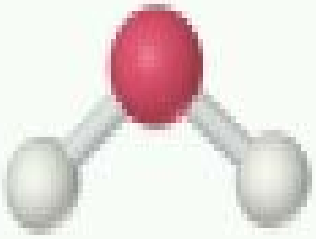
Moleküler Geometri

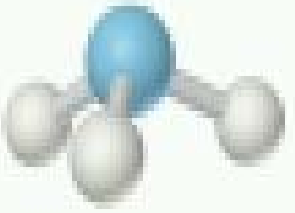
Bir molekülde; atomlar arası oluşan bağlar, çevre atomların merkez atom etrafında üç boyutlu yerleşme düzeni, bağlar arası açılar molekülün geometrisini (şeklini-yapısını) belirler. Molekül geometrisi molekülün fiziksel ve kimyasal özelliklerini belirler. Molekül geometrisini açıklamak için farklı kuramlar mevcuttur. modeller

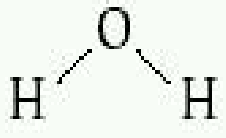
VSEPR Valens Bağ Teorisi Molekül Orbital Teori

Değerlik Kabuğu Elektron Çiftleri İtmesi (VSEPR) (Valence Shell Electron Pair Repulsion Theory)

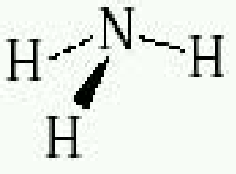
Molekül şeklini (geometrisini), merkez atom üzerindeki (bağ yapmış ve bağa katılmayan) elektron grupları üzerinden tahmin yapılabilir.



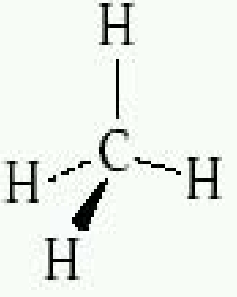




Water, H_2O



Ammonia, NH_3



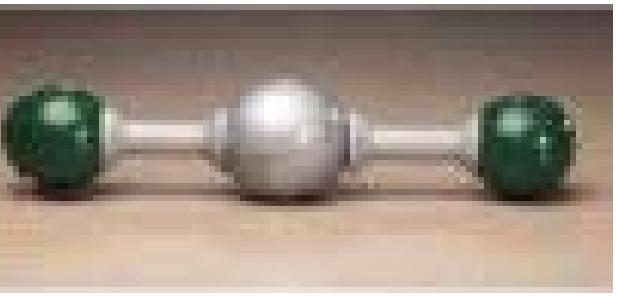
Methane, CH_4

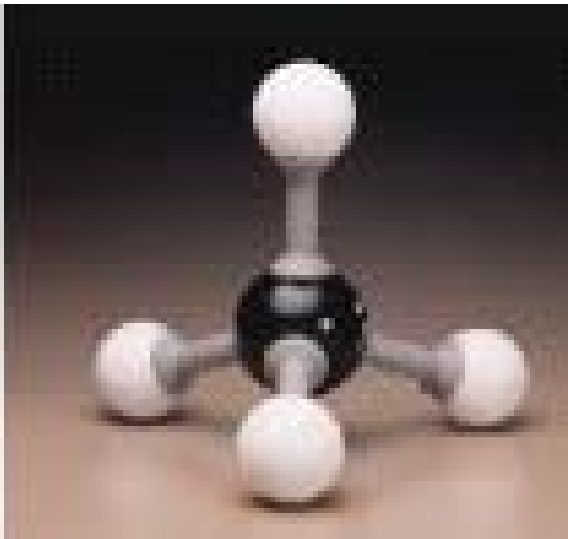
Elektron çiftleri (bağ yapmış ve bağa katılmayan) birbirlerini iterler. Bunun sonucunda, elektronlar birbirlerinden mümkün olduğunca uzakta yerleşirler (itme kuvvetlerinin en az olacak yerleşme düzeni)

- Son yörüngede 2 elektron çifti olması halinde **Çizgisel (lineer)**
- Son yörüngede 3 elektron çifti olması halinde **Üçgen düzlemsel**
- Son yörüngede 4 elektron çifti olması halinde **Düzgün dört yüzlü (tetrahedral)**
- Son yörüngede 5 elektron çifti olması halinde **Üçgen bipiramidal**
- Son yörüngede 6 elektron çifti olması halinde **Düzgün sekiz yüzlü (Oktahedral)**

Bağ yapmamış elektron çiftlerinin diğer elektron çiftlerini itme gücü, bağ elektronlarının itme gücünden daha yüksektir.

Elektron çiftleri birbirleri arasındaki itme kuvvetlerinin en az olacağı geometride yerleşir



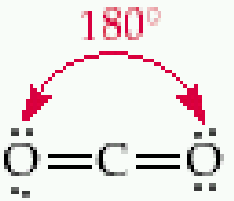


VSEPR teorisinin uygulanması

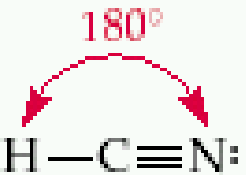
- Molekül veya iyon için Lewis yapısı çizilir.
- Merkez atomun bağ yapmamış elektron çifti sayısı ile tekli bağ sayısı belirlenir.
- $B_{\delta} + N_{o}$
- Elektron çifti sayısına karşılık gelen elektron çifti geometrisi belirtilir.
- molekül geometrisi bulunur.

VSEPR teorisine göre CO_2 HCN CH_4, NH_3 SO_2 PCl_5, SF_6 and H_2O bileşiklerinin şekillerini açıklayınız.

A CO_2 molecule is linear, with a bond angle of 180°.

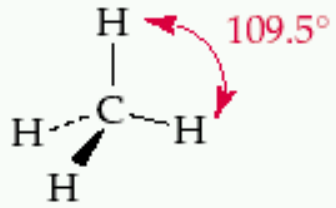


An HCN molecule is linear, with a bond angle of 180°.

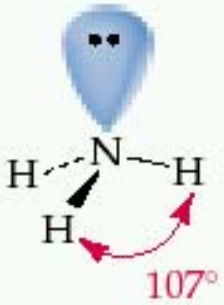


VSEPR teorisine göre CO_2 HCN CH_4, NH_3 SO_2 PCl_5, SF_6 and H_2O bileşiklerinin şekillerini açıklayınız.

A methane molecule is tetrahedral, with bond angles of 109.5°.



An ammonia molecule is trigonal pyramidal, with bond angles of 107°.



A water molecule is bent, with a bond angle of 104.5°.

İtme Kuvveti

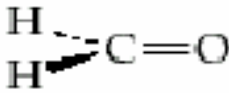
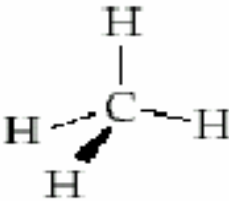
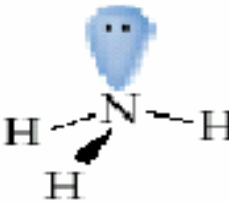
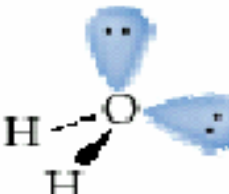
Bağ yapmamış e- Bağ yapmamış e> Bağ yapmamış e-bağ e > bağ e - bağ e

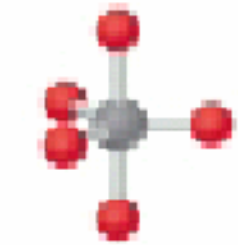
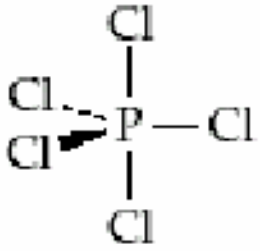
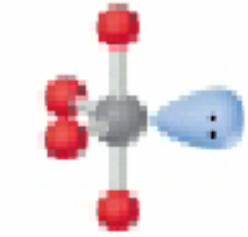
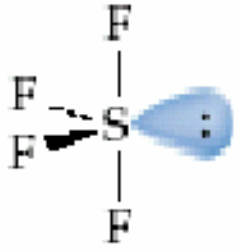
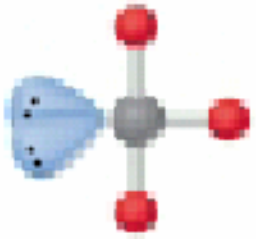
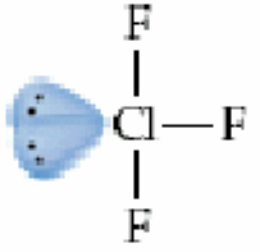
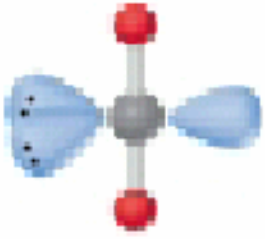
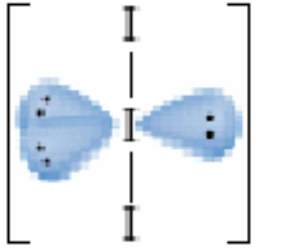
Bağ yapmamış e çiftleri molekülün yapısının belirlenmesinde bağa katılan elektronlar kadar önemlidir.

