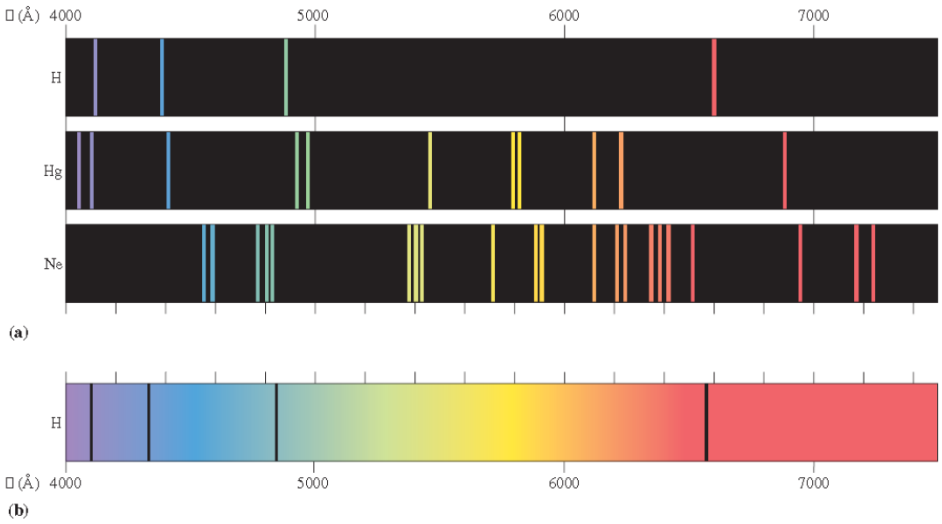
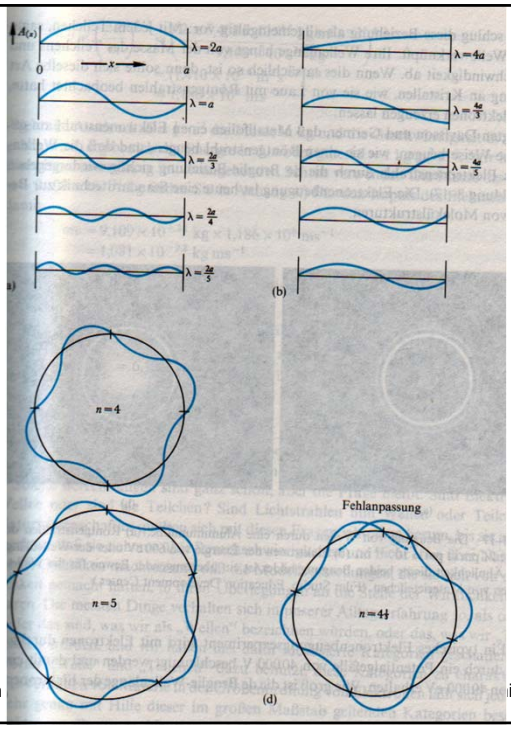
Lecture General Chemistry
Winter Term 2022/23

Dr. Lars Birlenbach
Physikalische Chemie 1 (PC1)
AR-F0102
Tel.: 0271 740 2817
eMail: birlenbach@chemie.uni-siegen.de

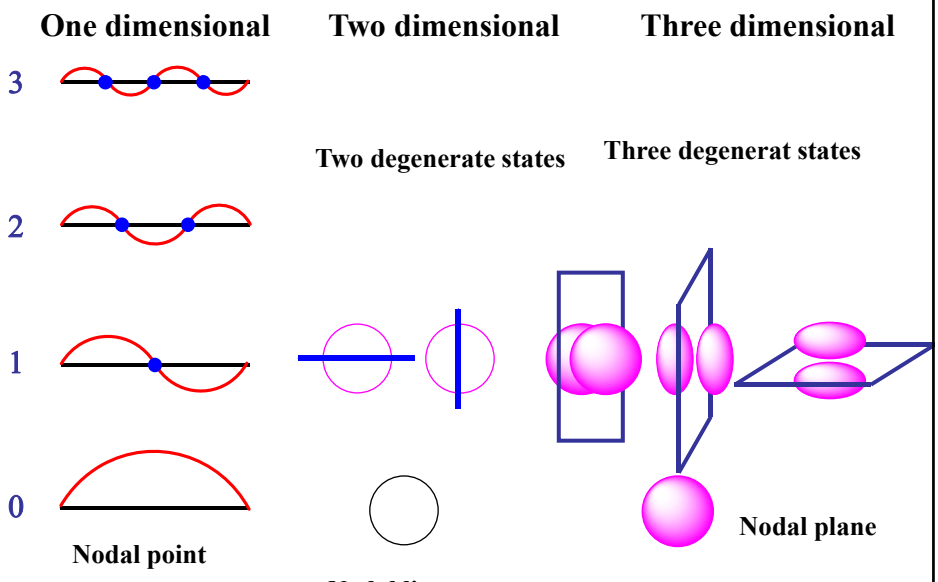
- Website (Slides, Excercises):
- http://www.chemie.uni-siegen.de/pc/lehre/nanoscitec/

