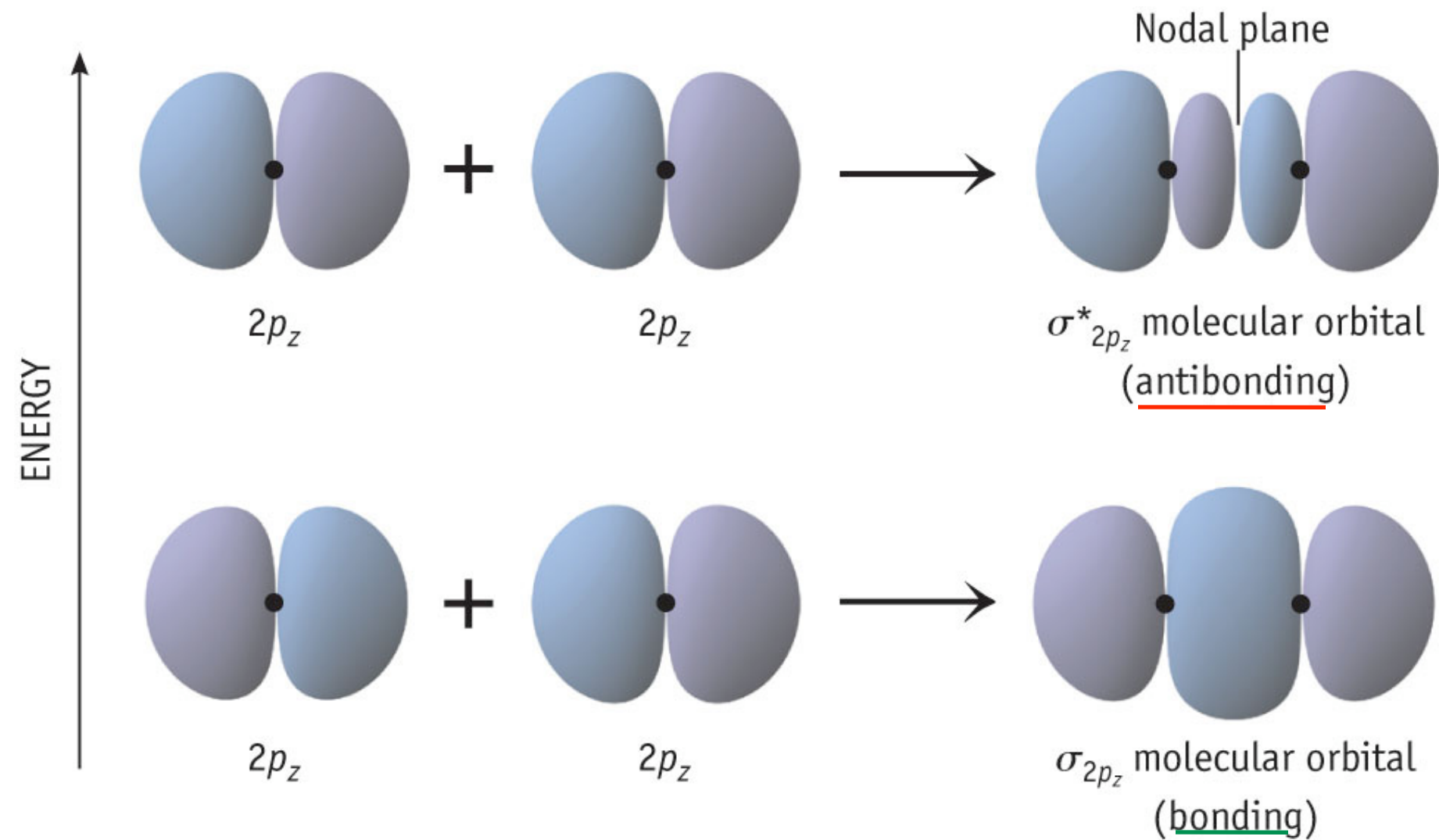


Li_2

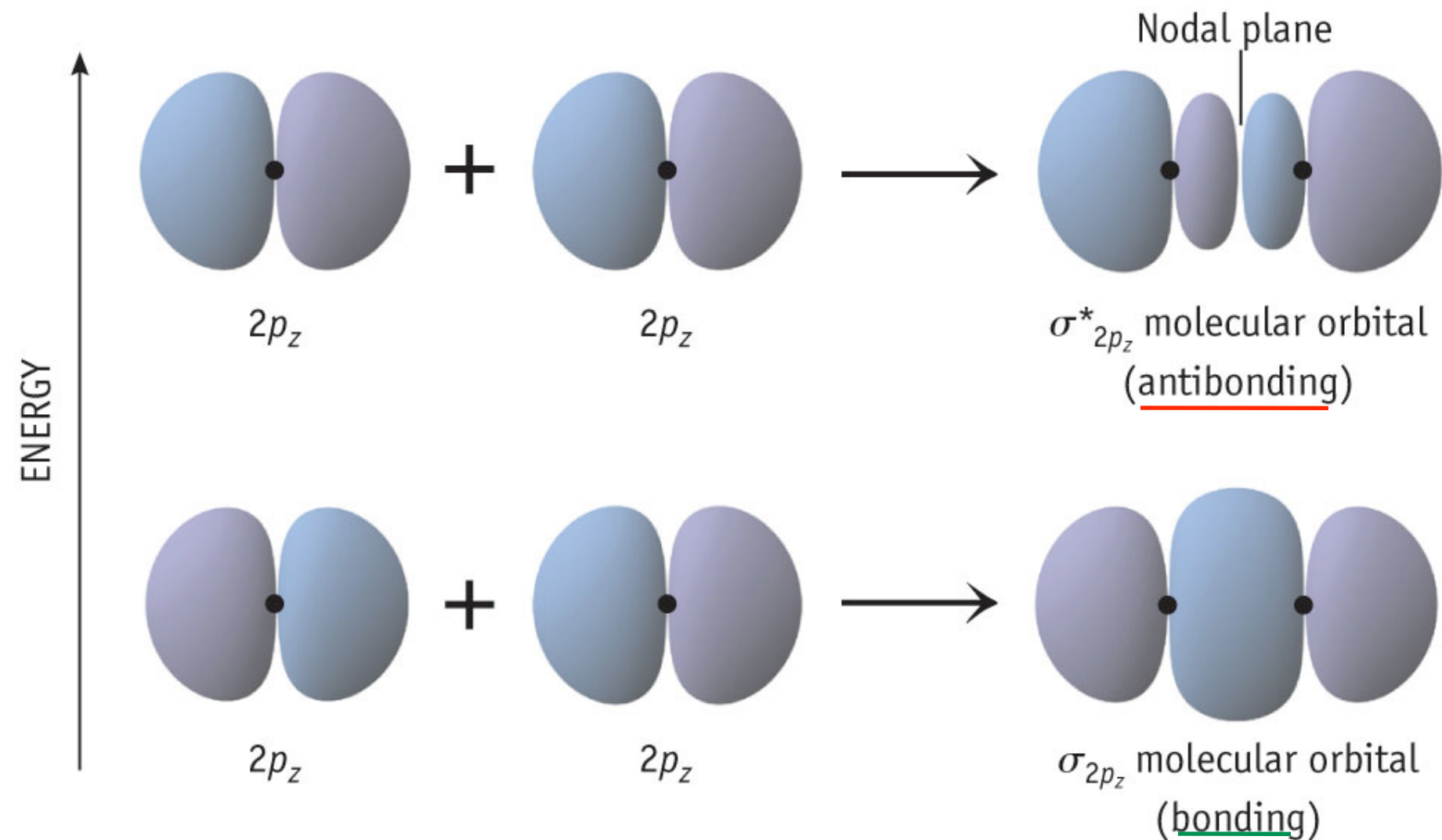
Does
exist

$\text{Li} - 1s^2 2s^1$



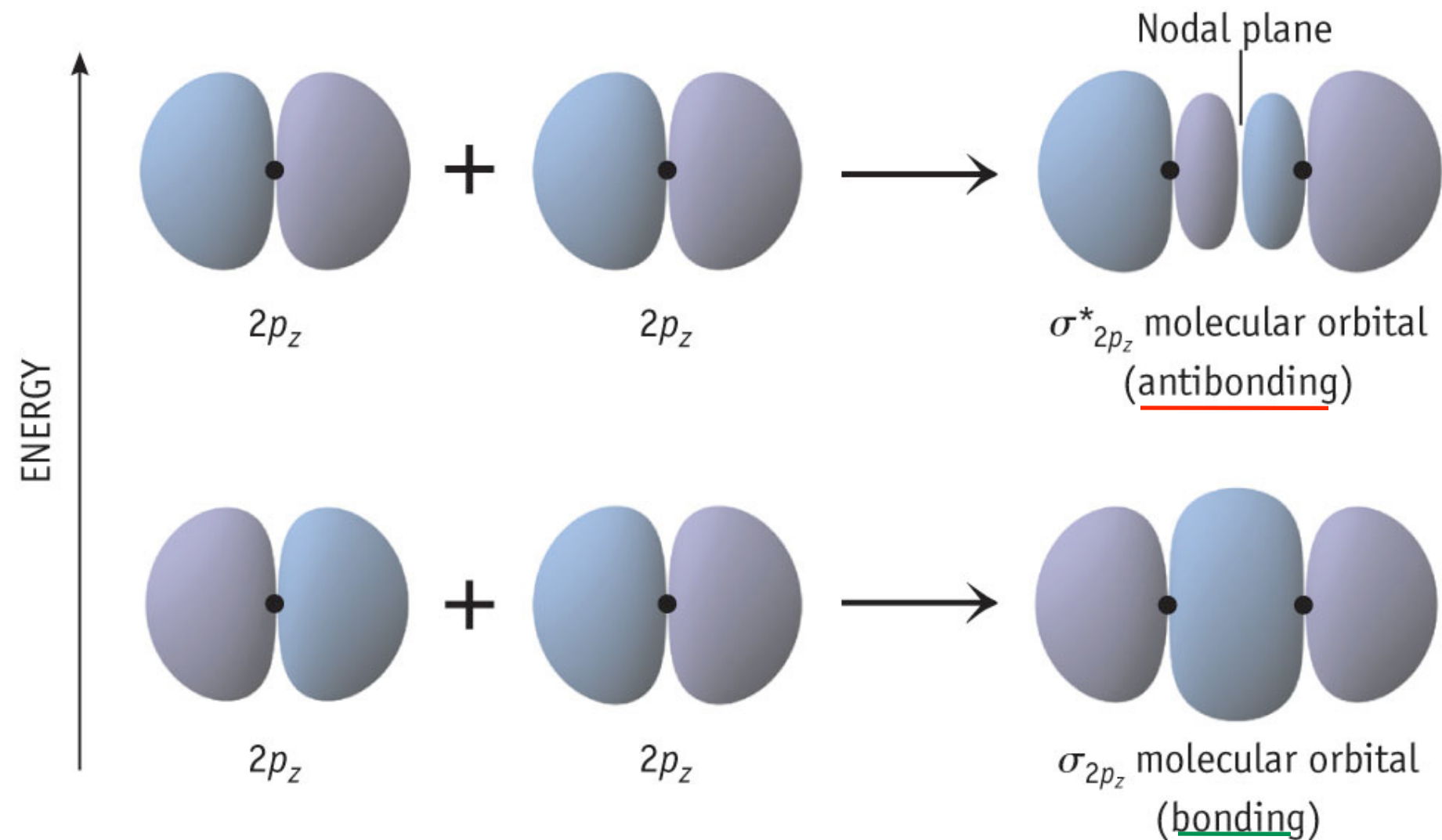


Atomic Orbitals



Atomic Orbitals

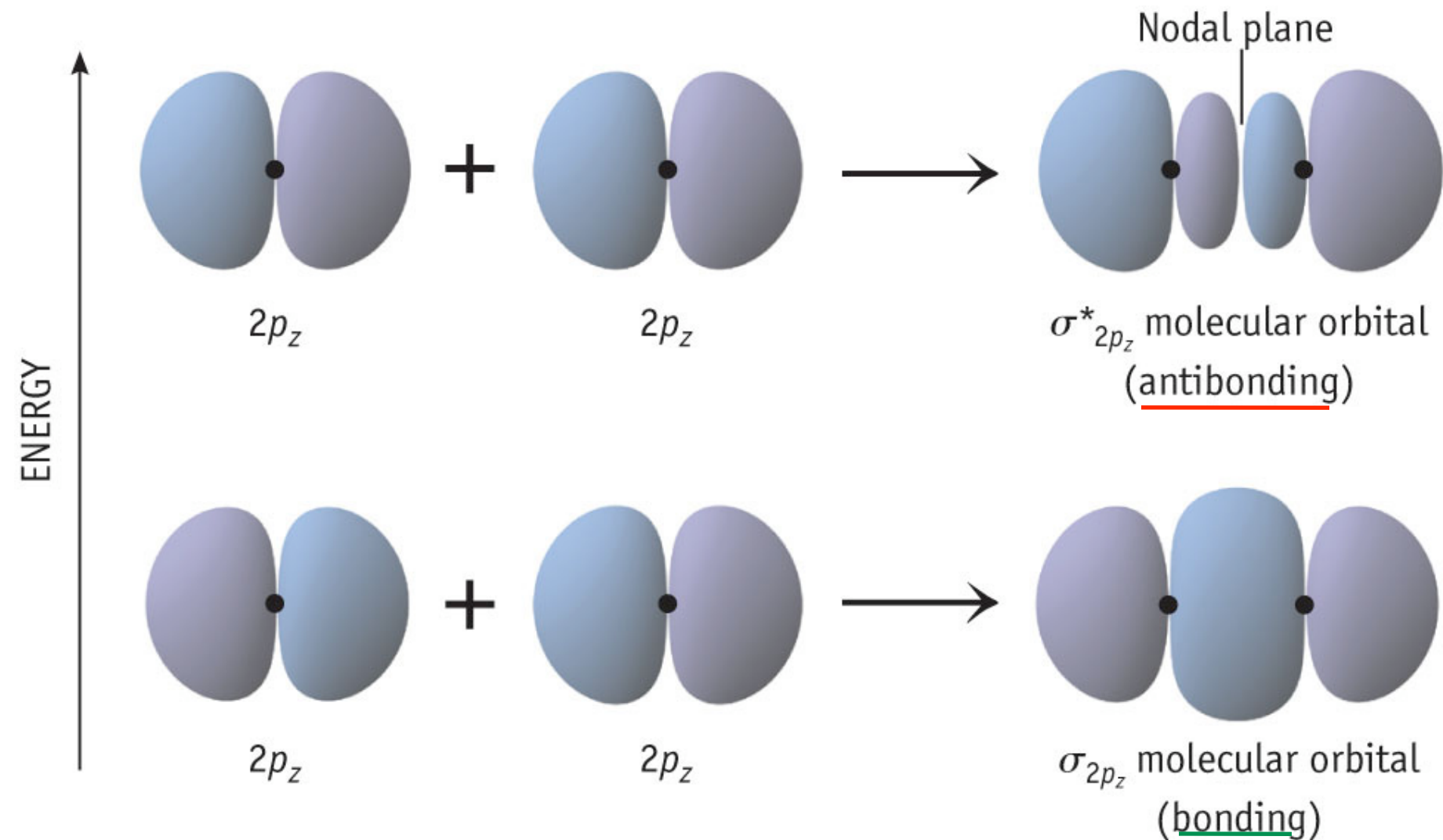
Bonding and Antibonding Orbitals

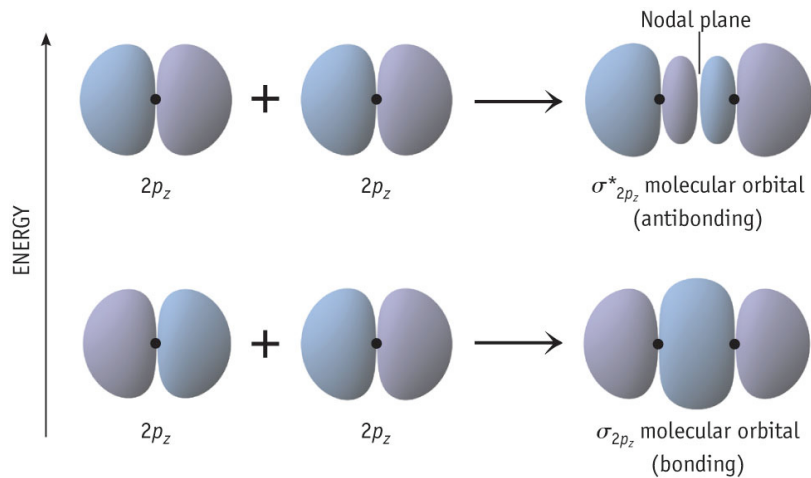


Sigma bonds

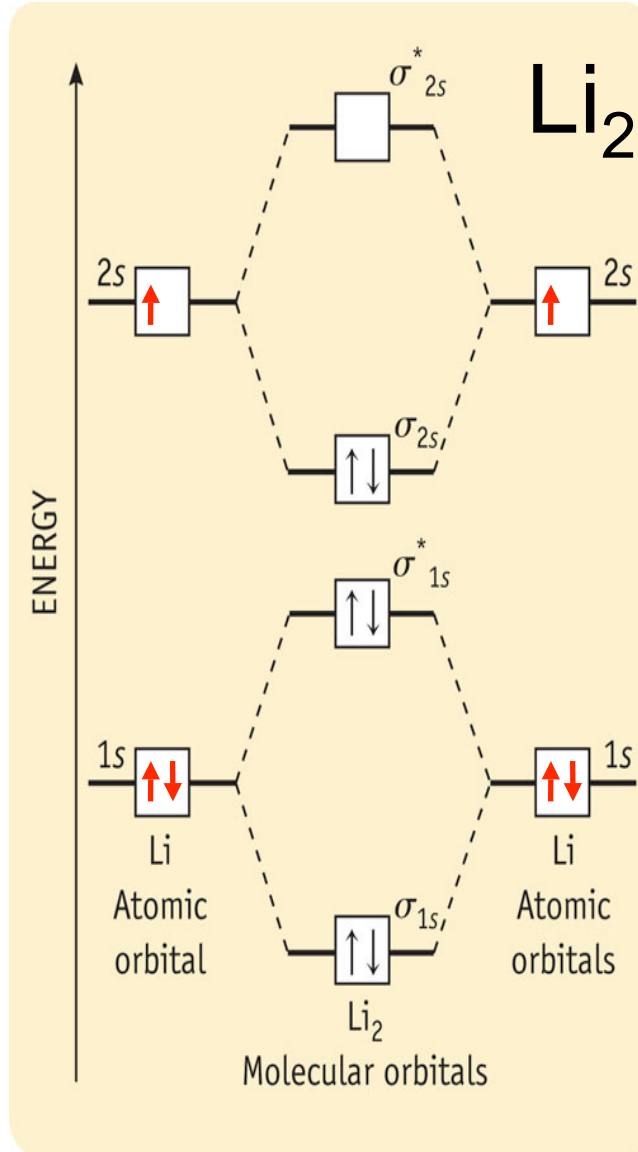
Atomic Orbitals

Bonding and Antibonding Orbitals



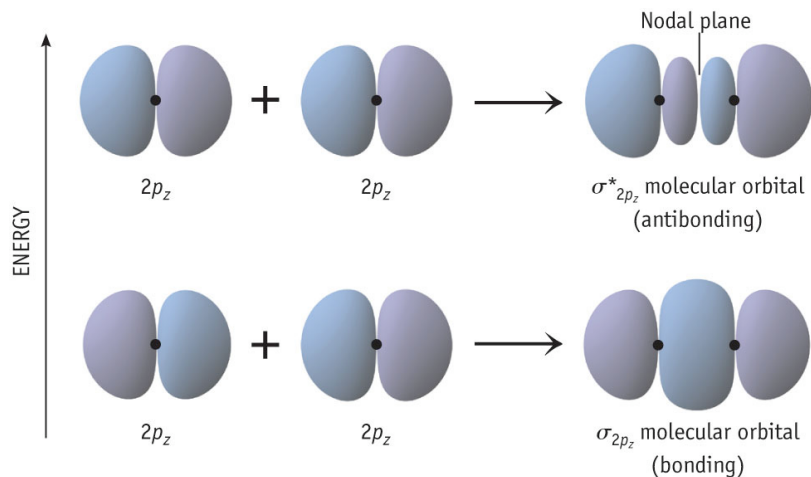


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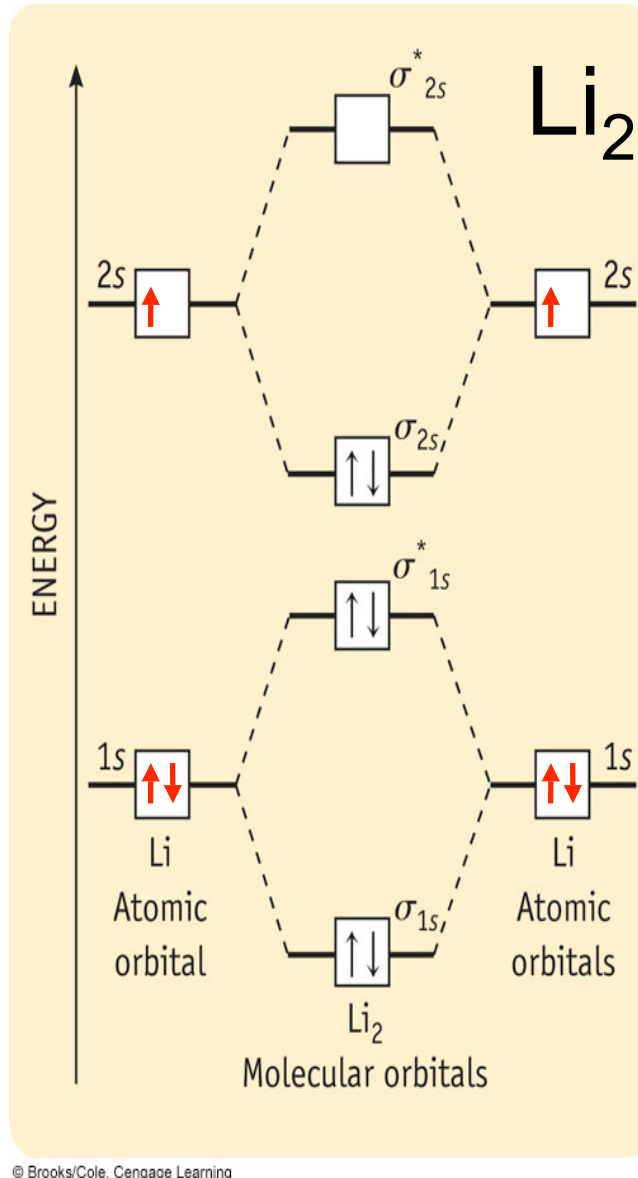


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Why not hybrid