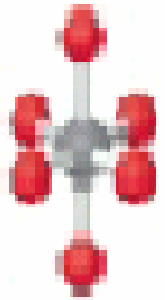
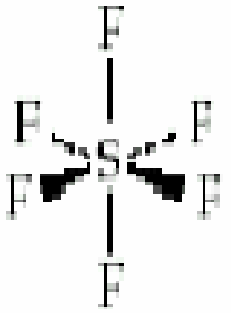
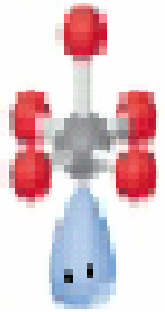
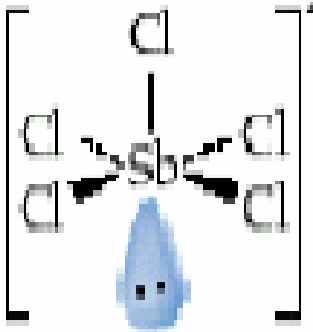
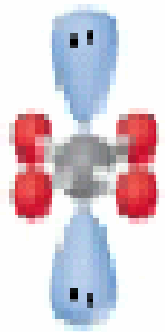
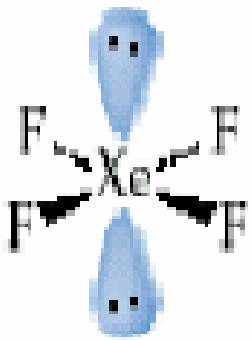
Bağ yapmamış elektronlar bağ elektronlarından daha fazla yer kaplarlar.

Merkez atom üzerinde bağ yapmamış elektron çifti mevcut ise, elektron çiftlerinin yerleşim düzeni,olduğu tüm elektron çiftlerinin bağ elektronları geometrik şekilden farklı olacaktır.

Bağ açıları molekülde bağ yapmayan elektron çiftleri sayısı arttıkça azalır.

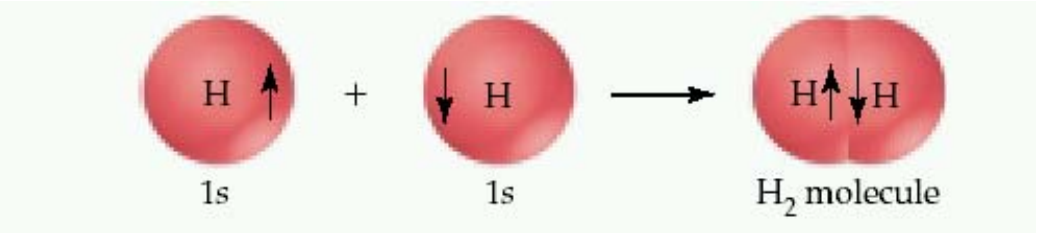
Bağ sayısı	Bağ yapmamış e çifti		molekül geometrisi	
2	0	2	 çizgisel	
3	0	3	 Üçgen düzlemsel	
2	1		 Açısal	
4	0	4	 Düzgün dörtyüzlü (Tetrahedral)	
3	1		 Üçgen piramidal	
2	2		 Açısal	

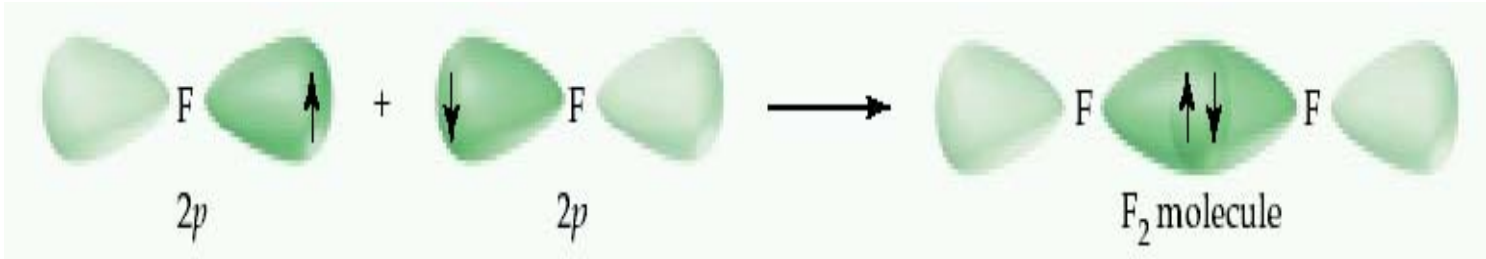
Bağ sayısı	Bağ yapmamış e çifti		molekül geometrisi	
5	0	5	 Üçgen bipiramidal	
4	1		 Tahterevalli	
3	2		 T şeklinde	
2	3		 Açısal	

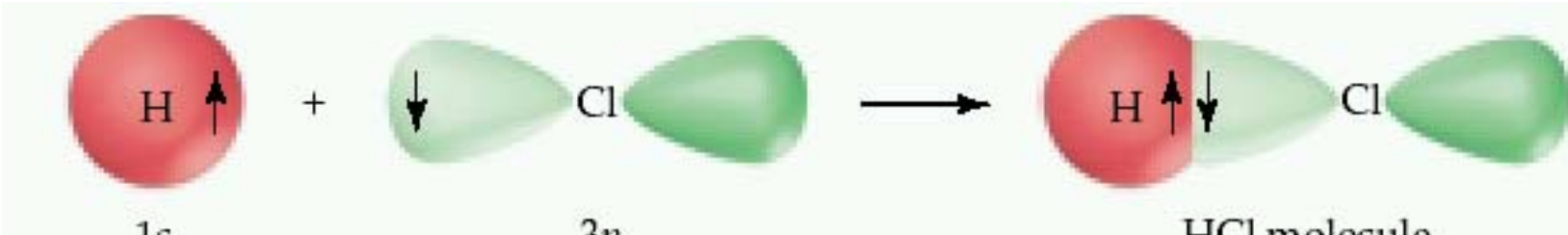
ğ sayısı	Bağ yapmamış e çifti		molekül geometrisi	
6	0	6	 Düzgün sekizyüzlü (oktahedral)	
5	1		 Kare piramidal	
4	2		 Kare Düzlemsel	