Login Data for slides:
User: Ludwig
Password: Boltzmann

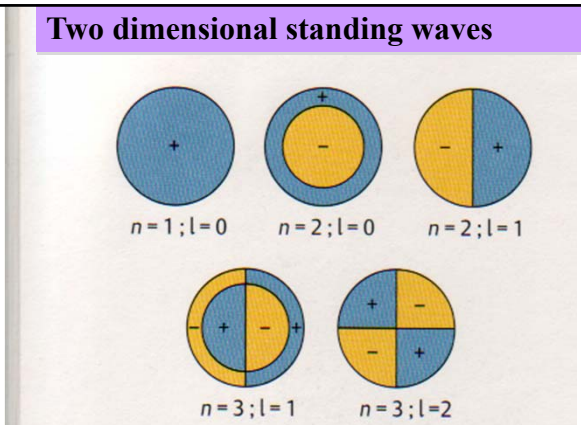




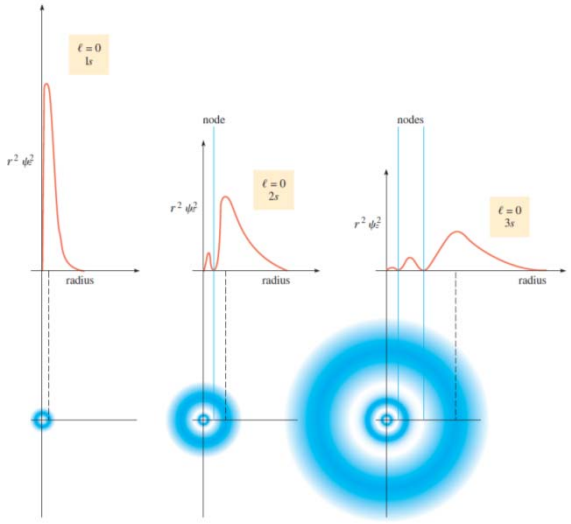
Standing waves



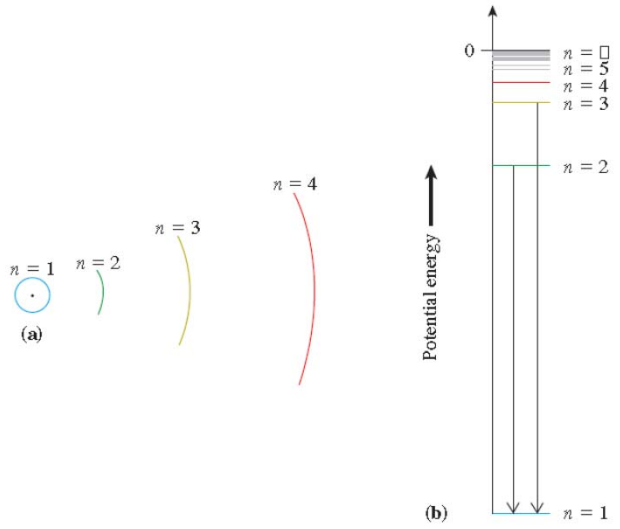
Two dimensional standing waves



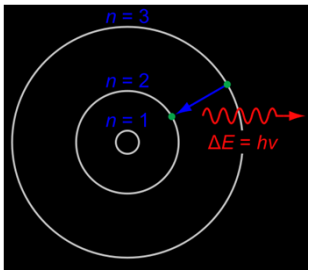
Three dimensional standing waves



Bohr‘s atomic model



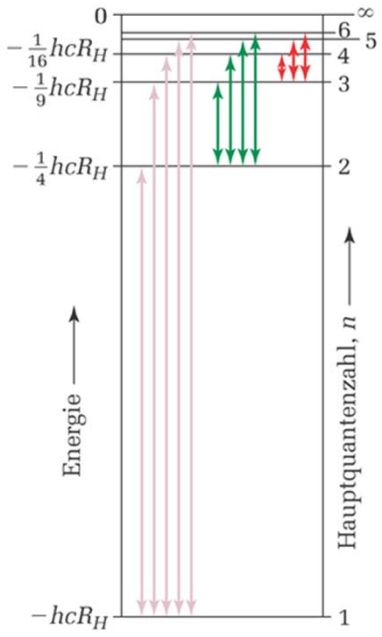