atomic orbitals?

Not worth it in
diatomics

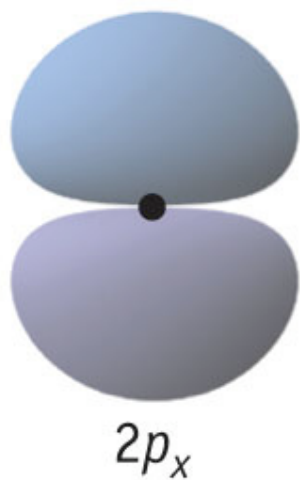
But we will in
everything larger



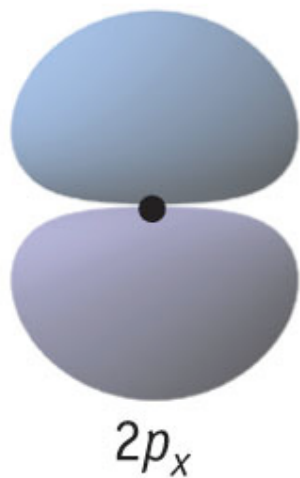
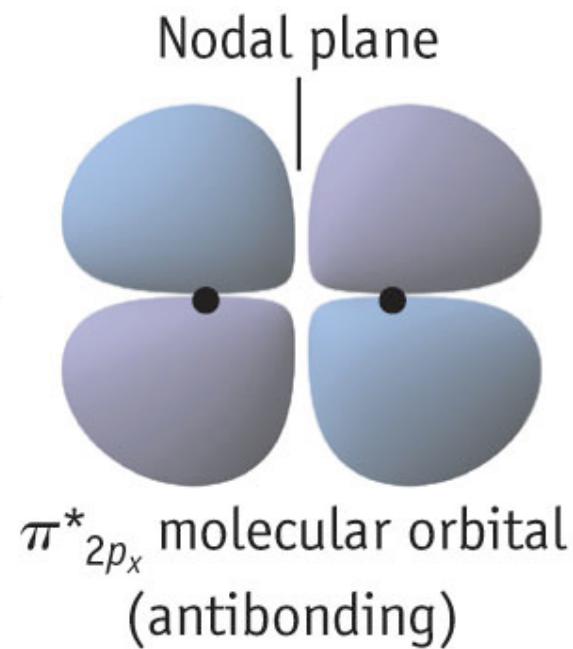
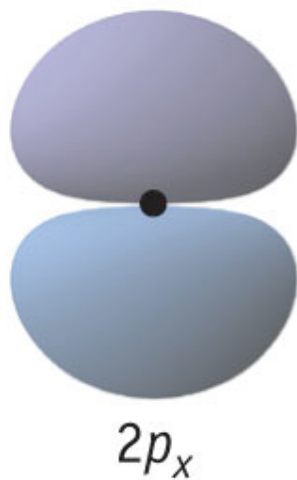
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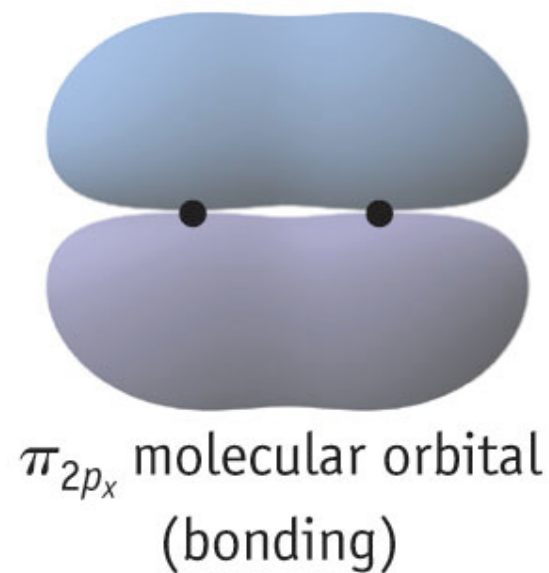
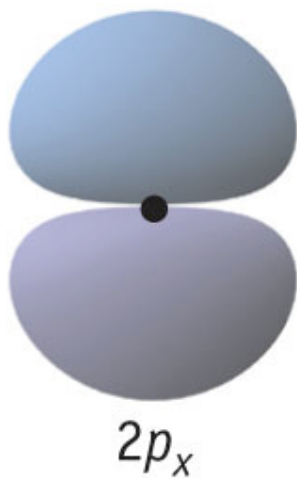
ENERGY ↑

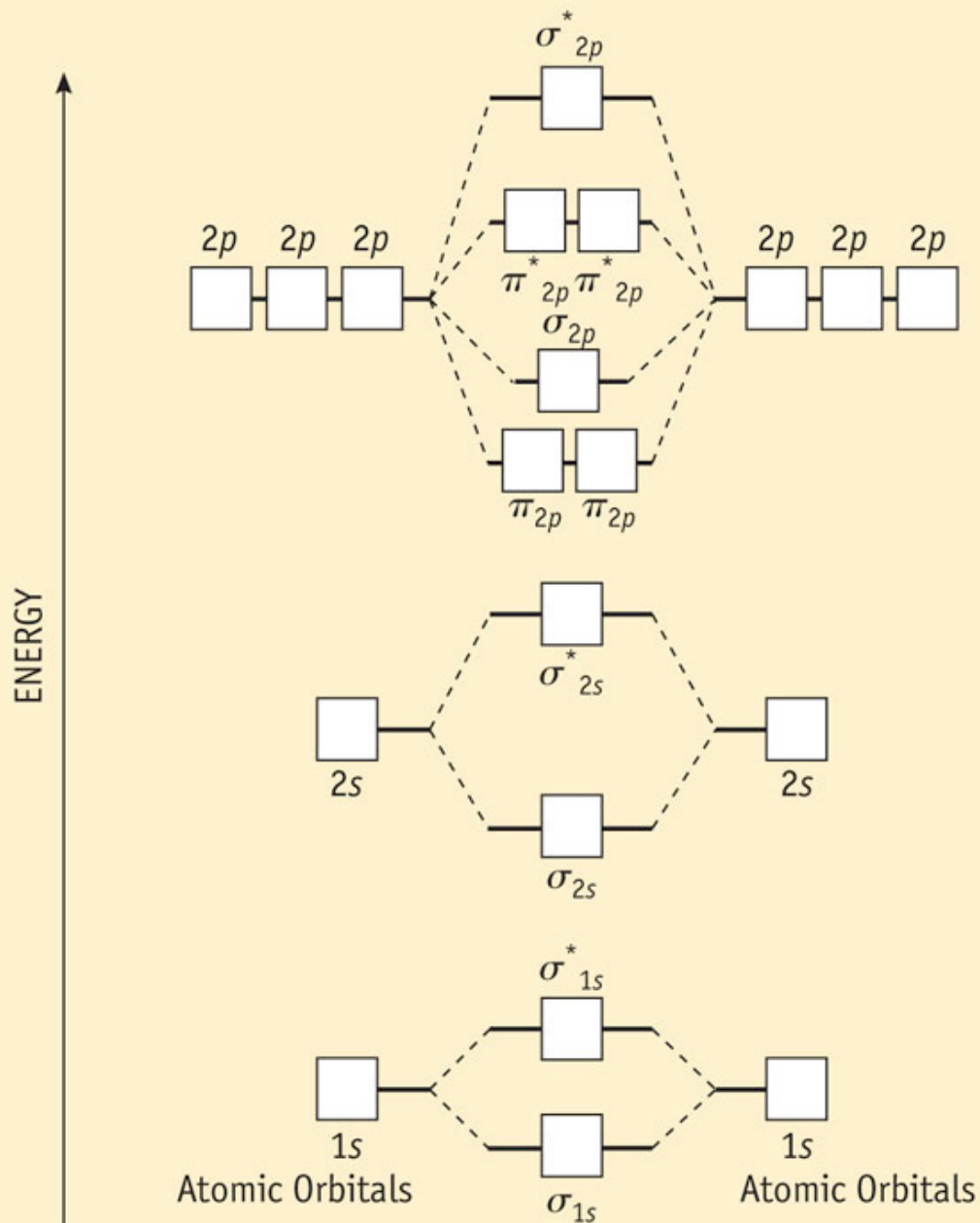


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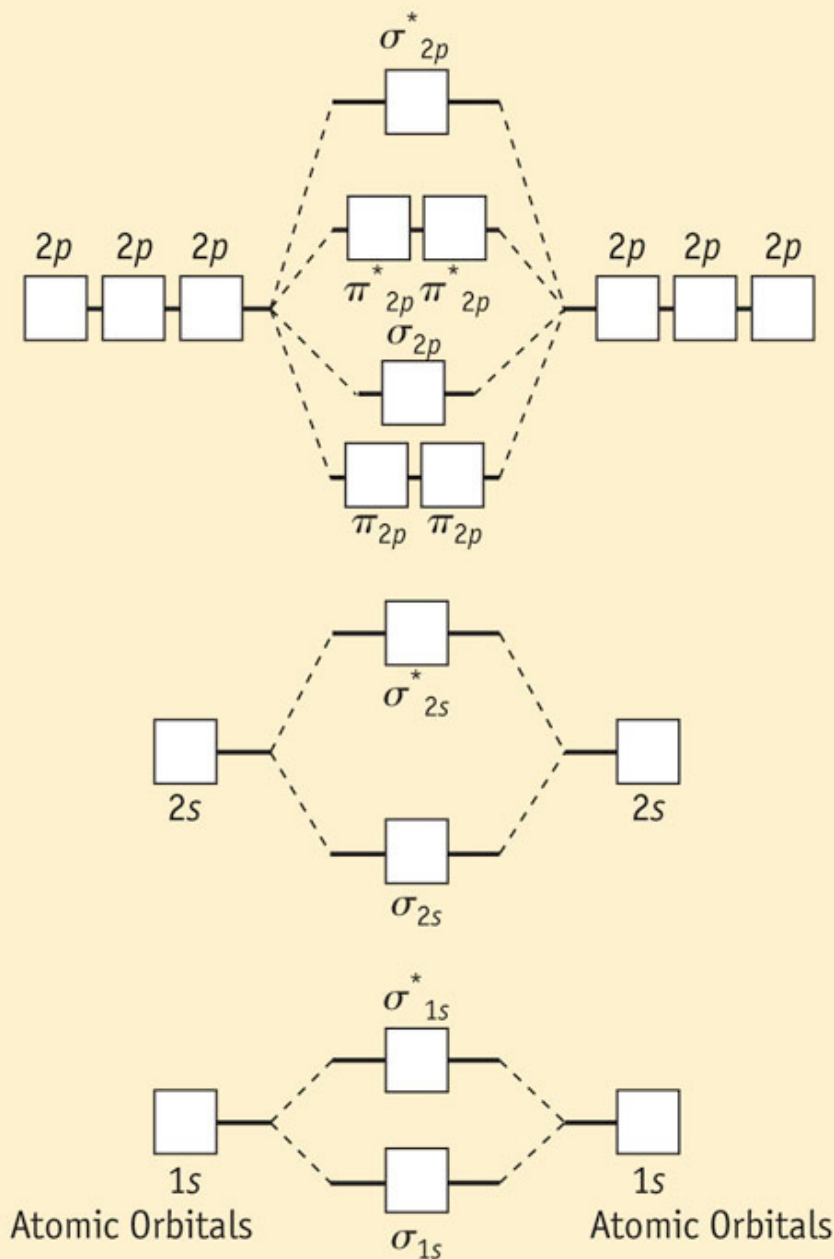
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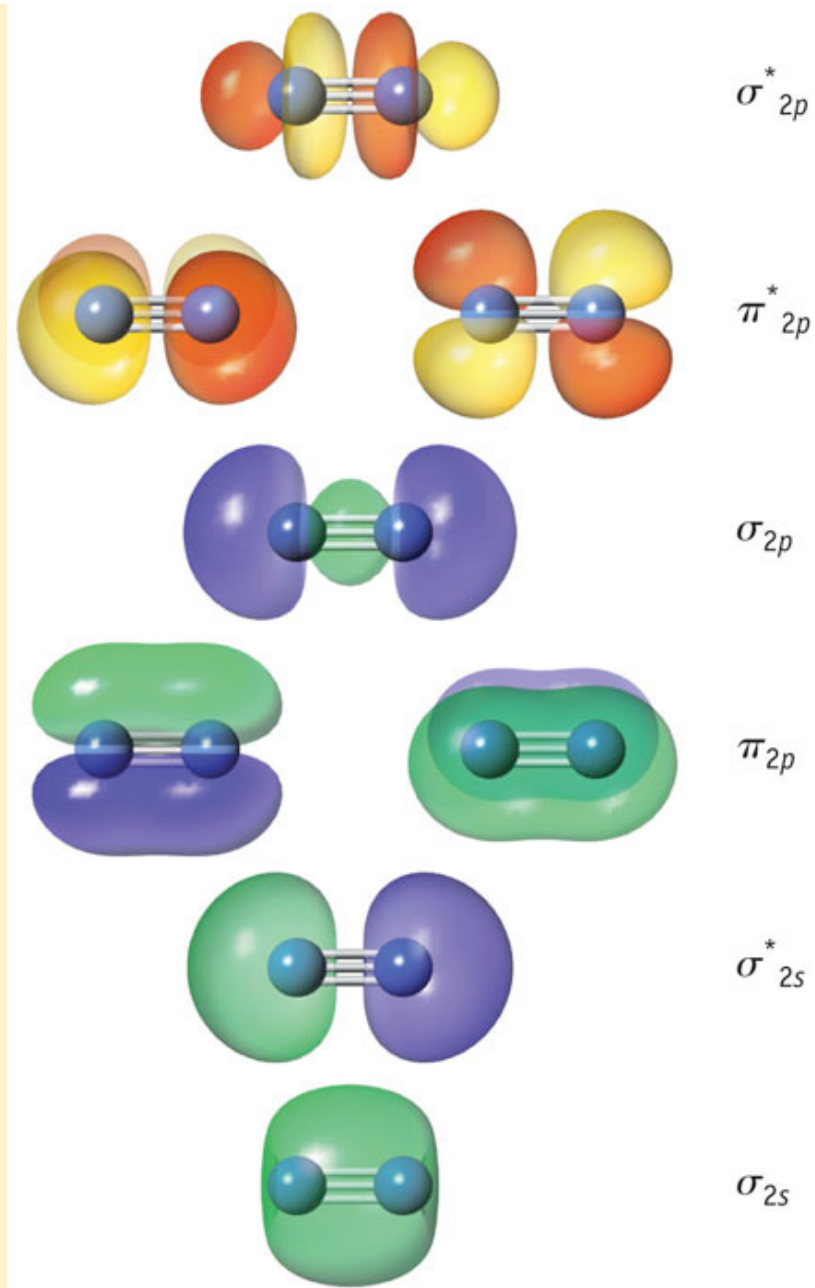