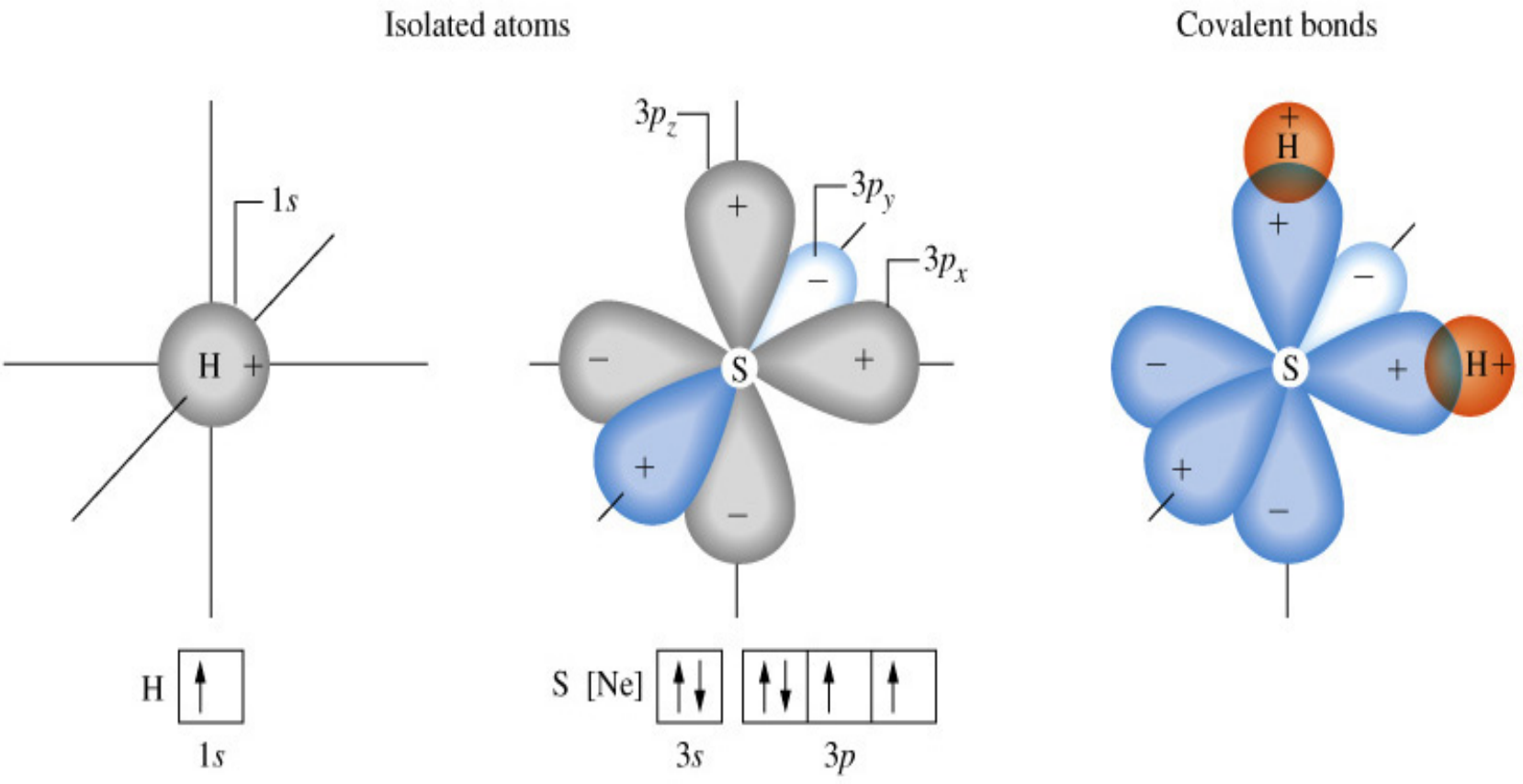
Valens (Değerlik) Bağ Teorisi

Kovalent bağ, iki atomun tek elektronlu orbitallerinin uygun şekilde üstüste çakışması (örtüşmesi) sonucunda (elektronların zıt spinli bir şekilde bu orbitalleri doldurması ile) oluşur.