Bohr‘s atomic model

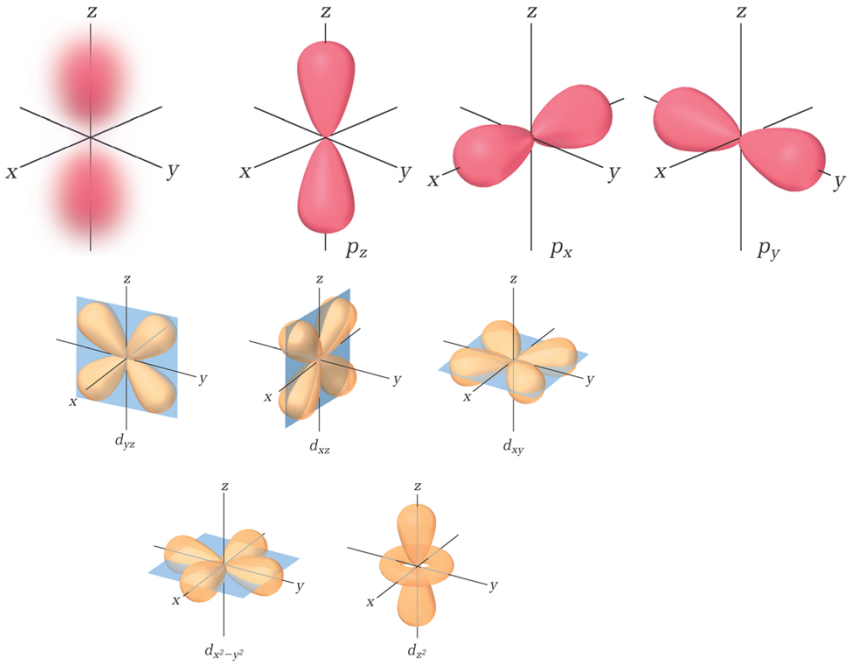


$$\frac{1}{\lambda} = R\left(\frac{1}{n_2^{\,2}} - \frac{1}{n_1^{\,2}}\right)$$

$R = 1{,}1 \cdot 10^{7}\,\mathrm{m}^{-1}$

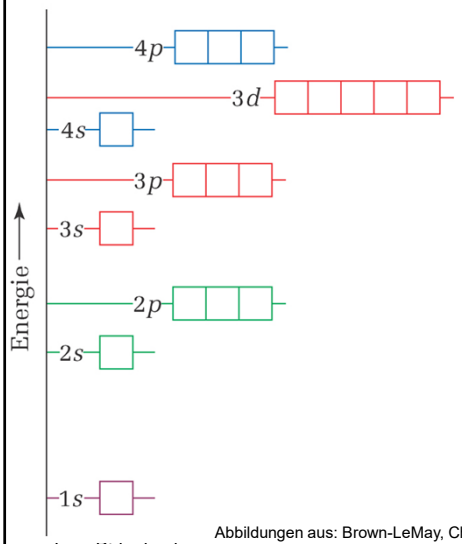
Rydberg-Konstant





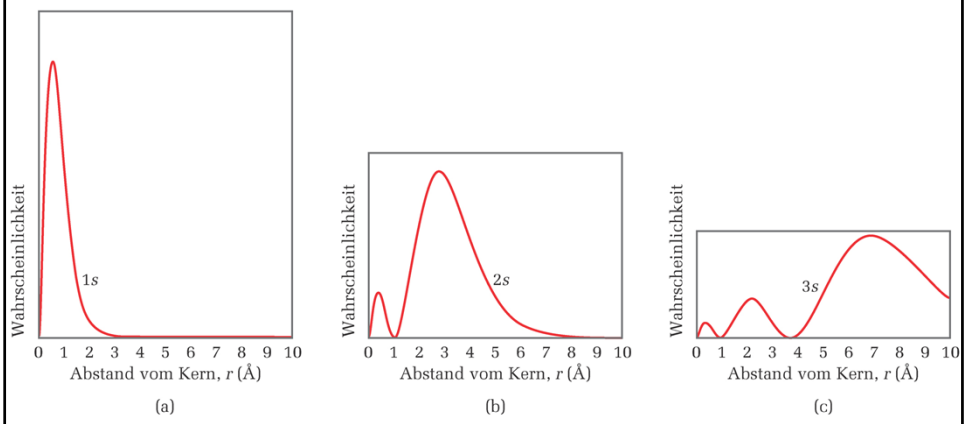
Abbildungen aus: Brown-LeMay, Chemie siehe www.pearson-studium.de

Energy levels of the orbitals