Molecular Orbitals for B_2 , C_2 , and N_2

ENERGY

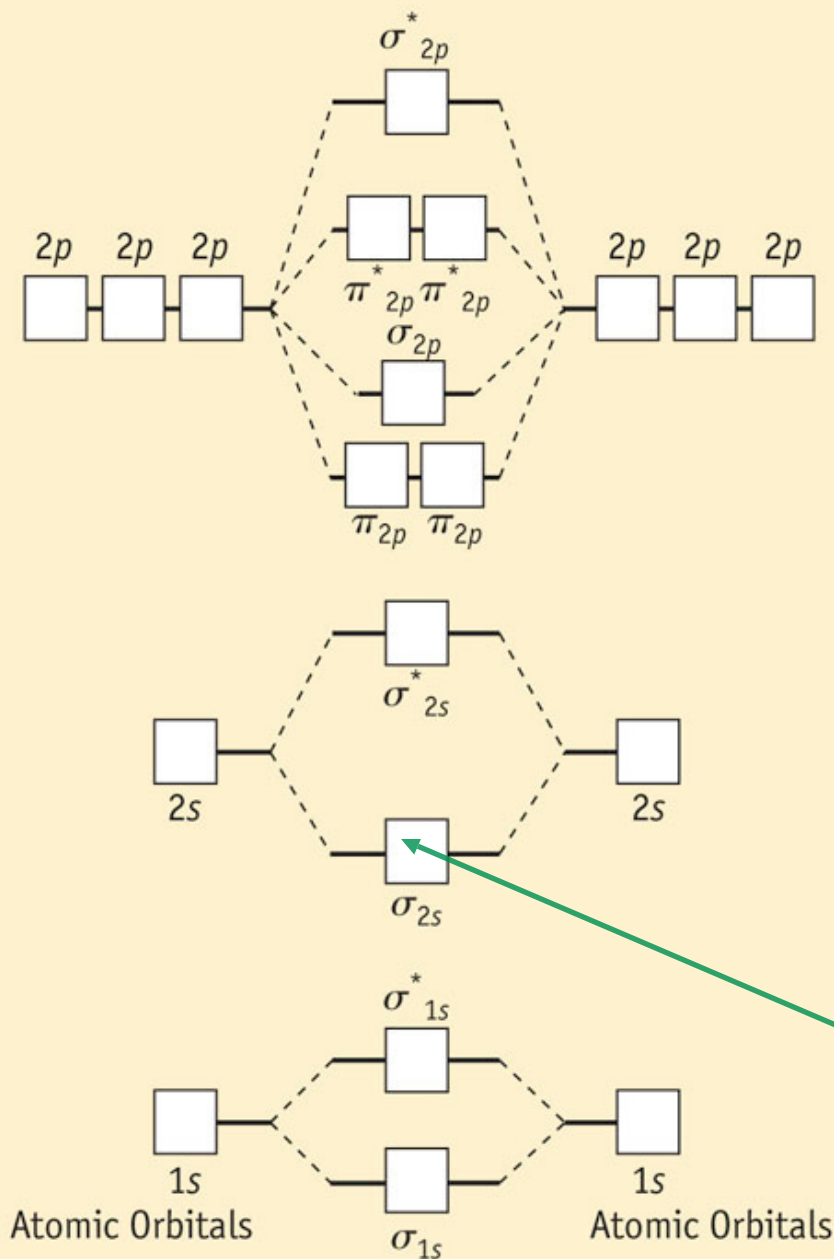


Molecular Orbitals for B_2 , C_2 , and N_2

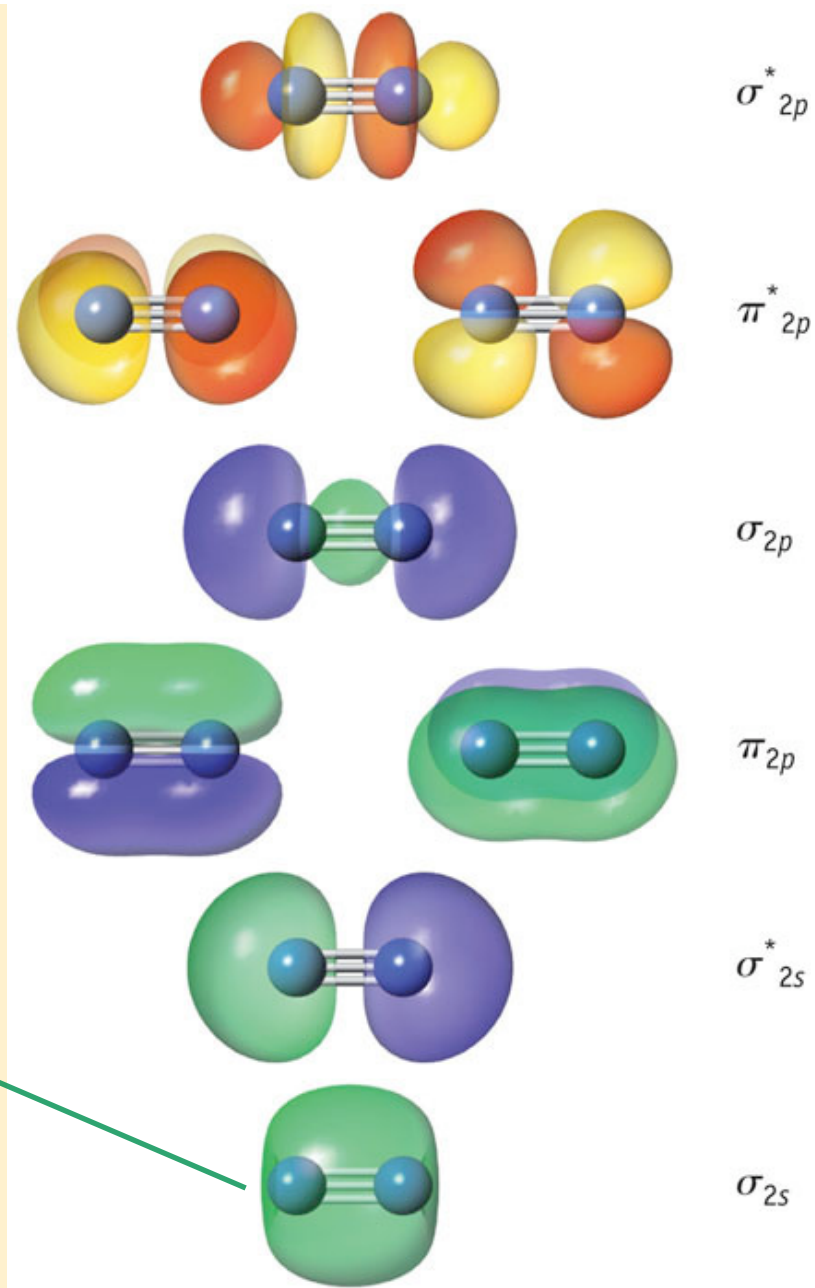


N_2 Molecular Orbitals

ENERGY

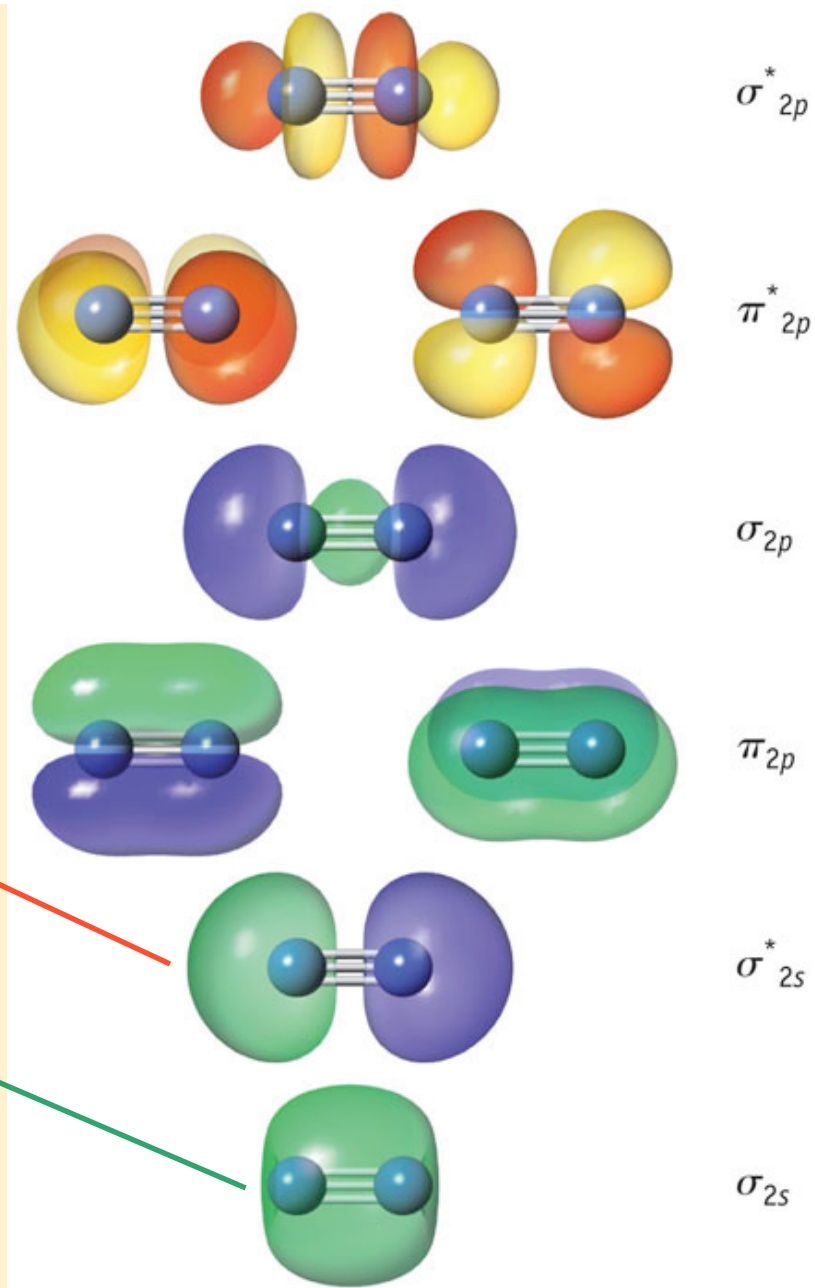
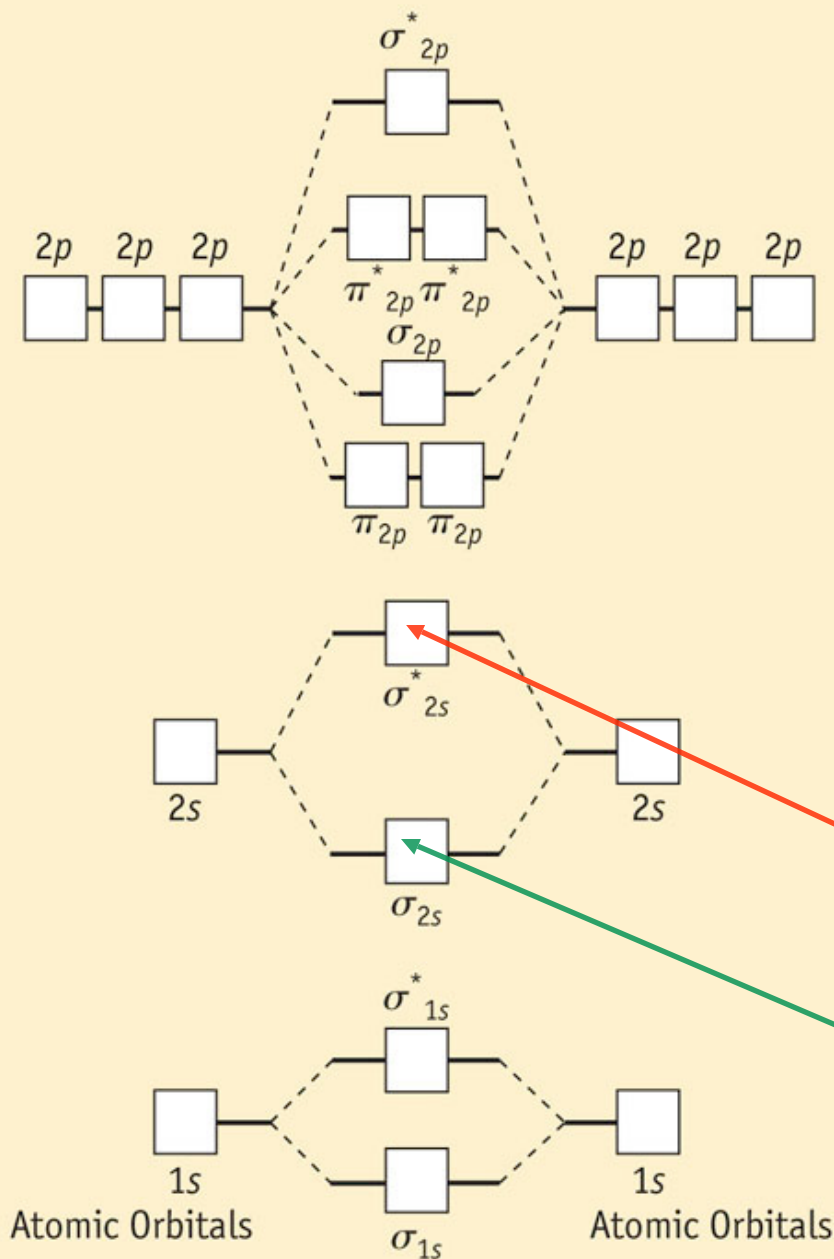