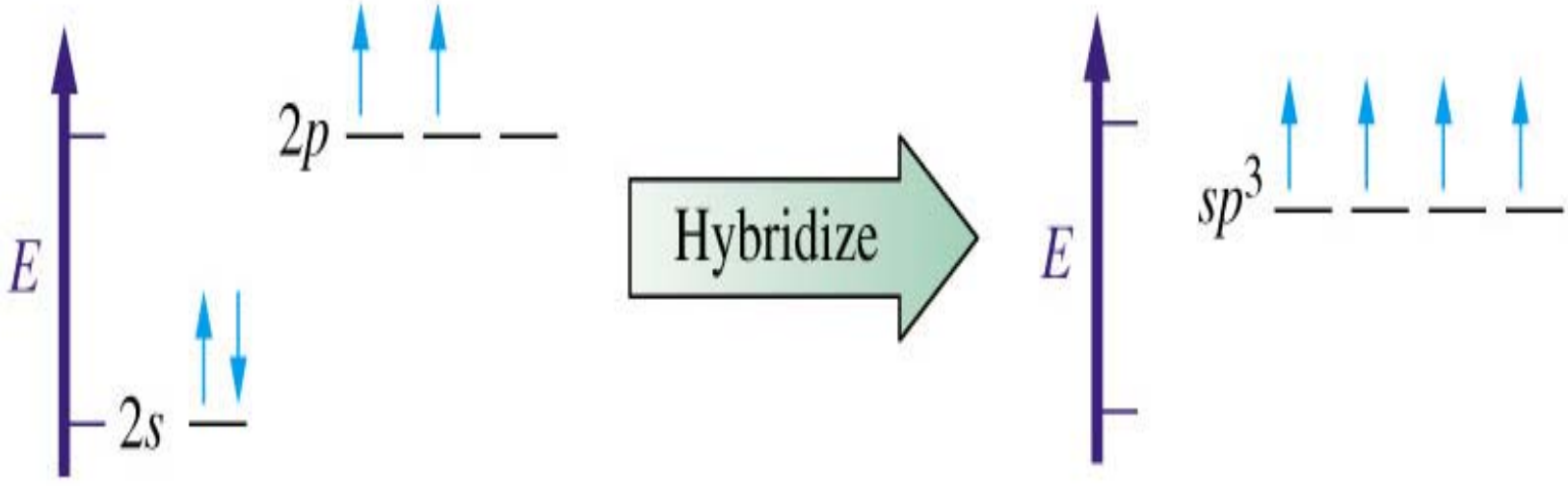


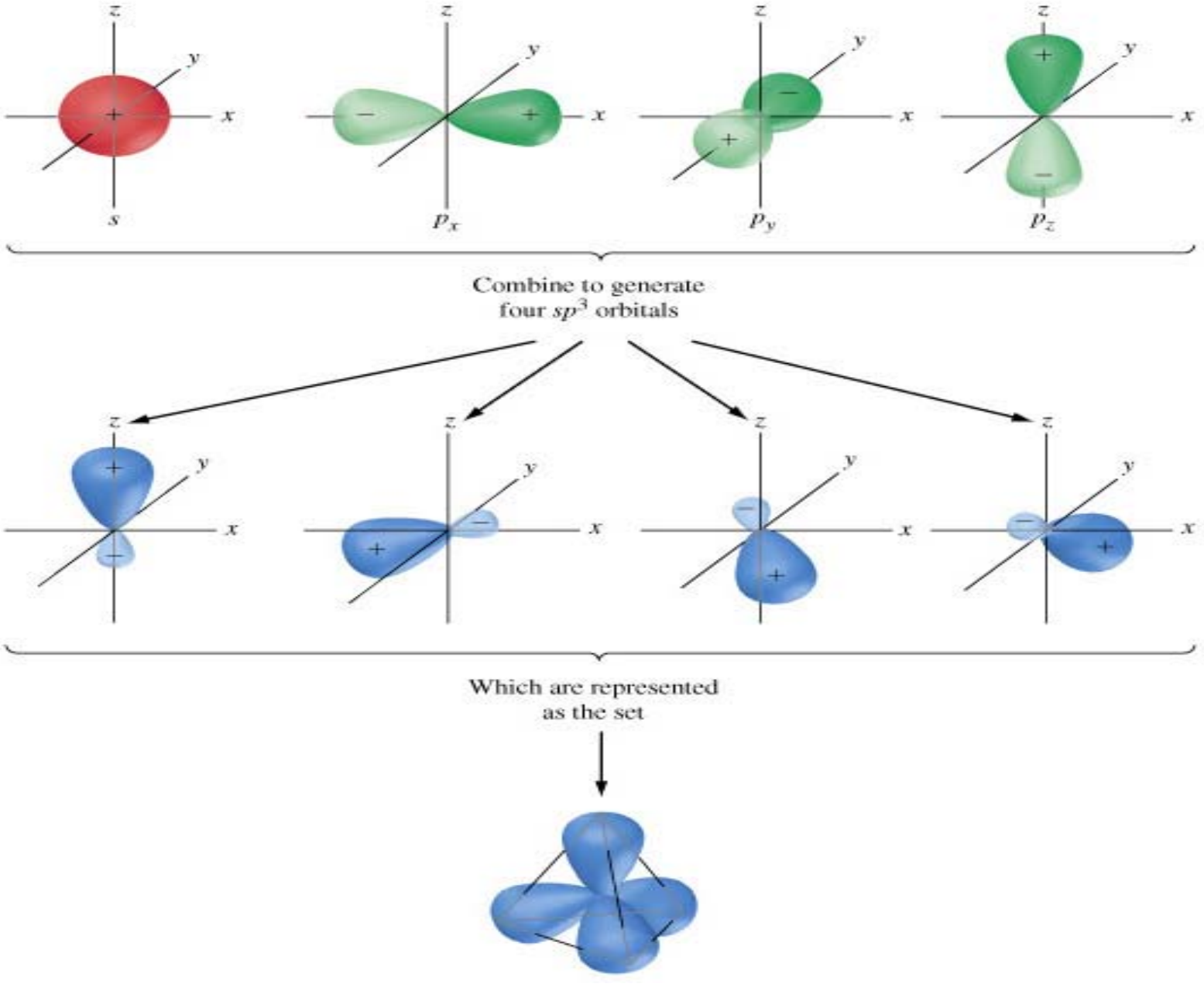



Isolated atoms
Covalent bonds
1s
H
+
H
1s
3p_z
3p_y
3p_x
S
S [Ne]
3s
3p
H
+
H+

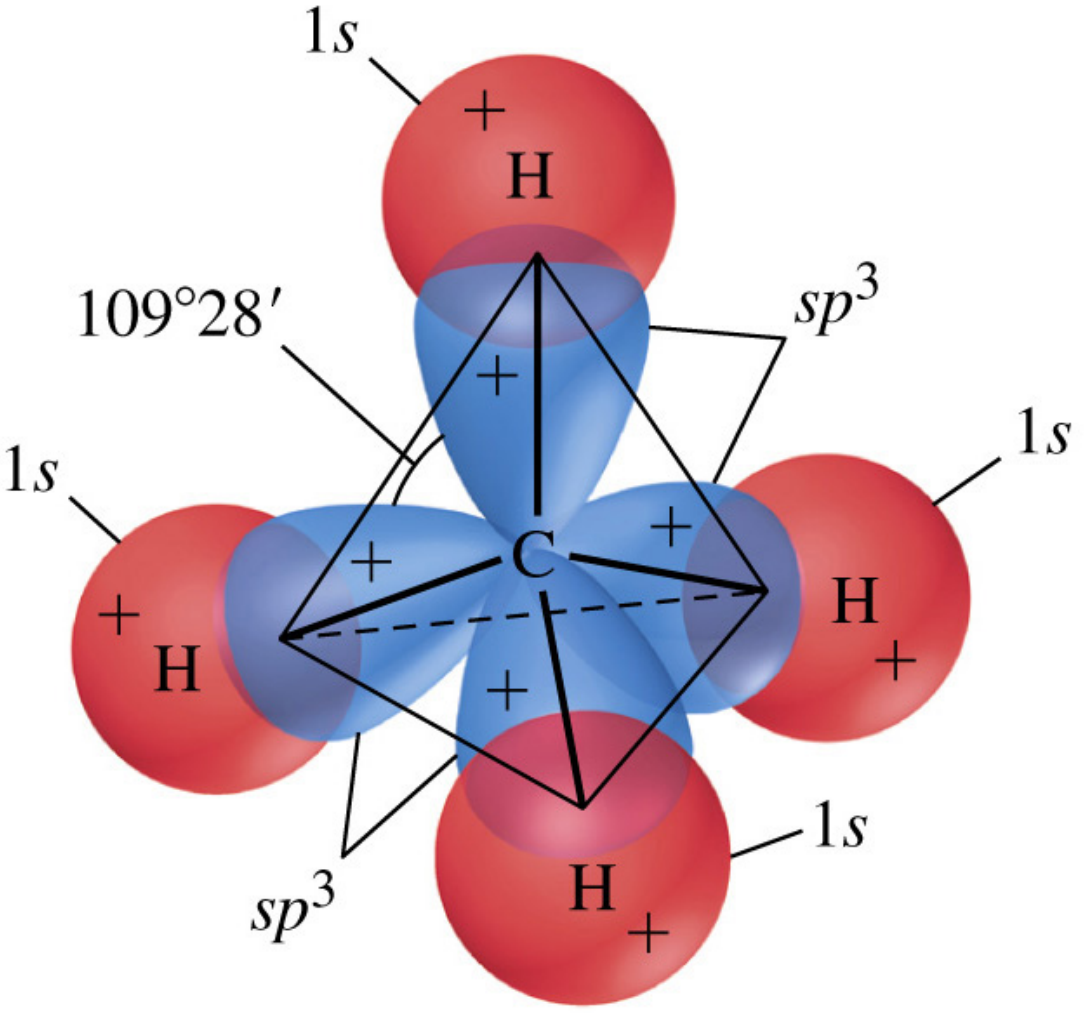
Valens Bağ molekülün şeklini çakışan orbitallerin şekli ve yerleşme düzenine göre açıklar.

Çoğunlukla bağ oluşumu için atomlarda elektron düzenlemesi ve orbitaleri şeklinin değişmesi olur. Bunun sonucunda merkez atomda hibrit orbitaller meydana gelir.




z
y
x
s
p_x
p_y
p_z
Combine to generate four sp^3 orbitals
Which are represented as the set

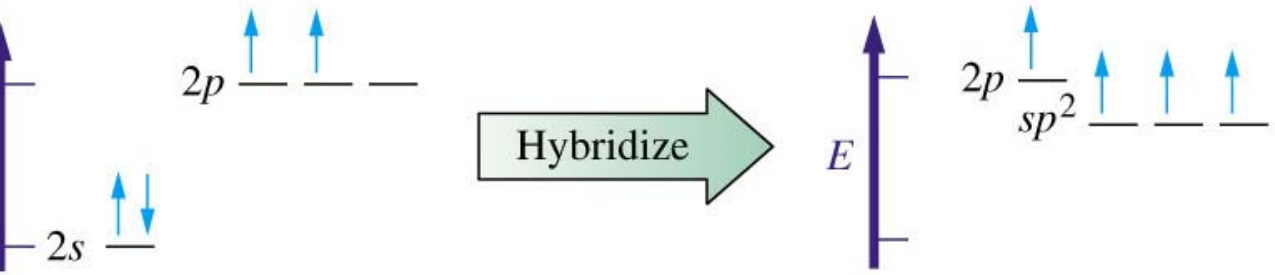
Metan ın hibritleşmesi ve bağ yapması

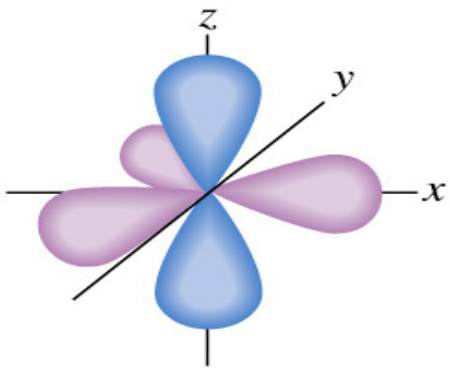


Geometri	Orbital sayısı	Hibritleşme tipi
Çizgisel (lineer)	2	sp
Üçgen düzlemsel	3	sp^2
Düzgün dört yüzlü (tetrahedral)	4	sp^3
Üçgen bipiramidal	5	sp^3d
Düzgün sekiz yüzlü (Oktahedral)	6	sp^3d^2

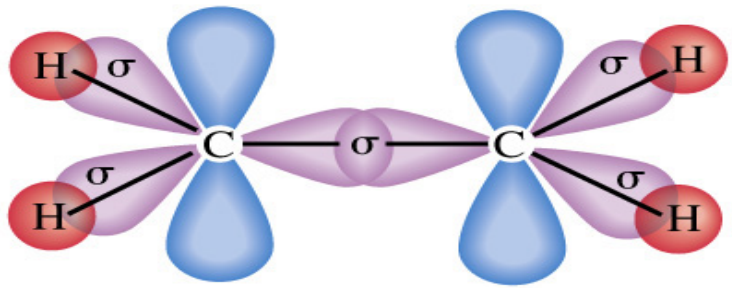
CH_4, PCl_5, SF_6. NH_3 BeF_2 bileşiklerinin hibritleşme türü ve molekül geometrilerini bulunuz.

oklu bağlar: tek elektronlu orbitallerin çakışması sonucu δ bağı oluşur, eksenlerd
eri kalan e ların paralel örtüşmesi sonucu ise π bağları oluşur.