Molecular Orbitals for B_2 , C_2 , and N_2



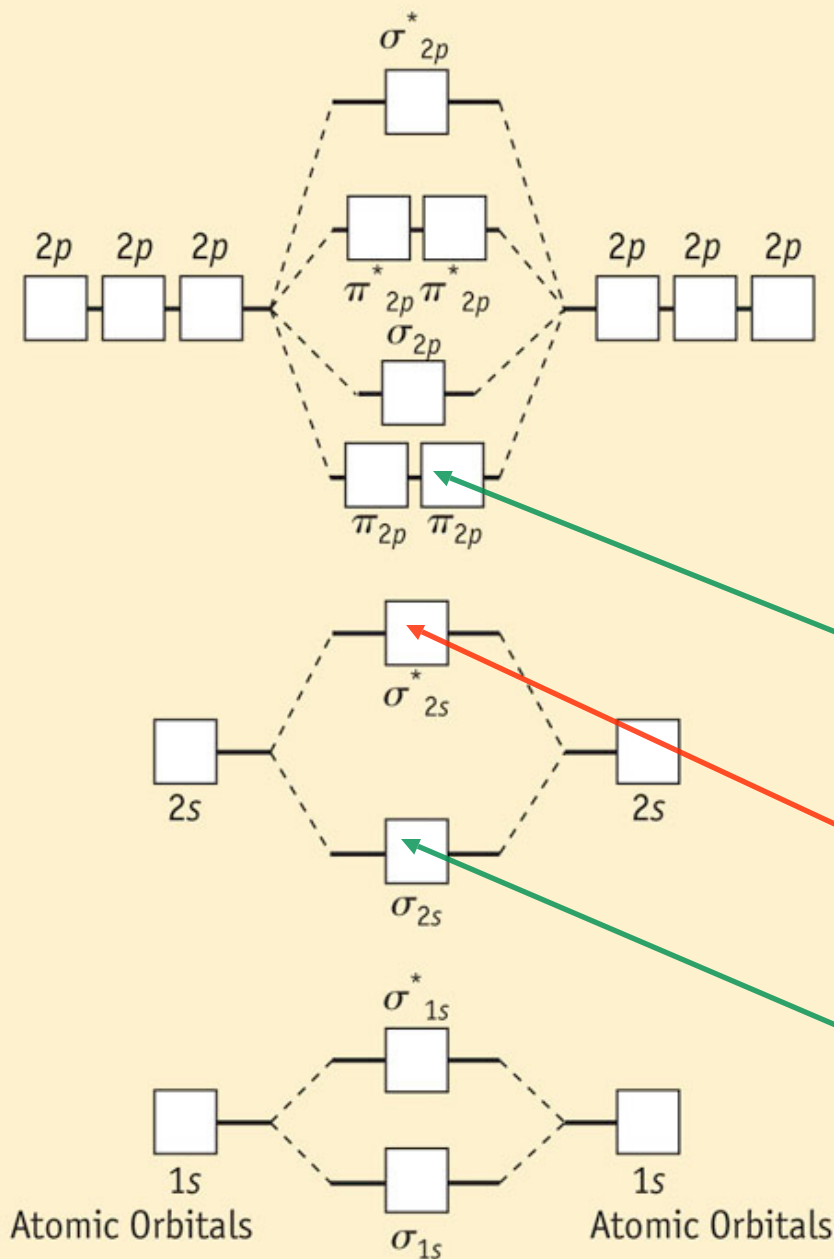
N_2 Molecular Orbitals

ENERGY

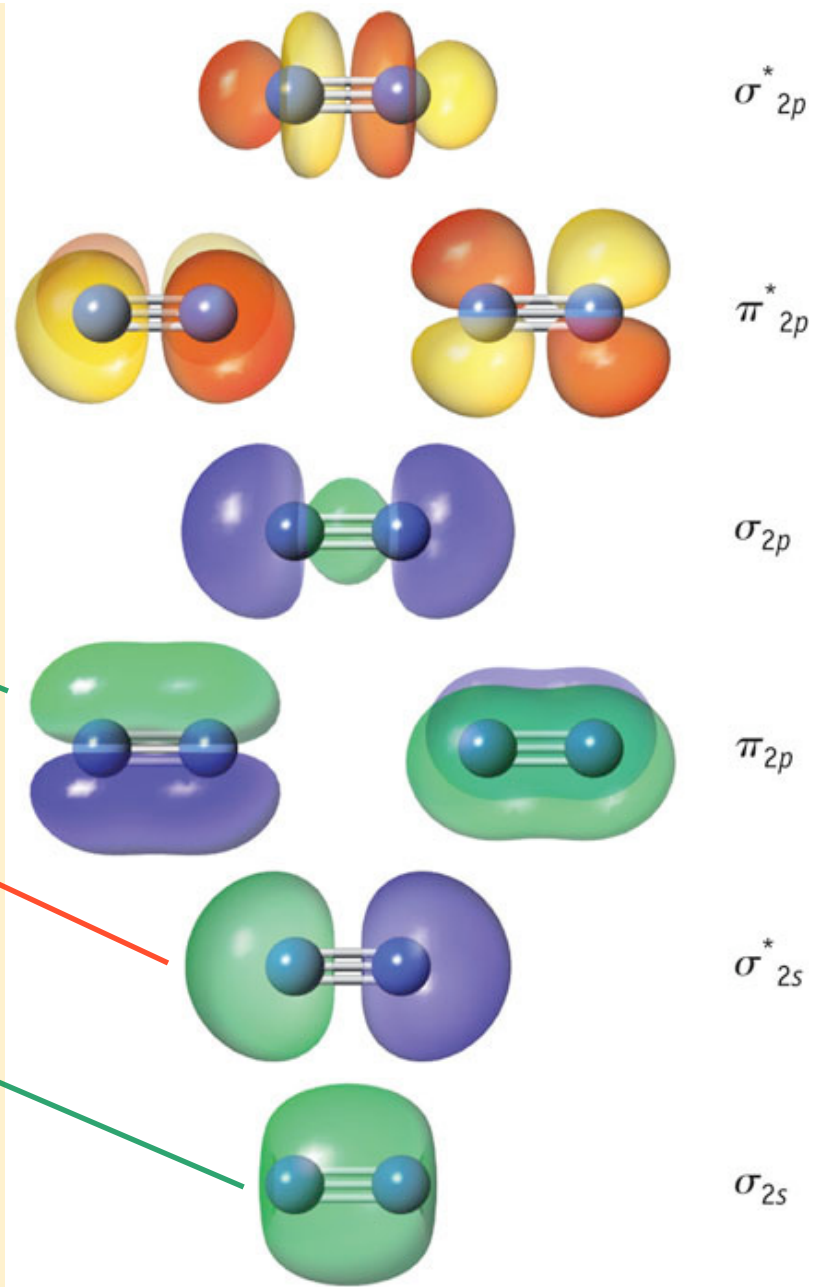


N_2 Molecular Orbitals

ENERGY

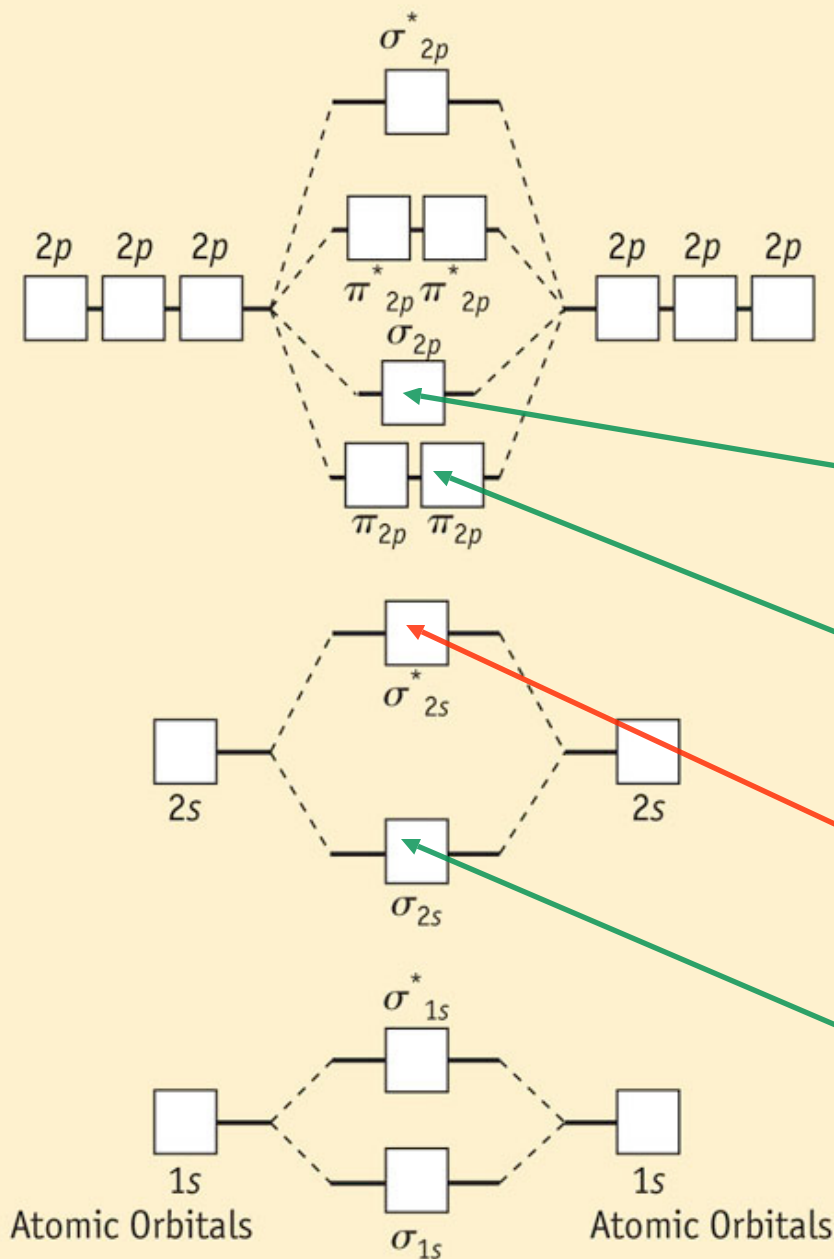


Molecular Orbitals for B_2 , C_2 , and N_2

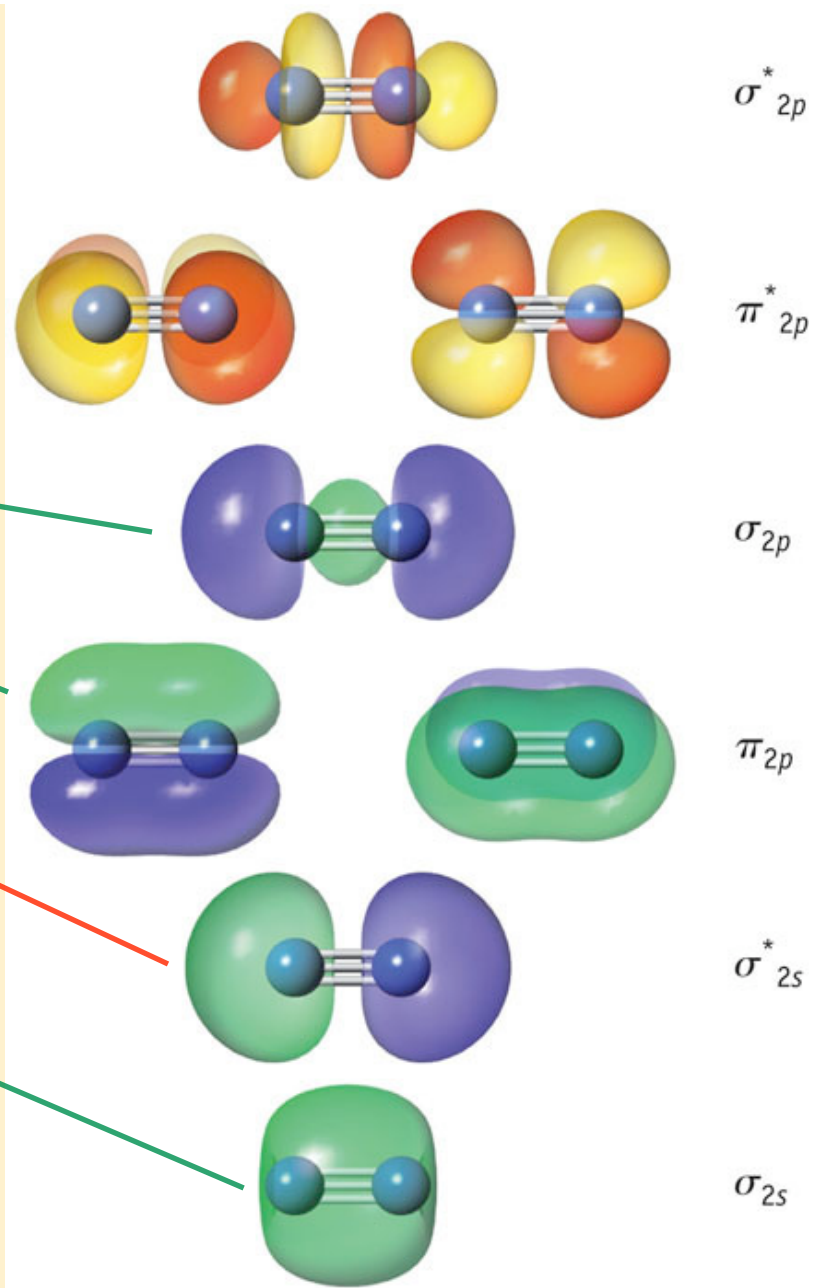


N_2 Molecular Orbitals

ENERGY

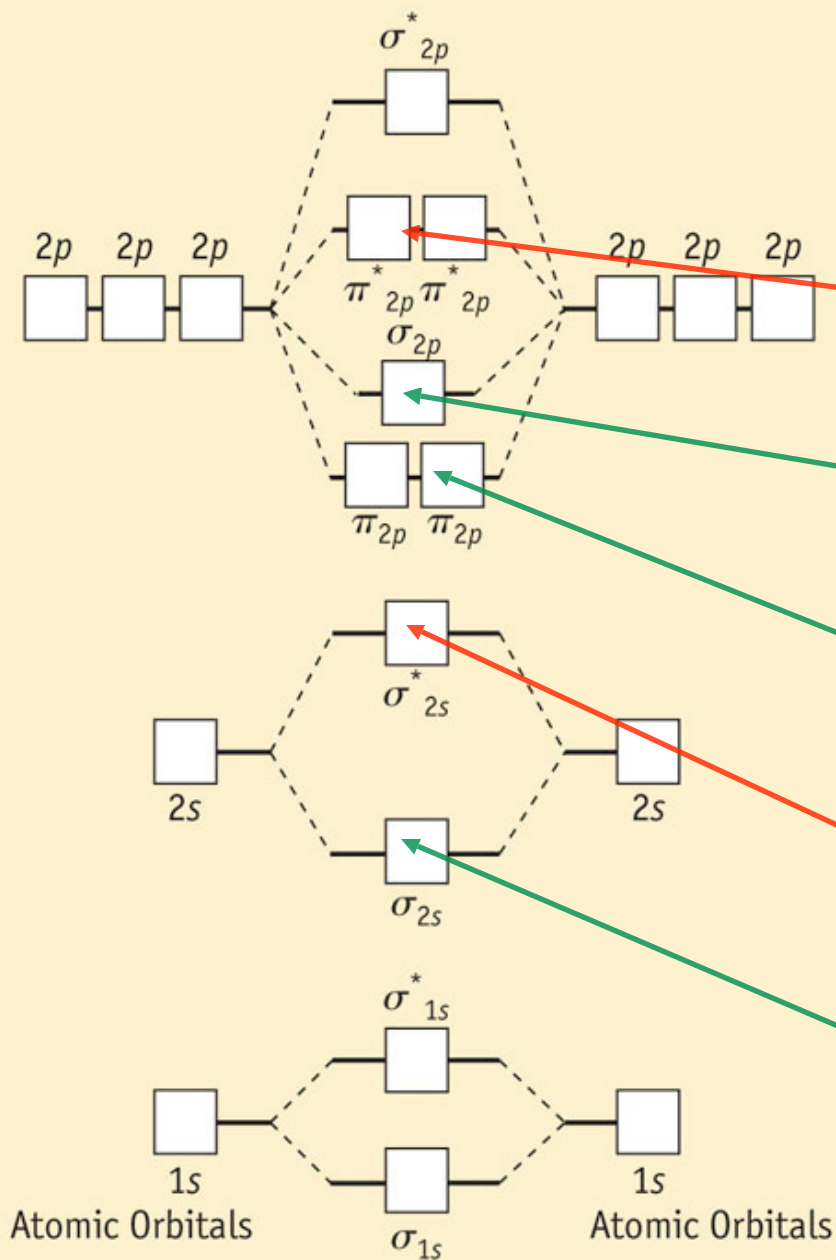


Molecular Orbitals for B_2 , C_2 , and N_2

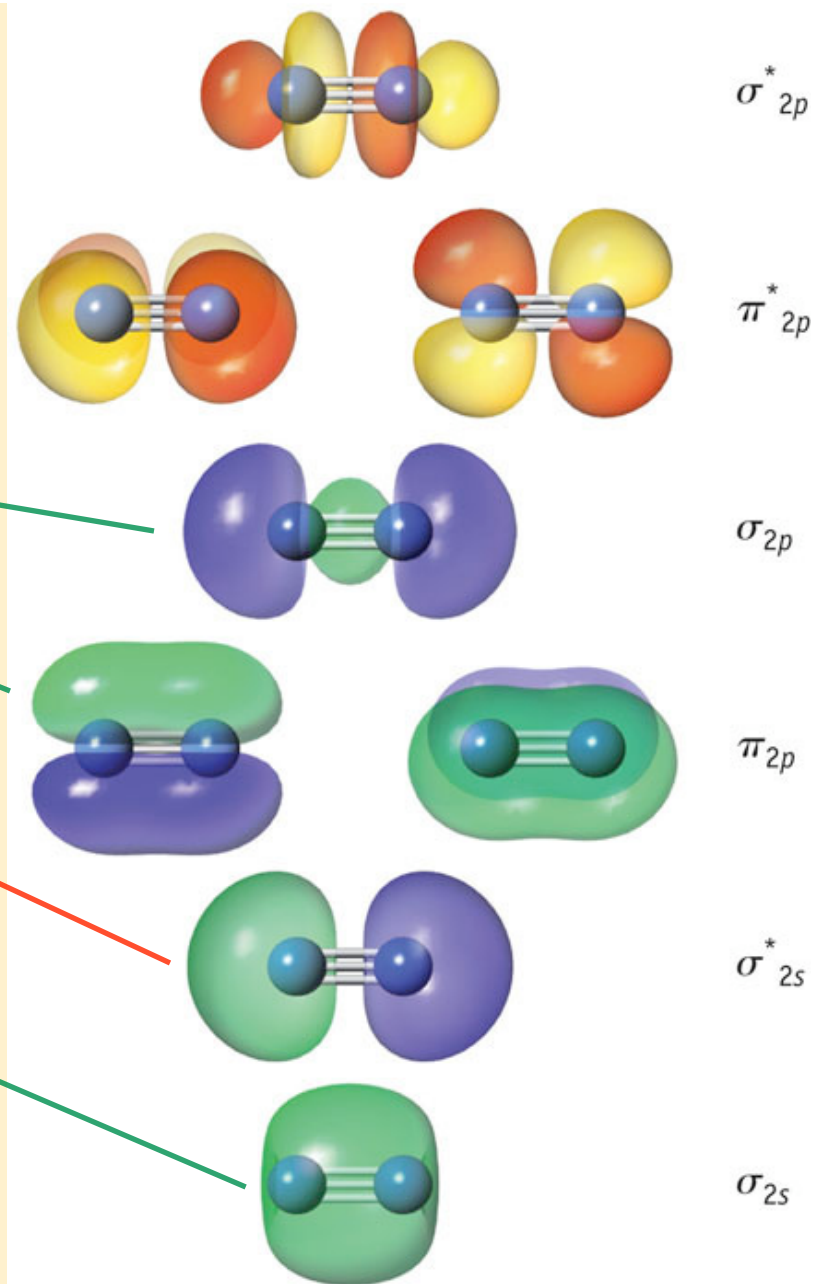


N_2 Molecular Orbitals

ENERGY

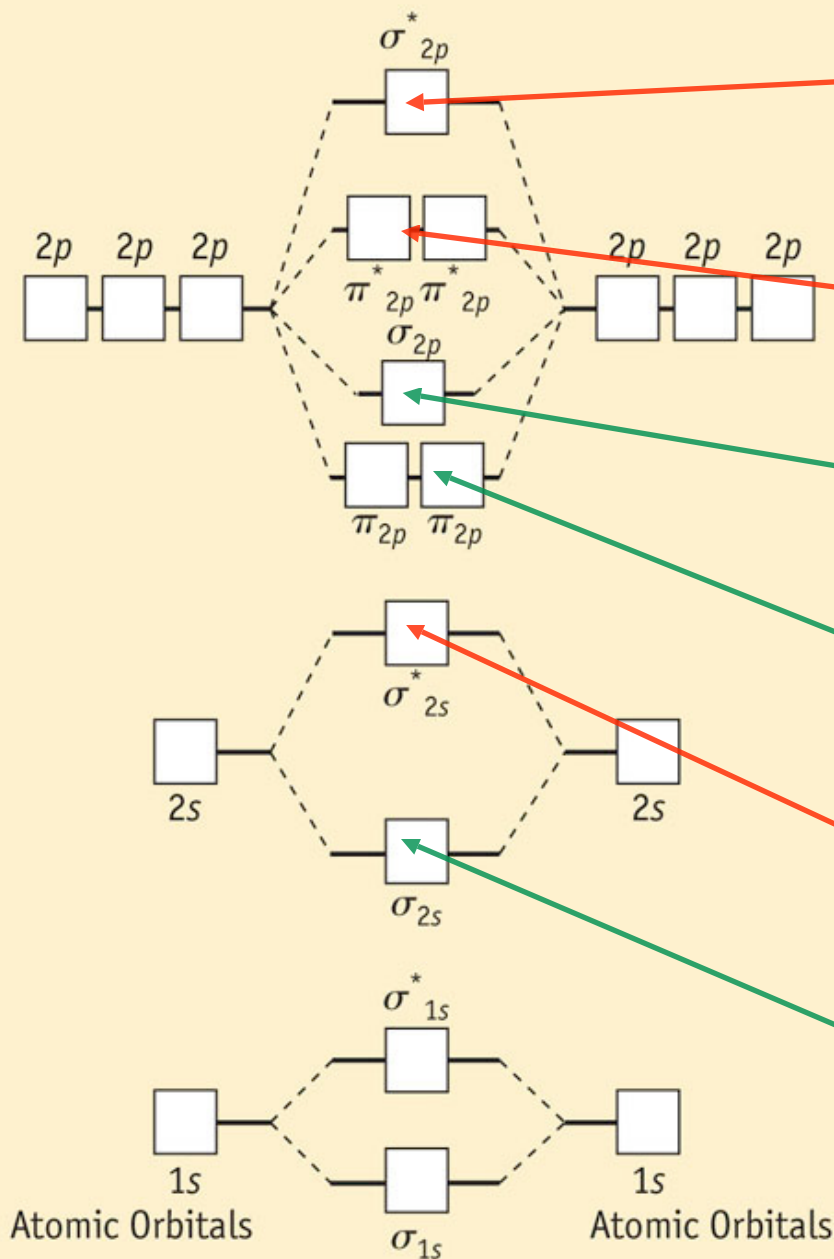


Molecular Orbitals for B_2 , C_2 , and N_2

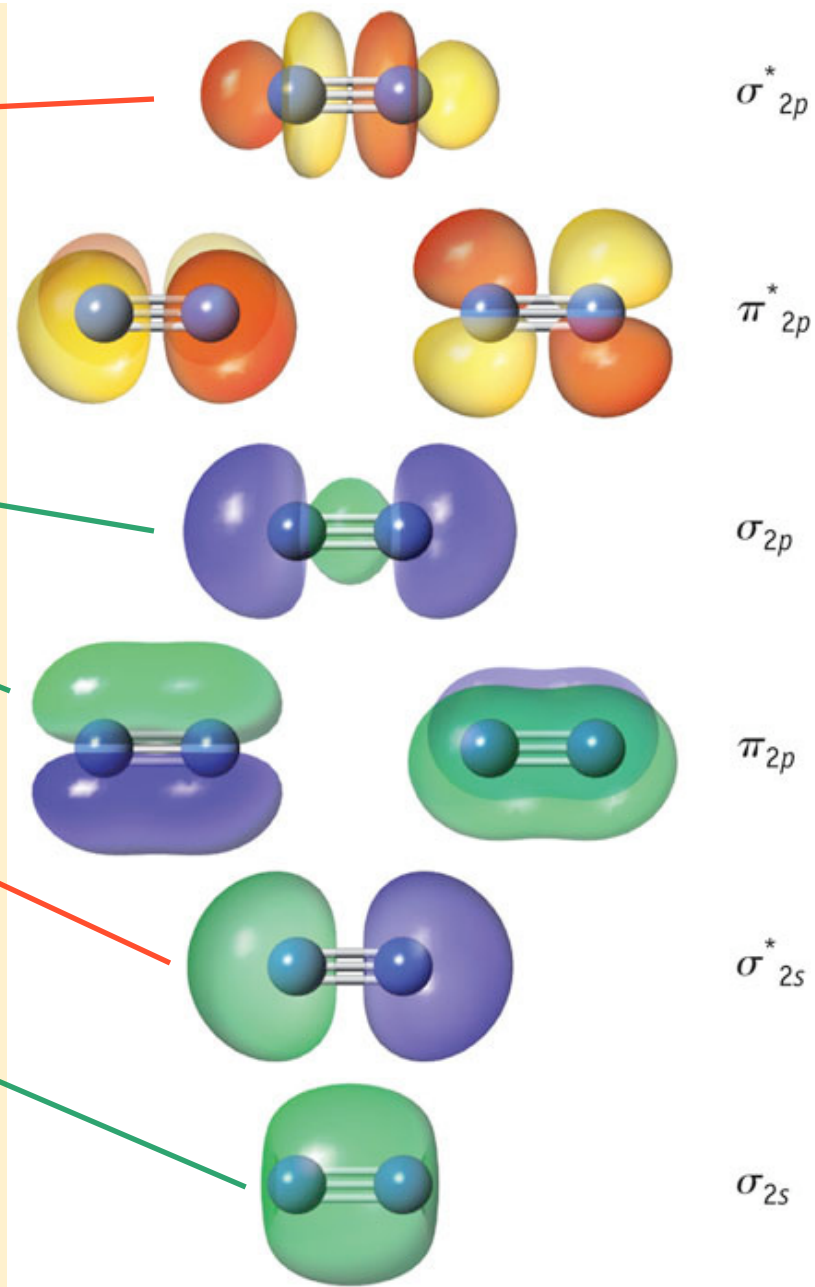


N_2 Molecular Orbitals

ENERGY

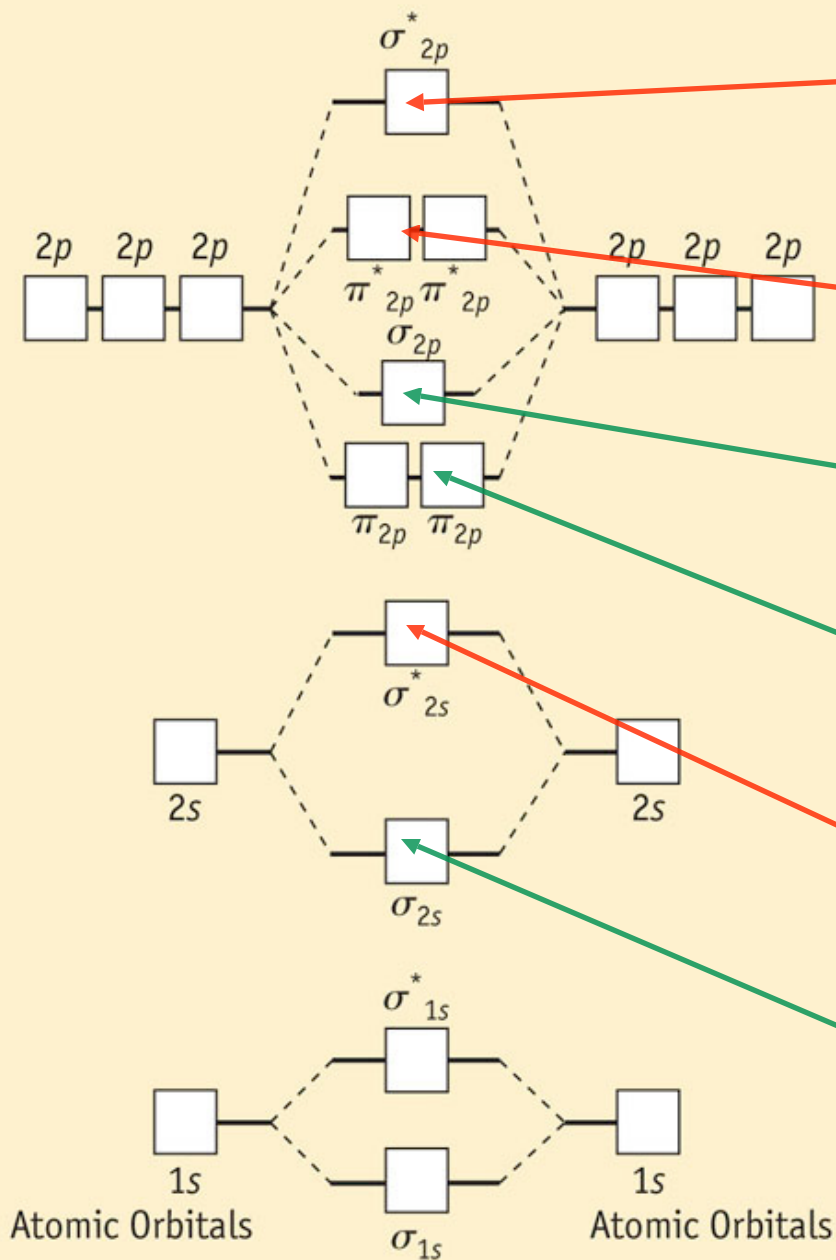


Molecular Orbitals for B_2 , C_2 , and N_2

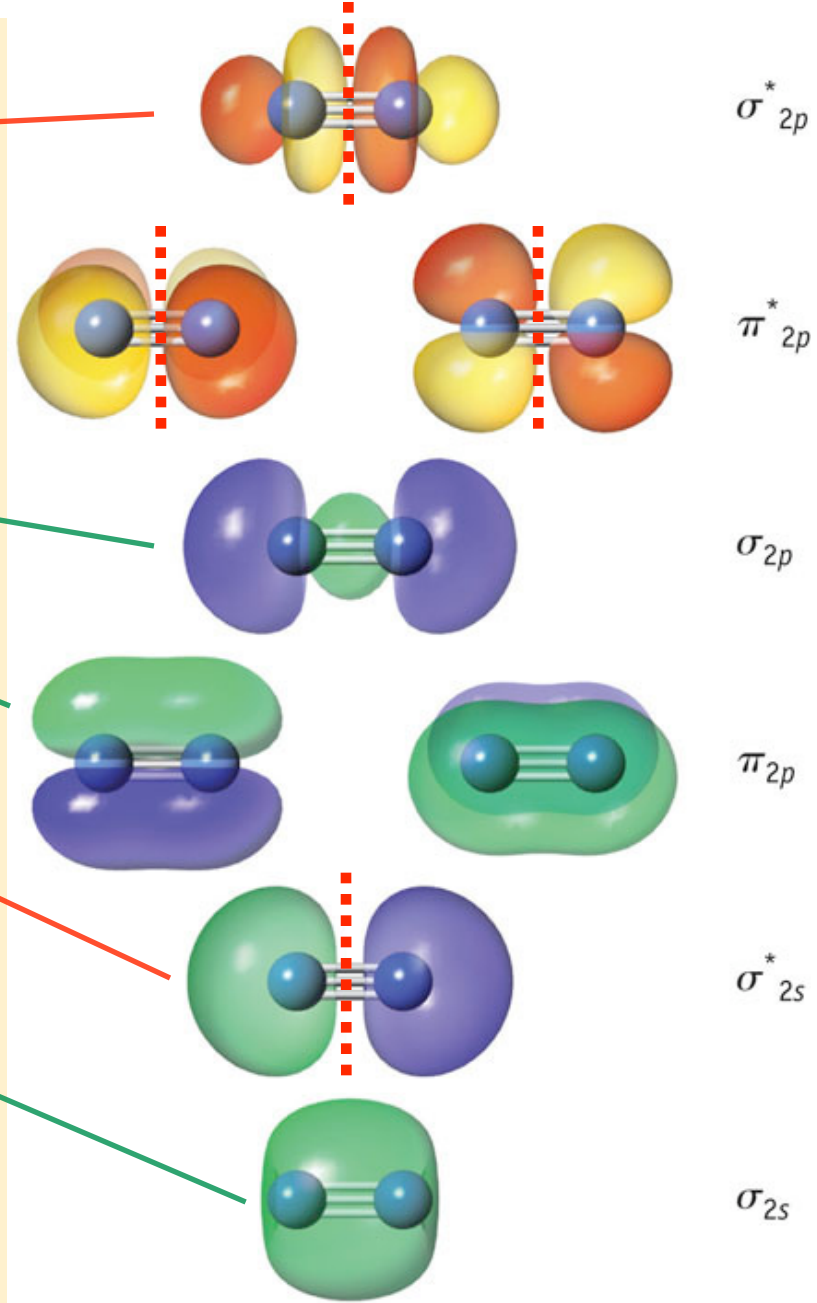


N_2 Molecular Orbitals

ENERGY

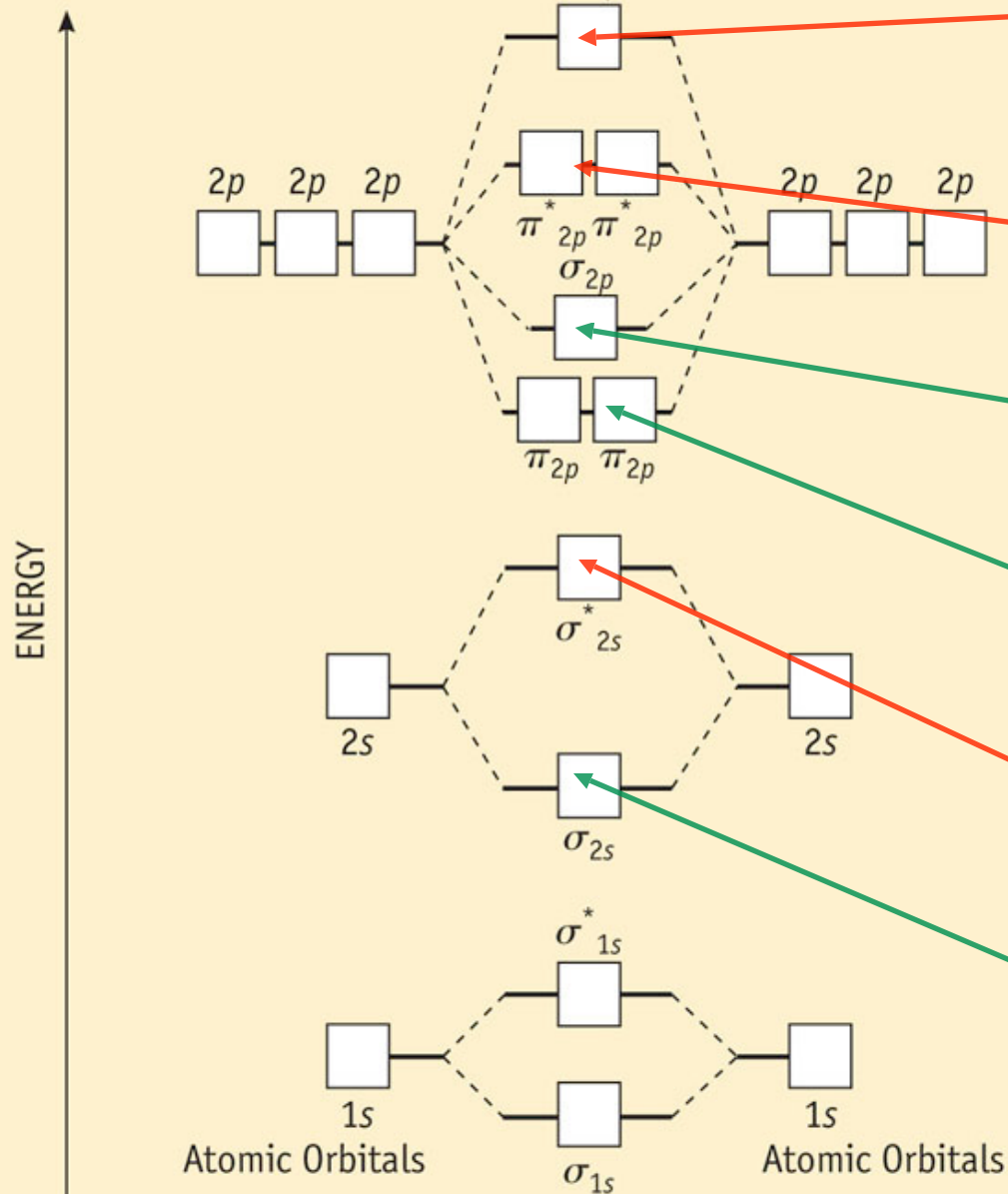


Molecular Orbitals for B_2 , C_2 , and N_2

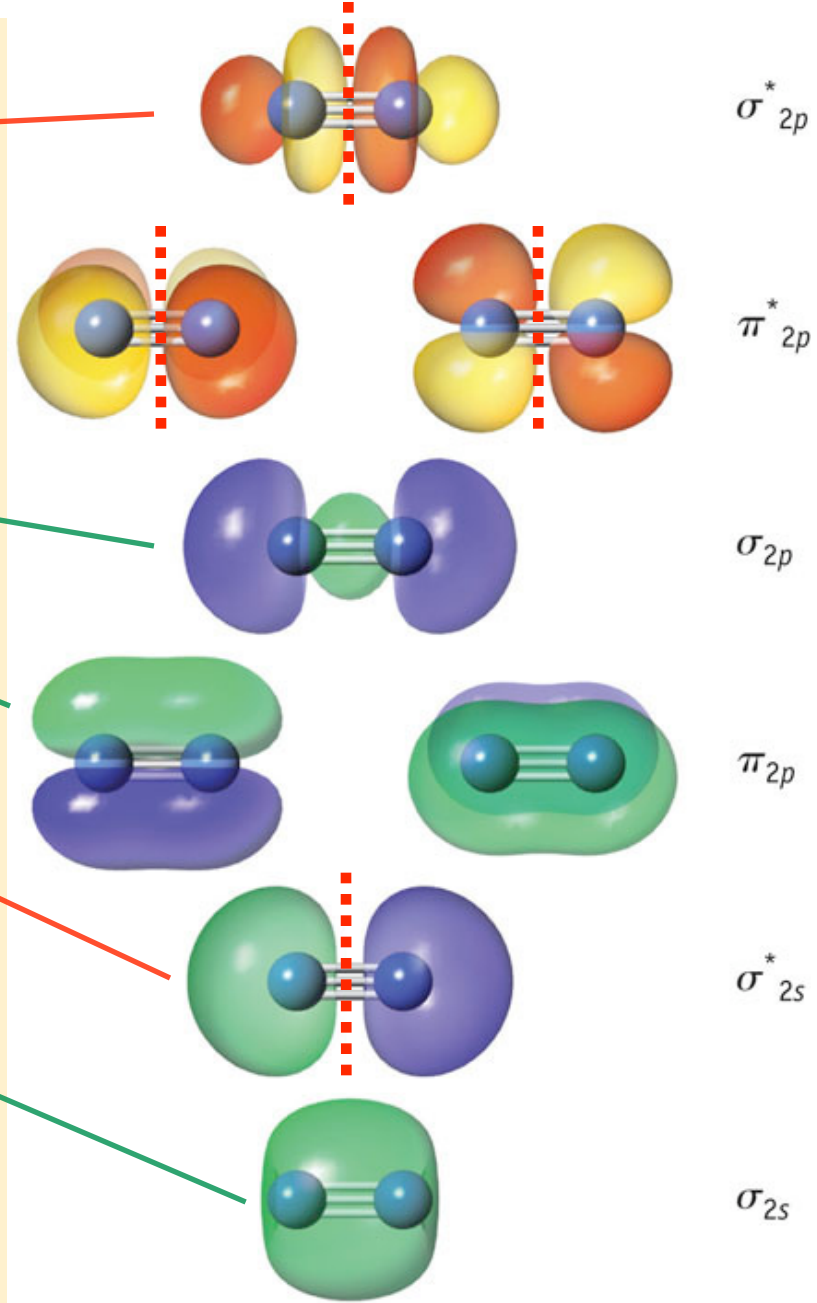


N_2 Molecular Orbitals