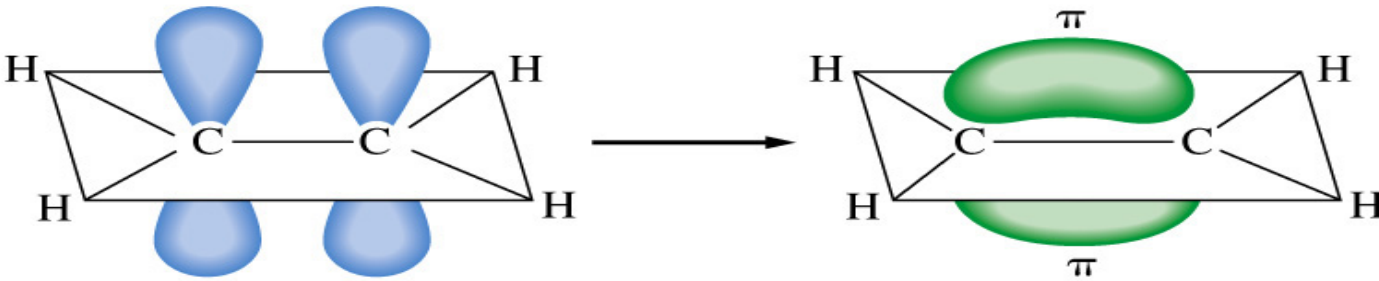




The set of orbitals $sp^2 + p$



Sigma (σ) bonds

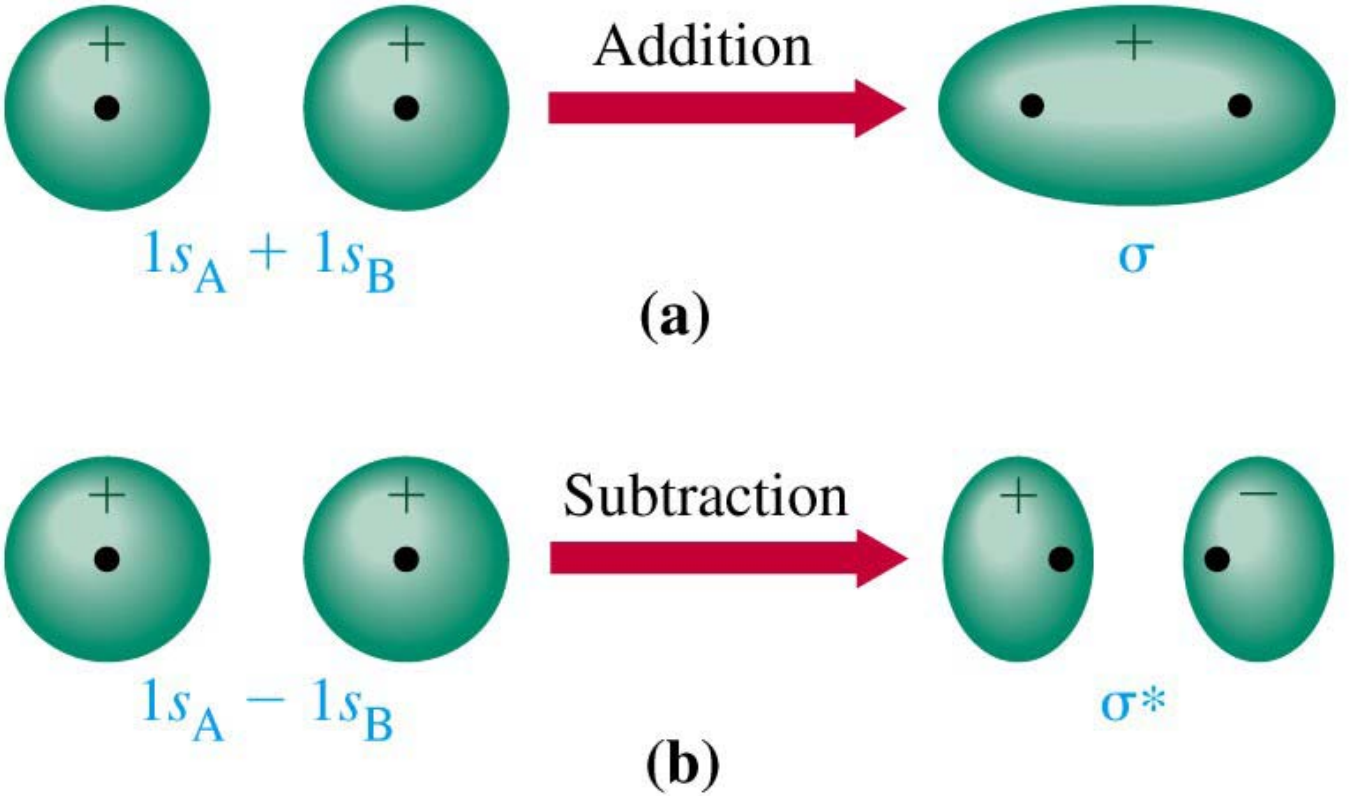


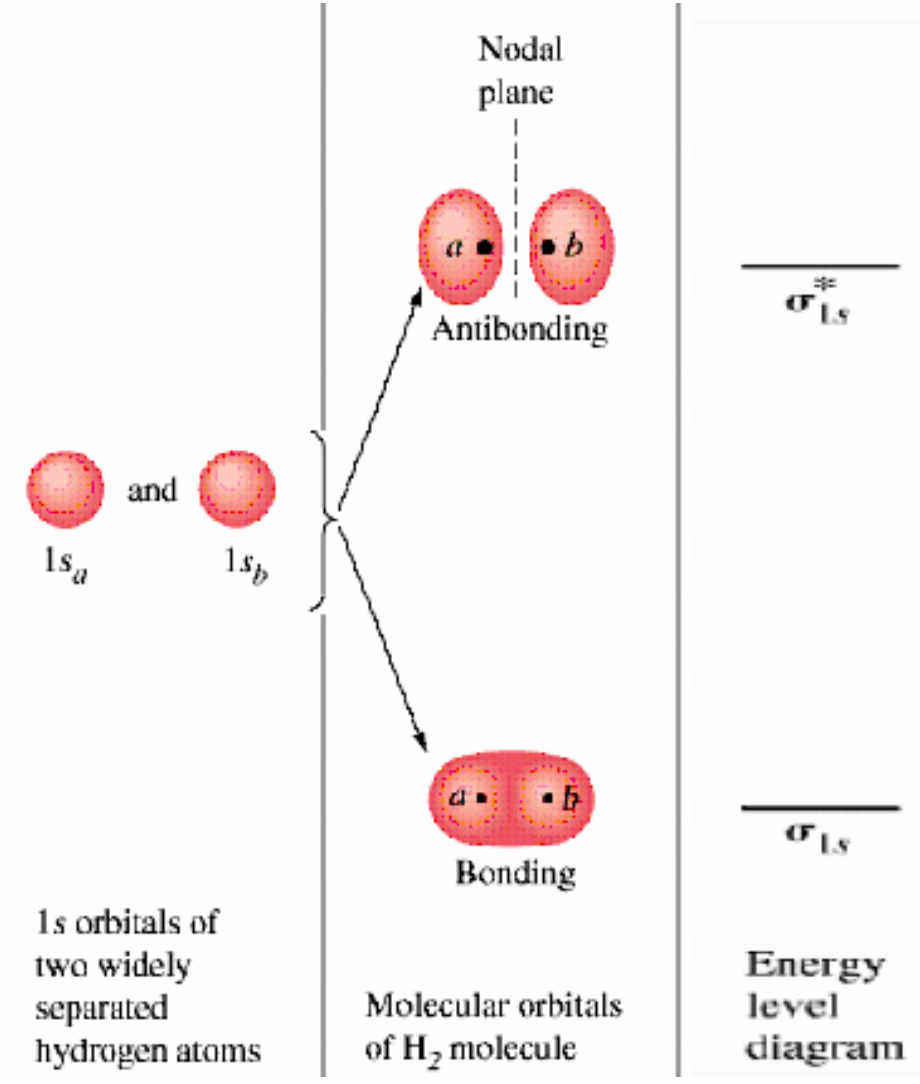
Molekül Orbital Teori

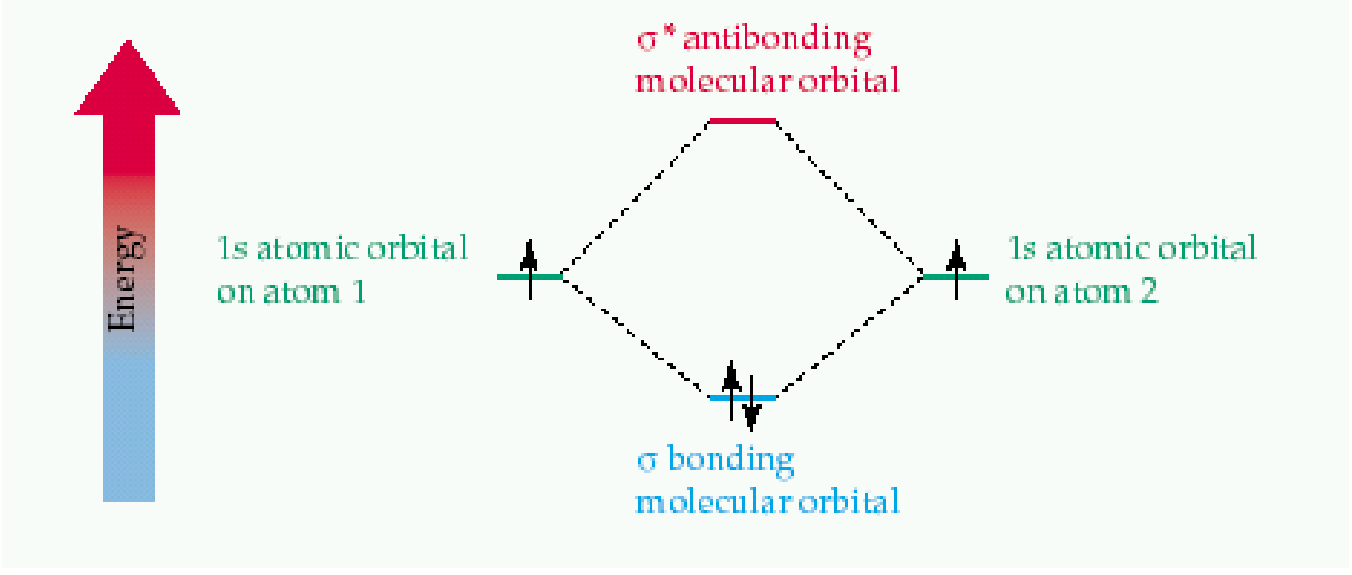
Bir molekülde atom çekirdeklerinin etrafında molekül yörüngeleri bulunur. A molecular orbital describes a region of space in a molecule where electrons are most likely to be found.