Each N brings 7 total electrons: 14 total

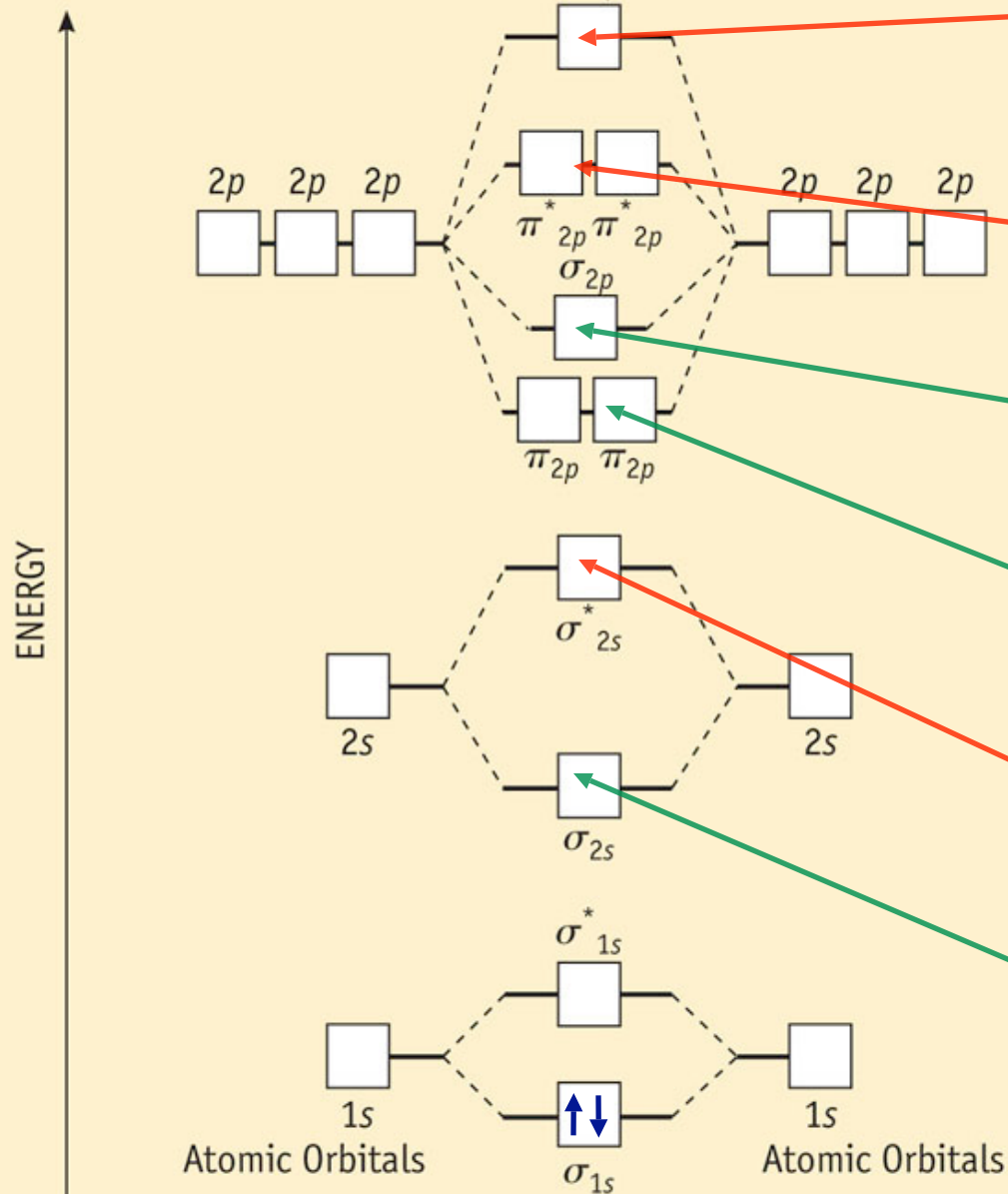


Molecular Orbitals for B_2 , C_2 , and N_2

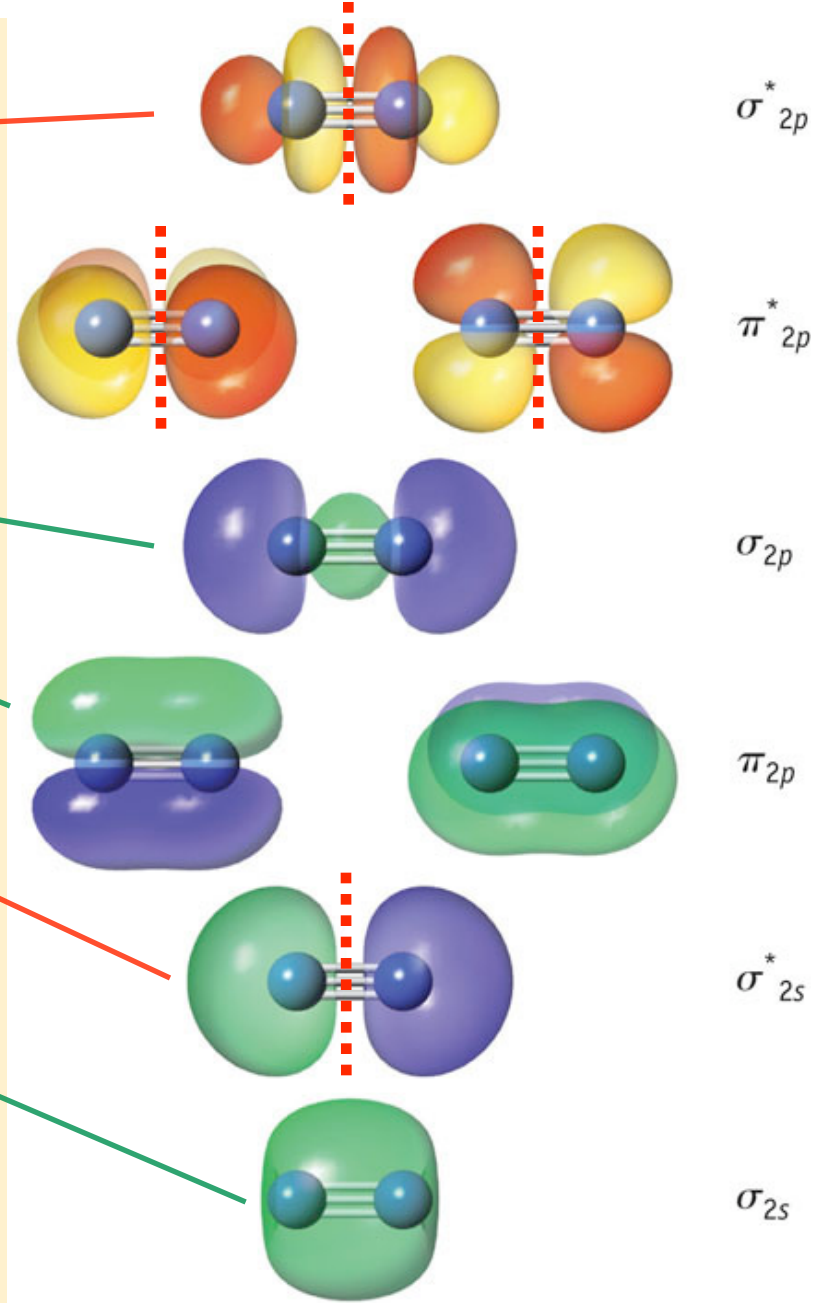


N_2 Molecular Orbitals

Each N brings 7 total electrons: 14 total

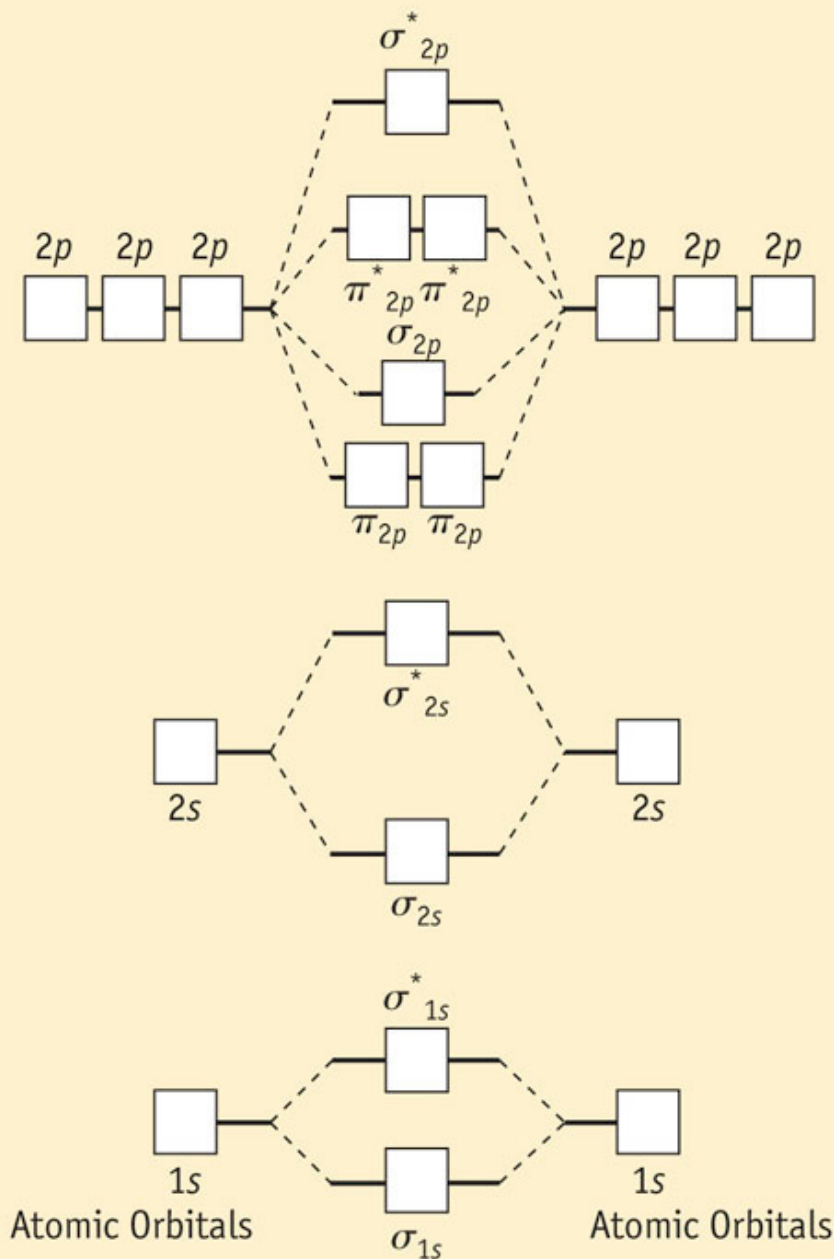


Molecular Orbitals for B_2 , C_2 , and N_2

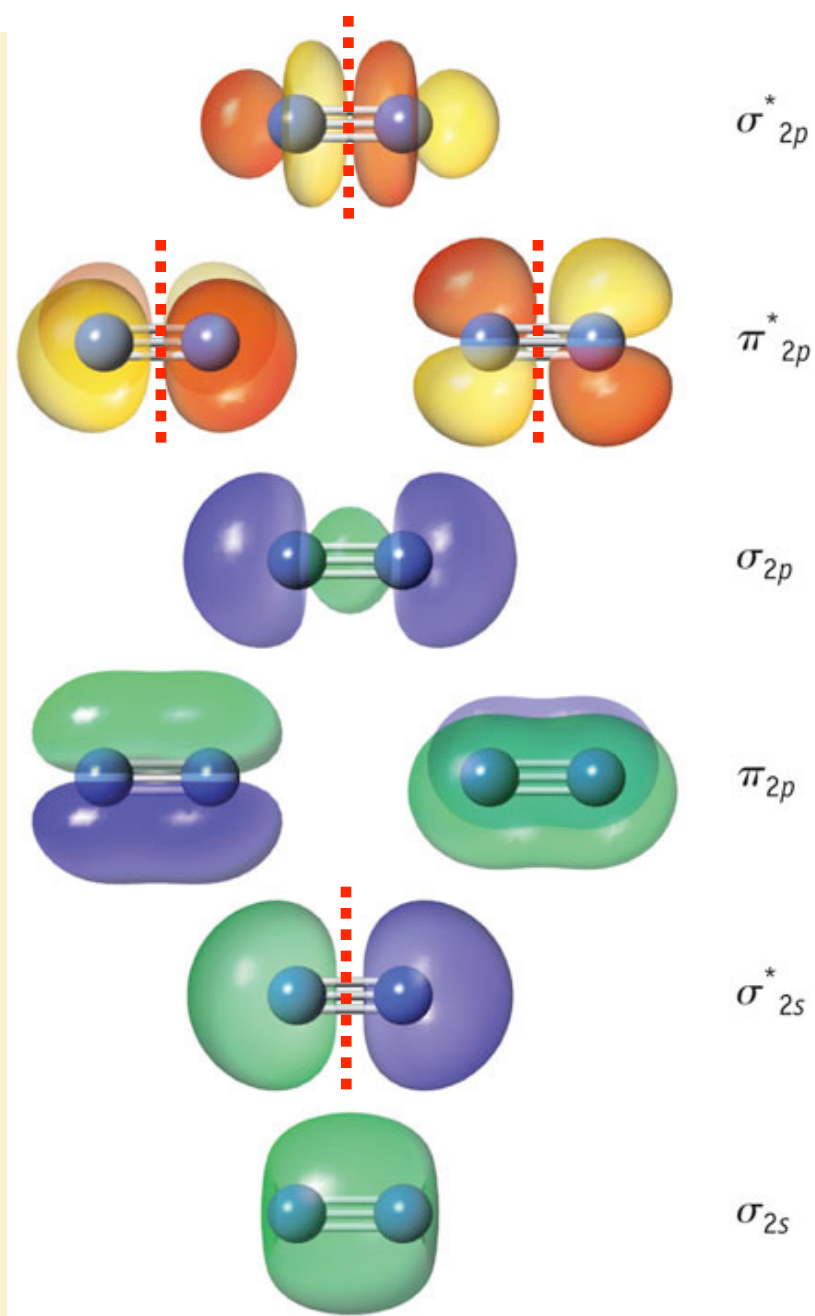


N_2 Molecular Orbitals

ENERGY



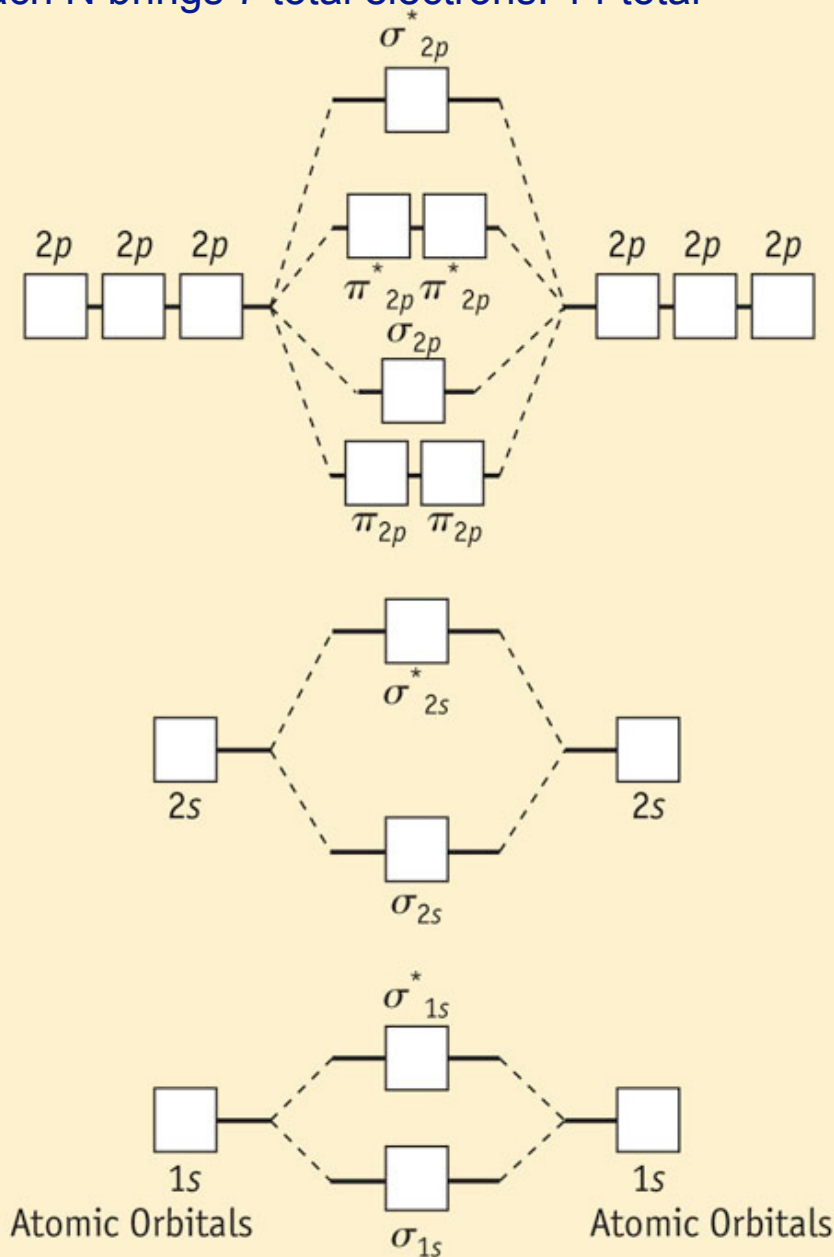
Molecular Orbitals for B_2 , C_2 , and N_2



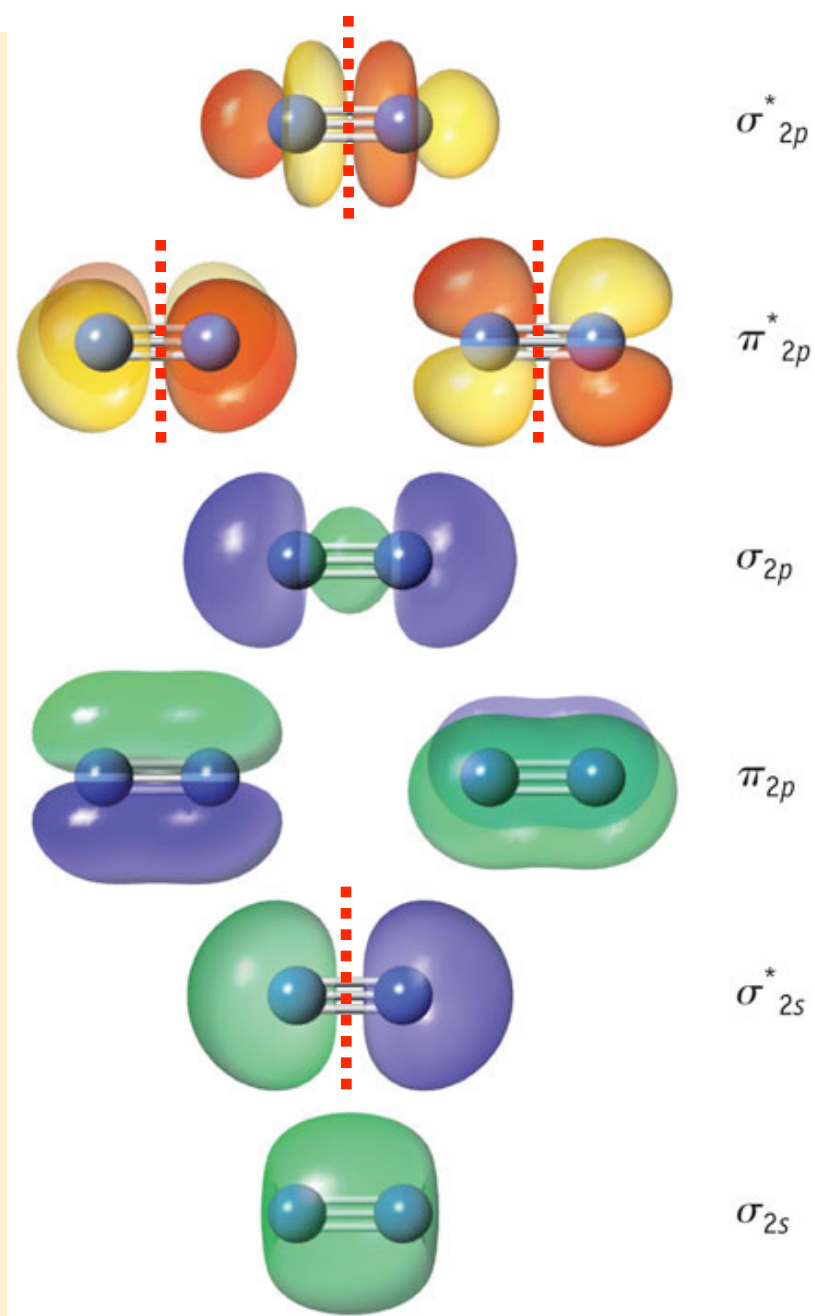
N_2 Molecular Orbitals

Each N brings 7 total electrons: 14 total

ENERGY

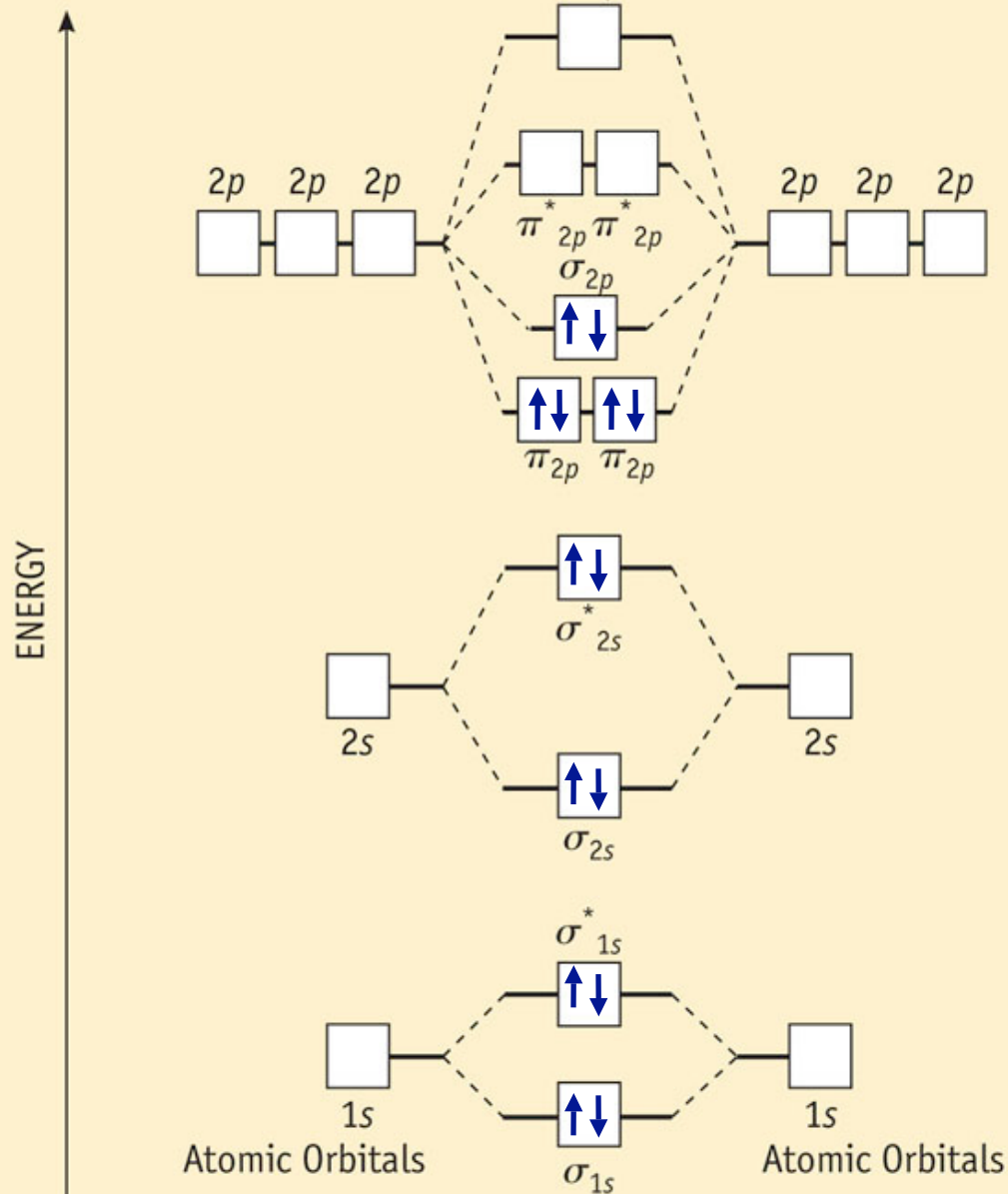


Molecular Orbitals for B_2 , C_2 , and N_2

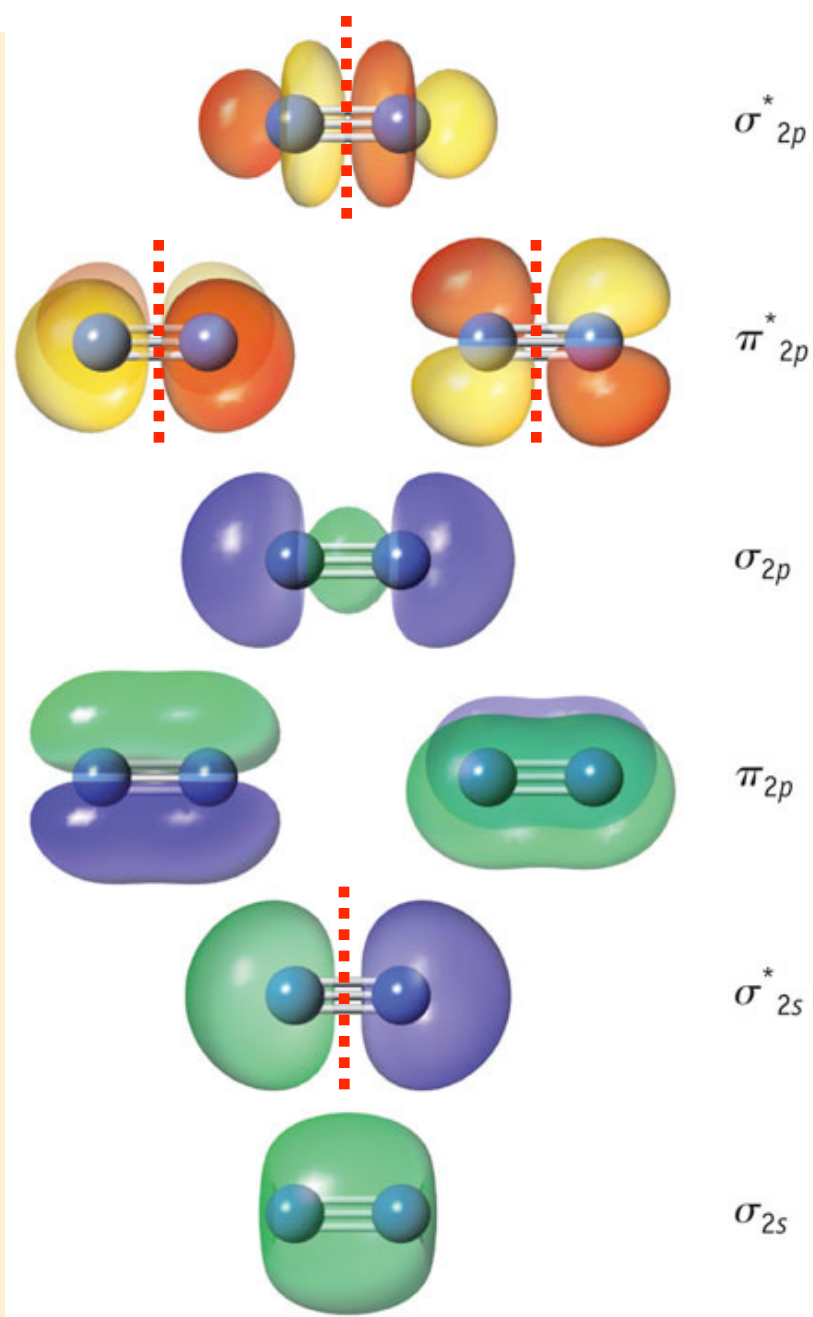


N_2 Molecular Orbitals

Each N brings 7 total electrons: 14 total

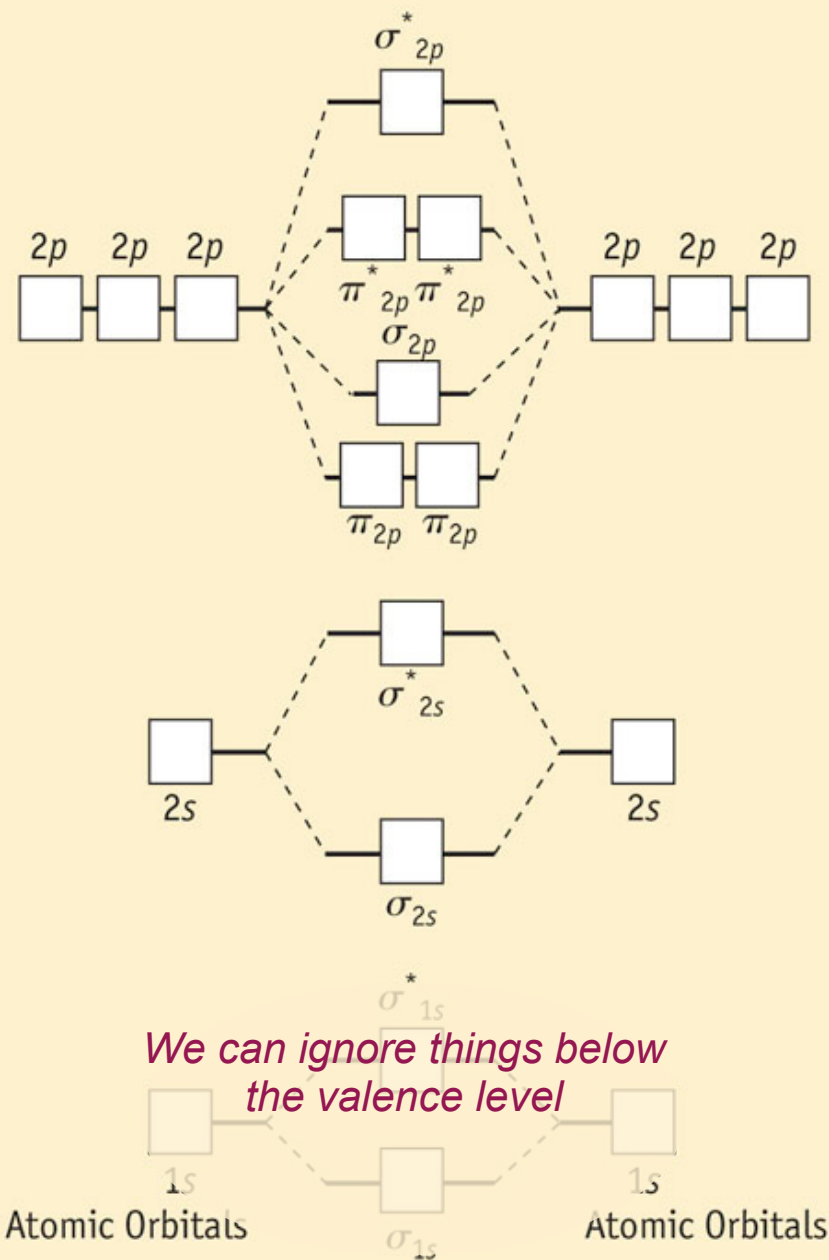


Molecular Orbitals for B_2 , C_2 , and N_2

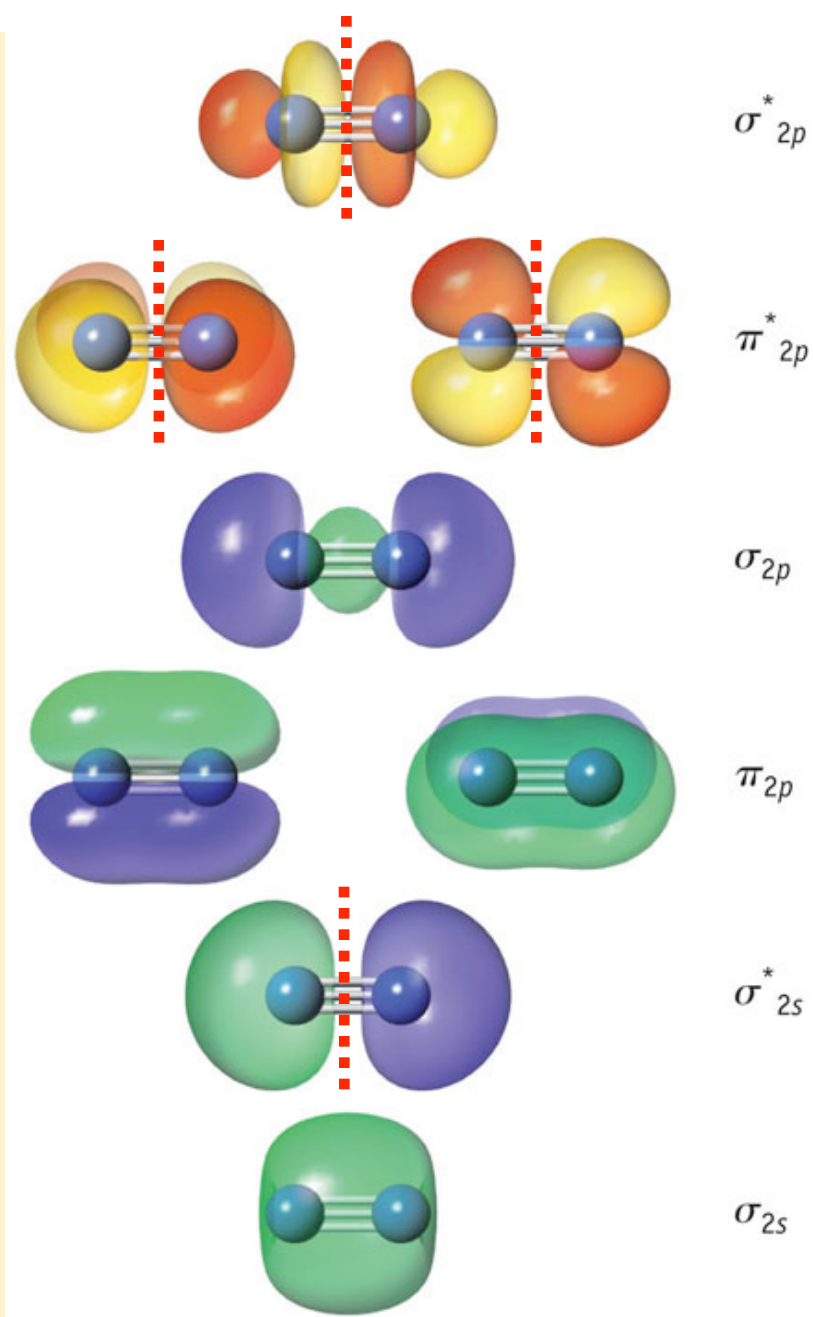


N_2 Molecular Orbitals

ENERGY



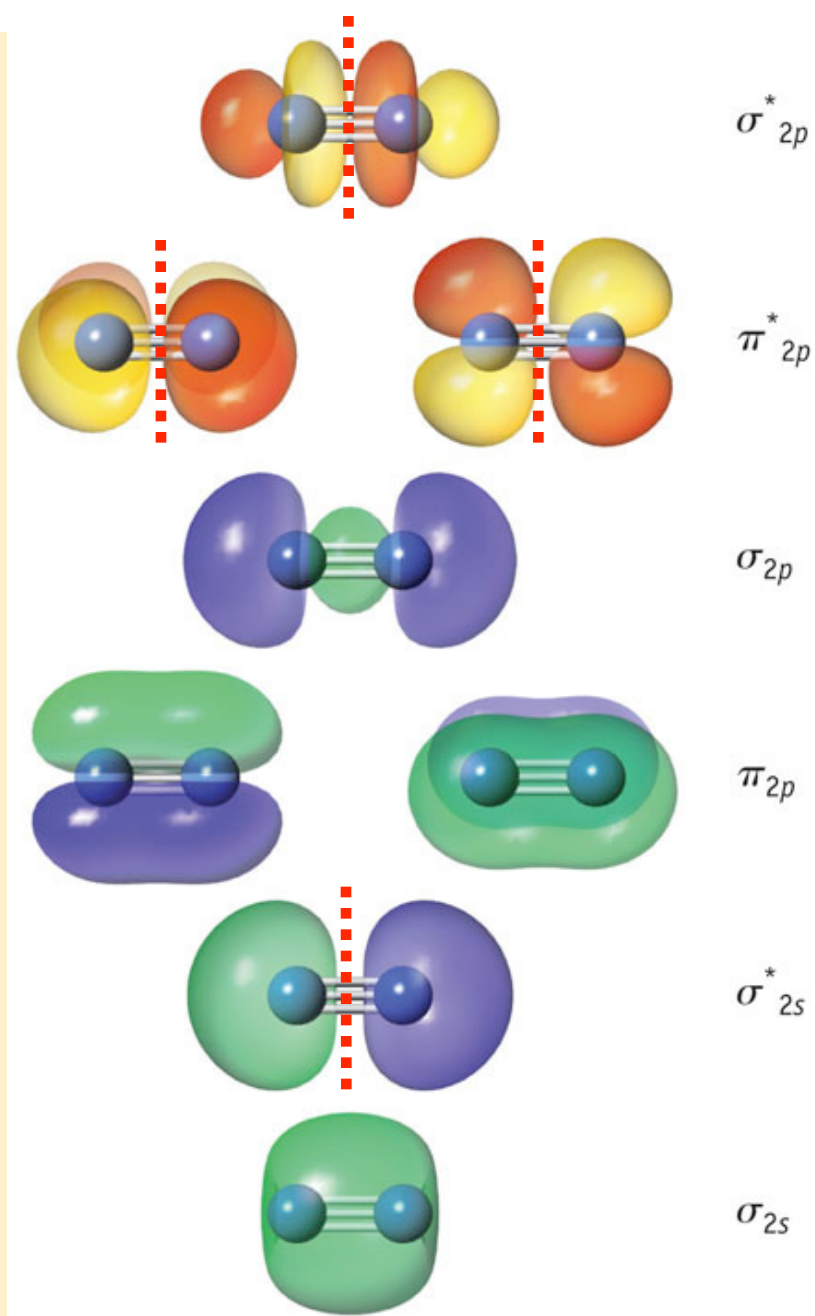
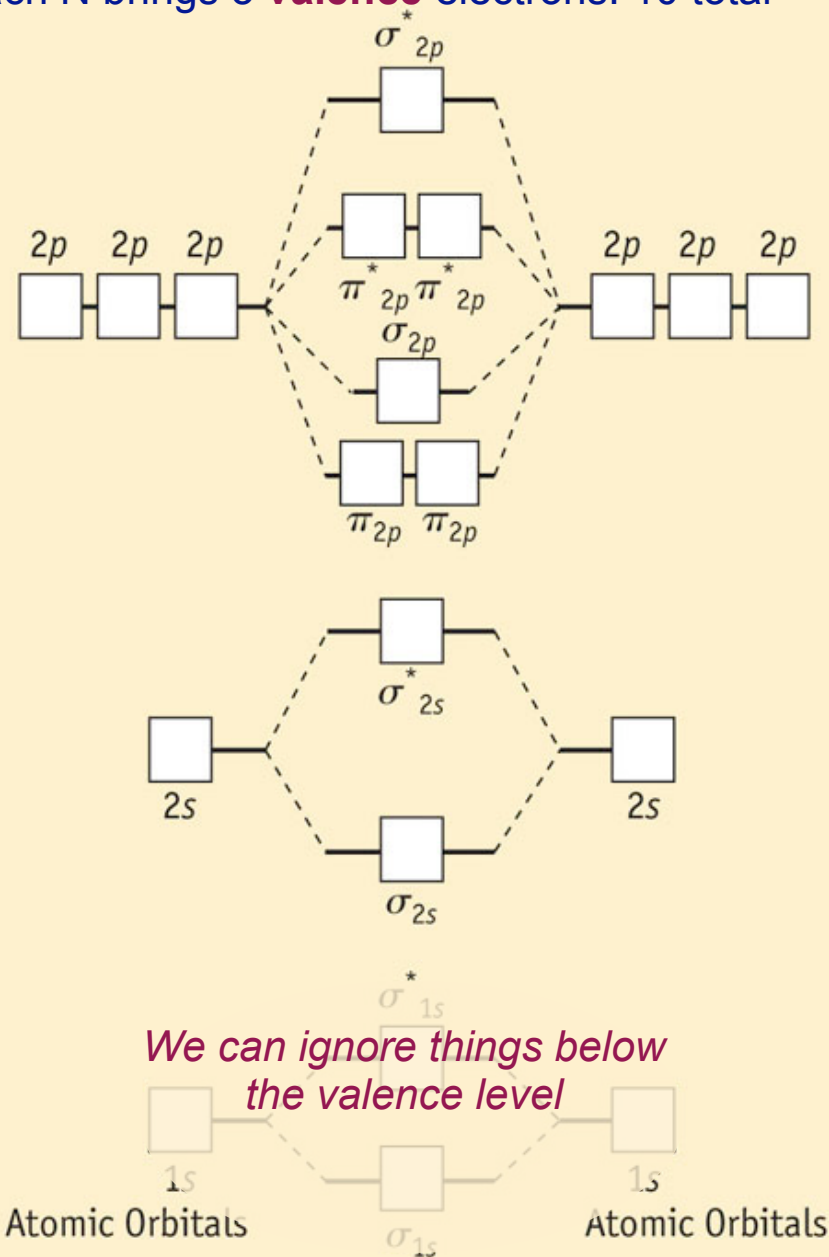
Molecular Orbitals for B_2 , C_2 , and N_2



N_2 Molecular Orbitals

Each N brings 5 **valence** electrons: 10 total

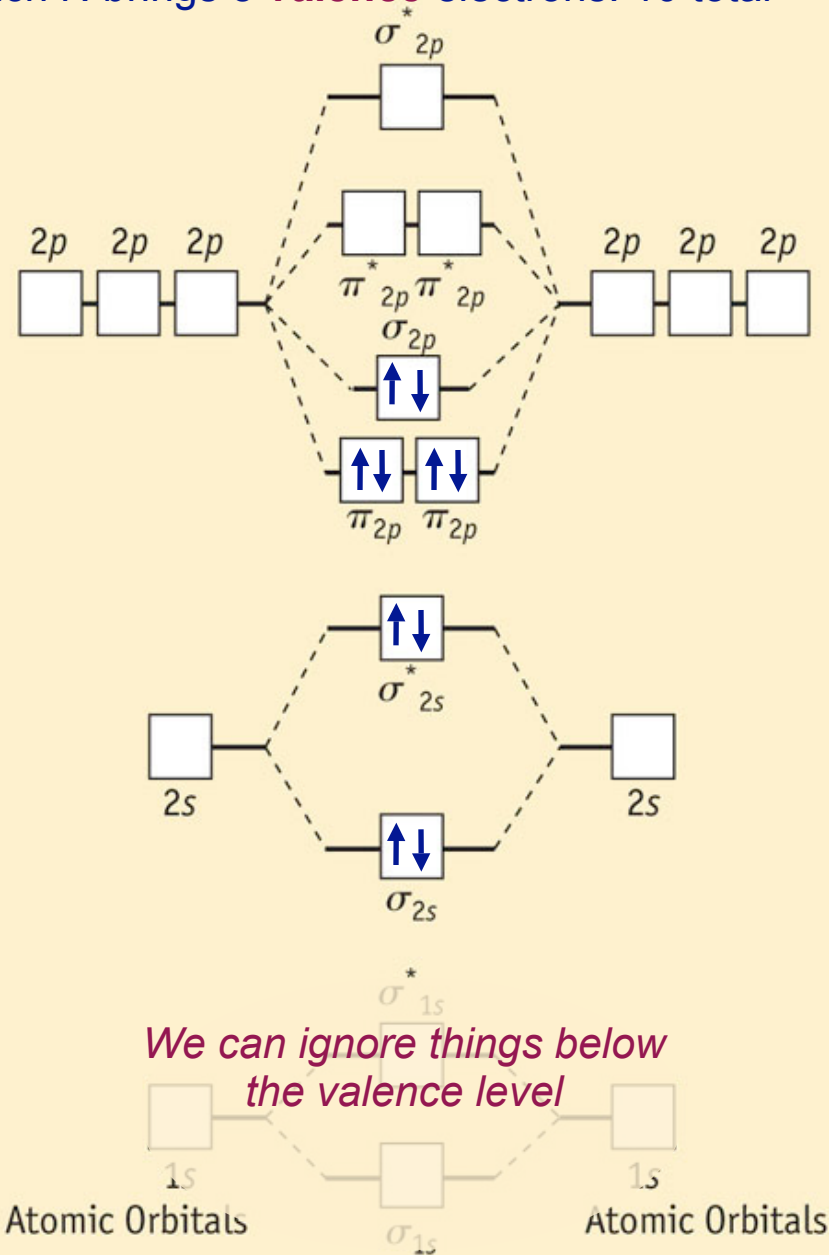
ENERGY



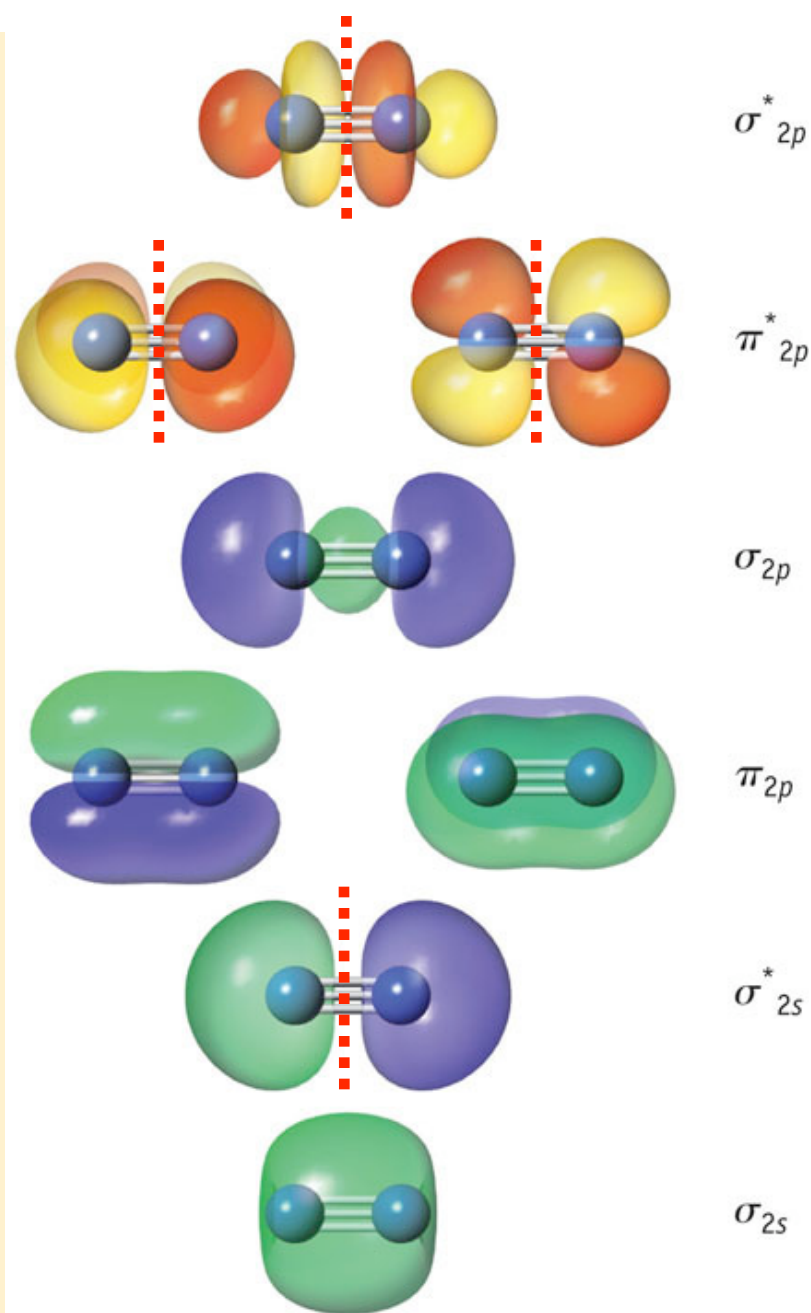
N_2 Molecular Orbitals

Each N brings 5 **valence** electrons: 10 total

ENERGY



Molecular Orbitals for B_2 , C_2 , and N_2



N_2 Molecular Orbitals

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

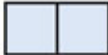
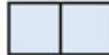
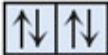
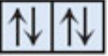
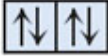
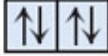
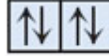
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}				σ^*_{2p}		
π^*_{2p}				π^*_{2p}		
σ_{2p}				π_{2p}		
π_{2p}				σ_{2p}		
σ^*_{2s}				σ^*_{2s}		
σ_{2s}				σ_{2s}		
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

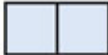
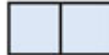
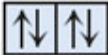
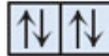
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s}						
σ_{2s} bonding						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

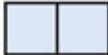
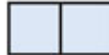
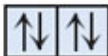
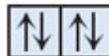
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s} antibonding						
σ_{2s} bonding						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear Diatomic Molecules of Second-Period Elements

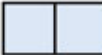
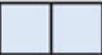
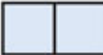
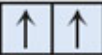
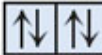
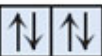
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s}						
σ_{2s}						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

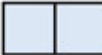
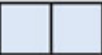