Molekül orbitaller atom yörüngelerinin birleştirilmesiyle oluşur.

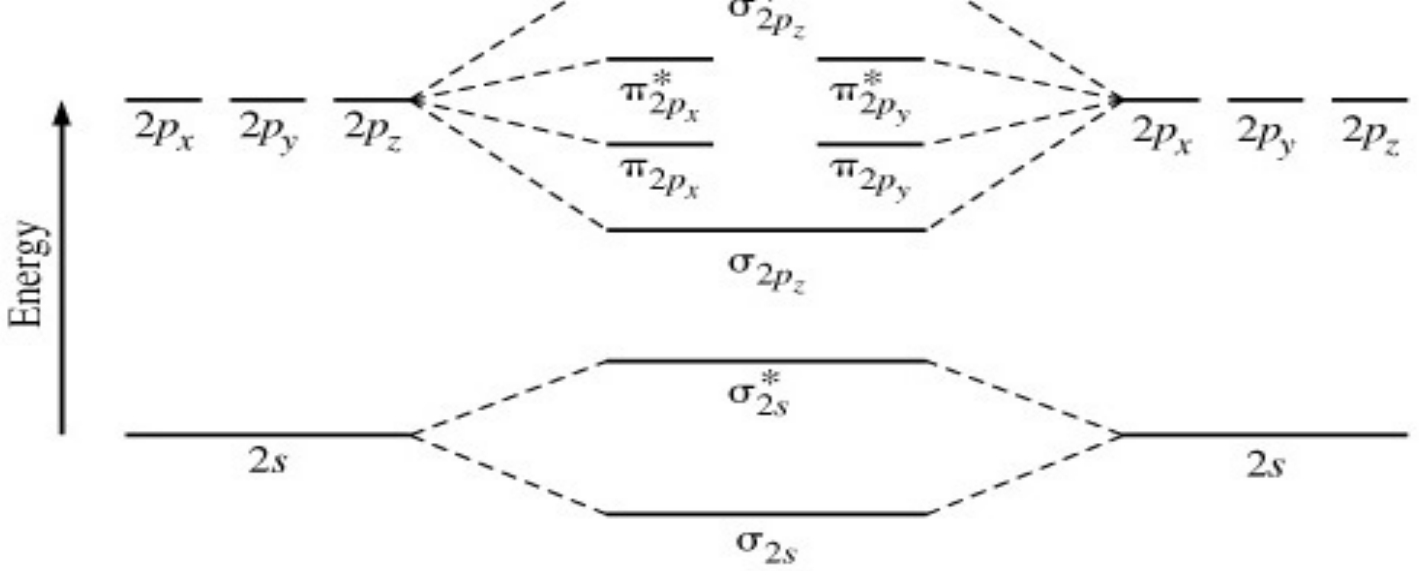
Atomik Orbitallerin birleşmesi



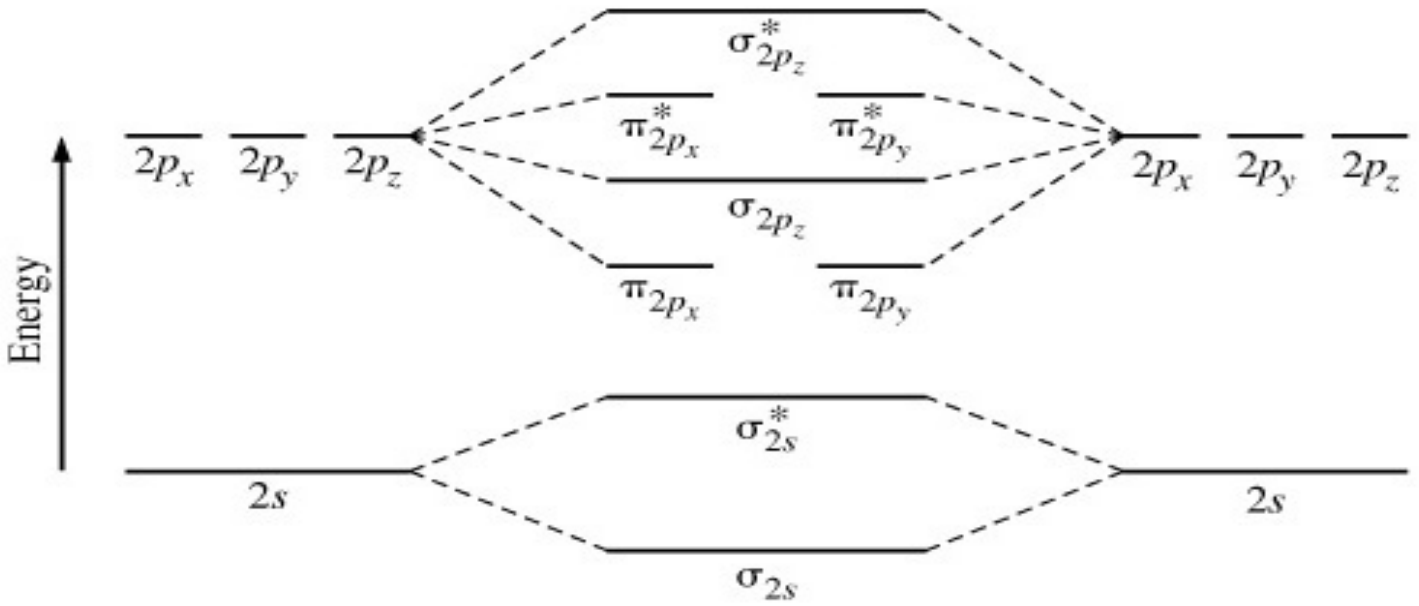

Nodal plane
a
b
Antibonding
and
$1s_a$
$1s_b$
a
b
Bonding
σ^*_{1s}
σ_{1s}
1s orbitals of two widely separated hydrogen atoms
Molecular orbitals of H_2 molecule
Energy level diagram

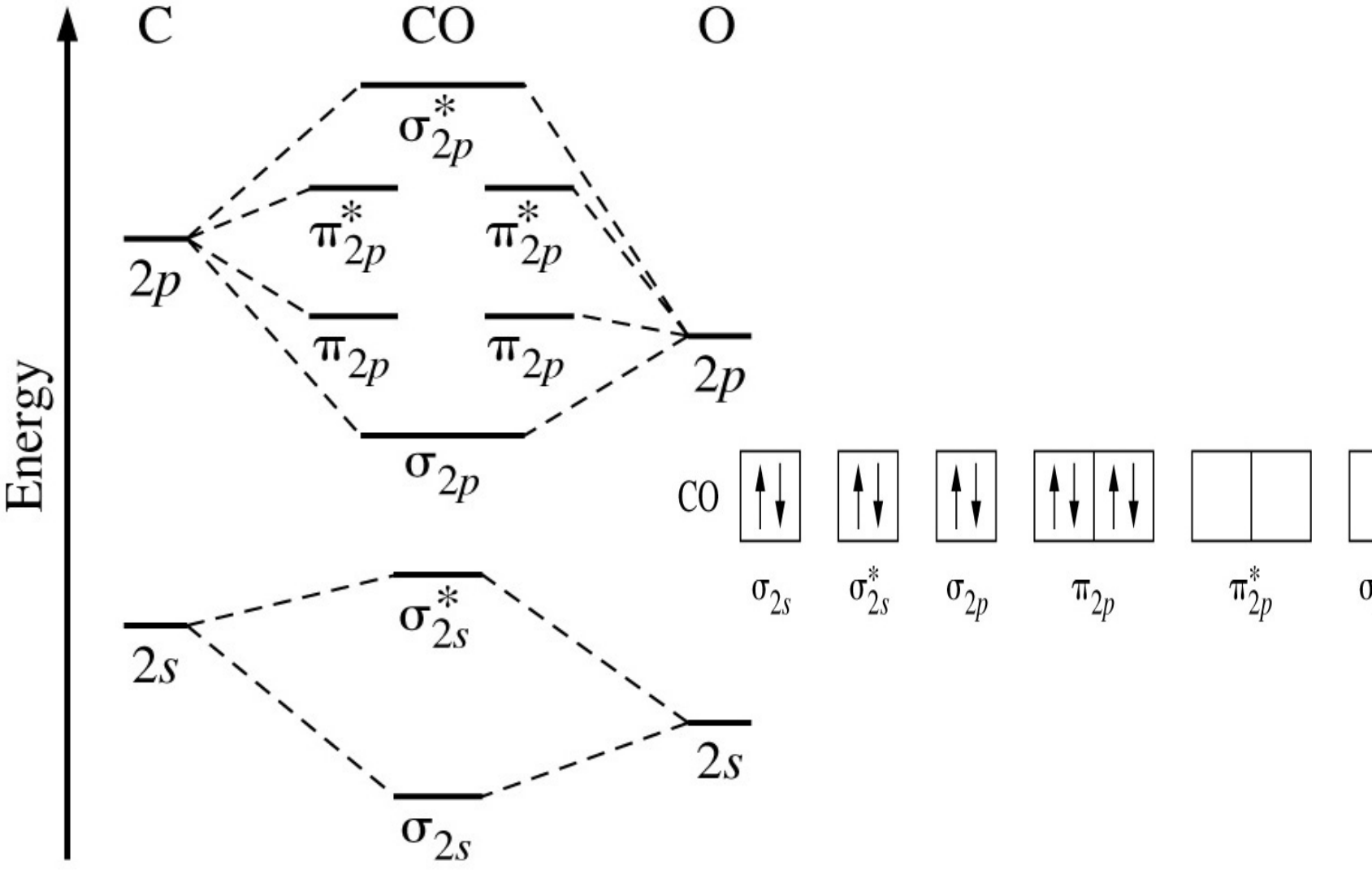


$$\text{Bağ derecesi} = \frac{\text{MO deki bağ elektronları sayısı - antibağ MO deki elektron sayı}}{2}$$


$\sigma^*_{2p_z}$
$\pi^*_{2p_x}$
$\pi^*_{2p_y}$
$2p_x$
$2p_y$
$2p_z$
π_{2p_x}
π_{2p_y}
$2p_x$
$2p_y$
$2p_z$
Energy
σ_{2p_z}
σ^*_{2s}
$2s$
$2s$
σ_{2s}

(a) $Z \geq 8$

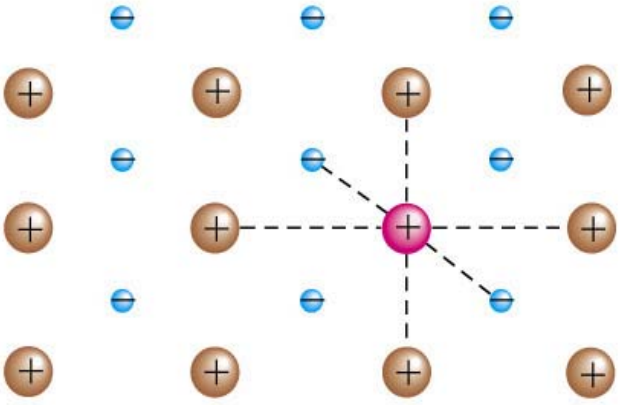

$\sigma^*_{2p_z}$
$\pi^*_{2p_x}$
$\pi^*_{2p_y}$
$2p_x$
$2p_y$
$2p_z$
σ_{2p_z}
$2p_x$
$2p_y$
$2p_z$
Energy
π_{2p_x}
π_{2p_y}
σ^*_{2s}
$2s$
$2s$
σ_{2s}

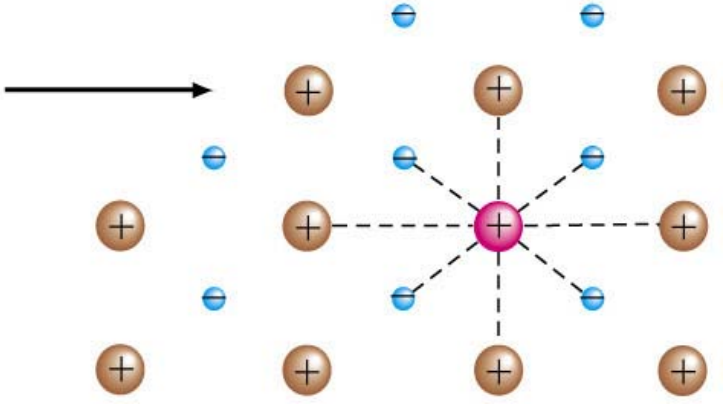

C
CO
O
Energy
σ^*_{2p}
π^*_{2p}
π^*_{2p}
2p
π_{2p}
π_{2p}
2p
σ_{2p}
CO
σ^*_{2s}
2s
2s
σ_{2s}
σ_{2s}
σ^*_{2s}
σ_{2p}
π_{2p}
π^*_{2p}