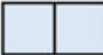
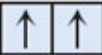
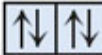
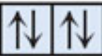
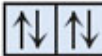
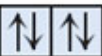
	1 bond					
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s}						
σ_{2s}						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

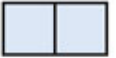
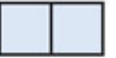
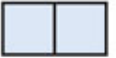
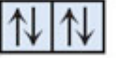
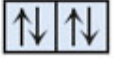
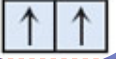
	1 bond	2 bonds			
	B ₂	C ₂	N ₂	O ₂	F ₂
σ^*_{2p}					
π^*_{2p}					
σ_{2p}					
π_{2p}					
σ^*_{2s}					
σ_{2s}					
Bond order	One	Two	Three	Two	One
Bond-dissociation energy (kJ/mol)	290	620	945	498	155
Bond distance (pm)	159	131	110	121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia	Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

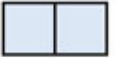
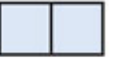
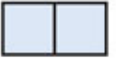
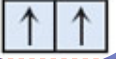
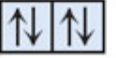
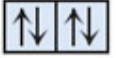
	1 bond	2 bonds	3 bonds			
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s}						
σ_{2s}						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

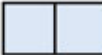
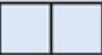
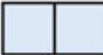
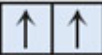
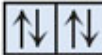
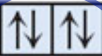
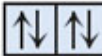
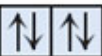
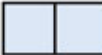
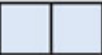
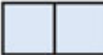
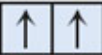
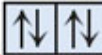
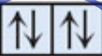
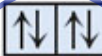
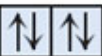
	1 bond	2 bonds	3 bonds		3-1=2	
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s}						
σ_{2s}						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia

TABLE 9.1 Molecular Orbital Occupations and Physical Data for Homonuclear

	1 bond	2 bonds	3 bonds		3-1=2	3-2=1
	B ₂	C ₂	N ₂		O ₂	F ₂
σ^*_{2p}						
π^*_{2p}						
σ_{2p}						
π_{2p}						
σ^*_{2s}						
σ_{2s}						
Bond order	One	Two	Three		Two	One
Bond-dissociation energy (kJ/mol)	290	620	945		498	155
Bond distance (pm)	159	131	110		121	143
Observed magnetic behavior (paramagnetic or diamagnetic)	Para	Dia	Dia		Para	Dia