Metalik Bağ	
Elektron denizi modeli	Band teori

Metalik Bağ

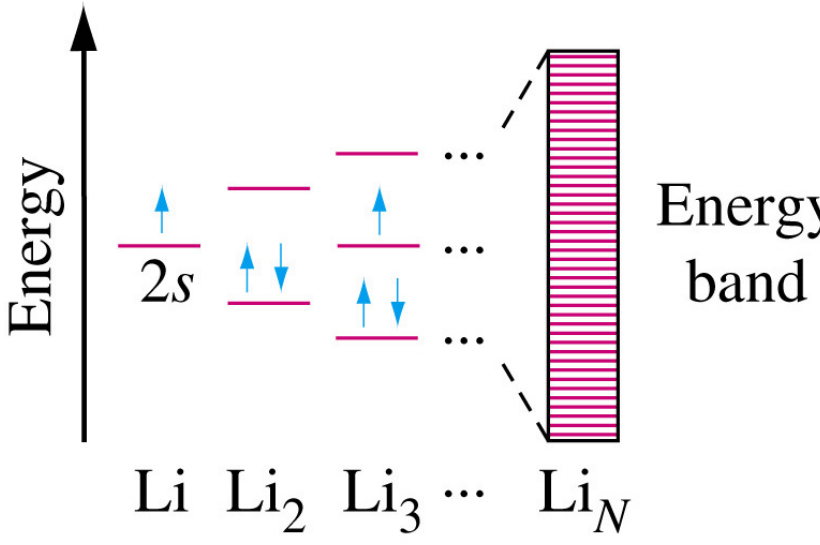
- Elektron denizi model



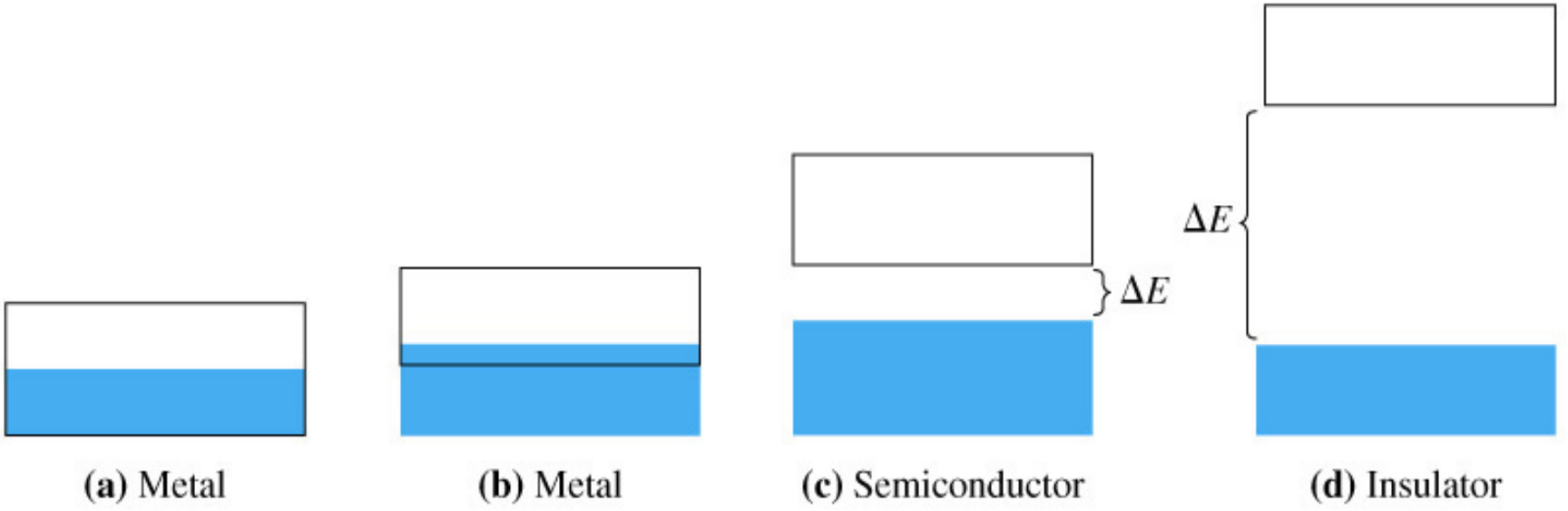


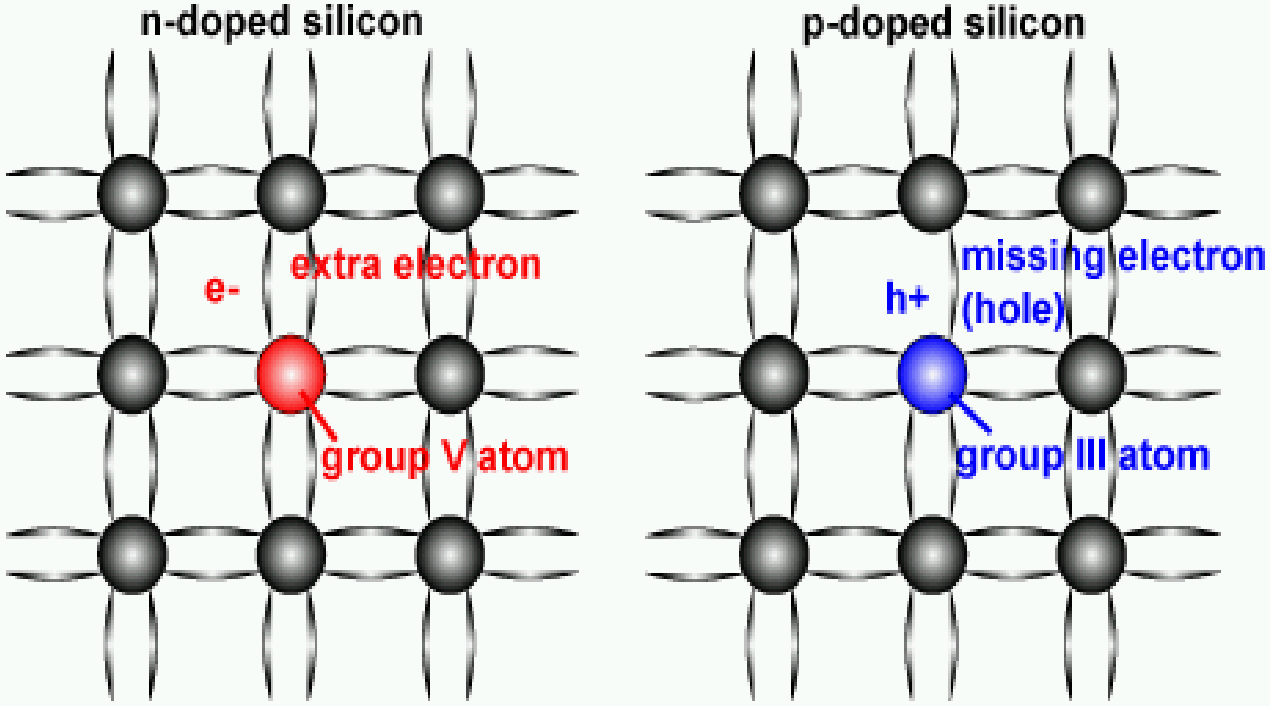
Metalik Bağ

Band teori



Band teori



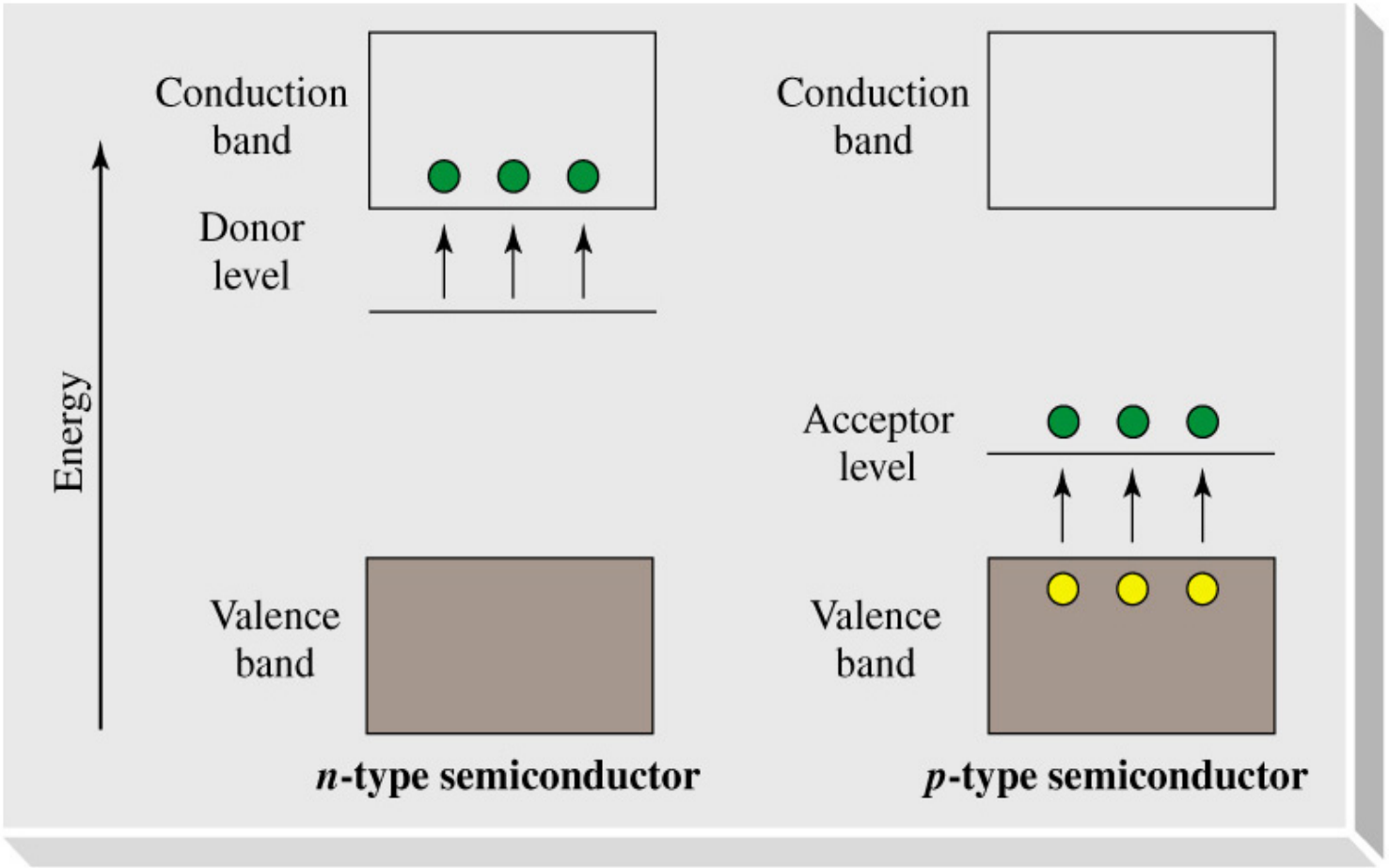


Schematic of a silicon crystal lattice doped with impurities to produce *n*-type and *p*-type semiconductor material.

e following table summarizes the properties of semiconductor types.

	P-type (positive)	N-type (negative)
Dopant	Group III (E.g. Boron)	Group V (e.g. Phosphorous)
Bonds	Missing Electrons (Holes)	Excess Electrons
Majority Carriers	Holes	Electrons
Minority Carriers	Electrons	Holes

Yarı iletkenler



Photovoltaic Cells