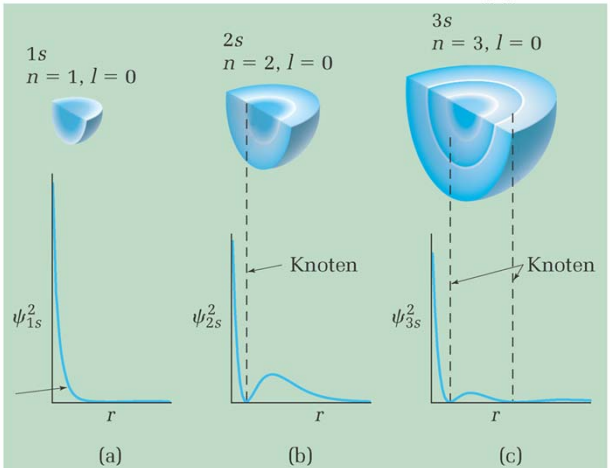
Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

Ions in s-Orbitals



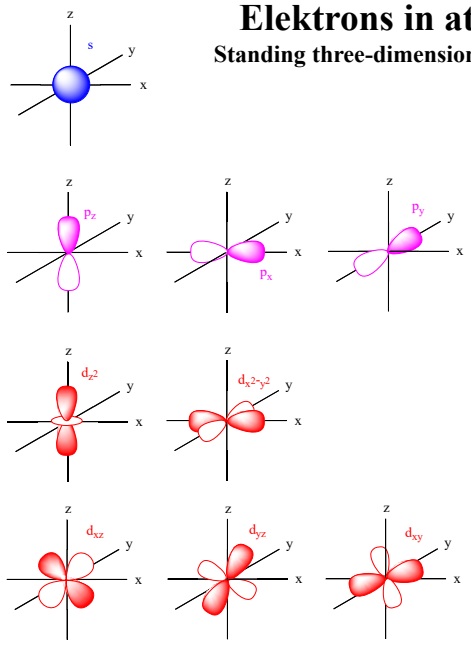
$$\text{probability} \propto 4\pi r^2 \Psi^2$$

Wave function $\Psi = f(r)$



Elektrons in atoms

Standing three-dimensional waves

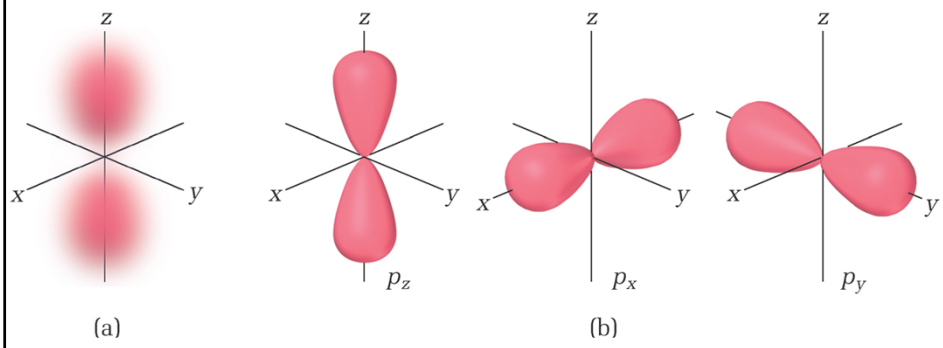


0 nodal planes
s-Orbitals

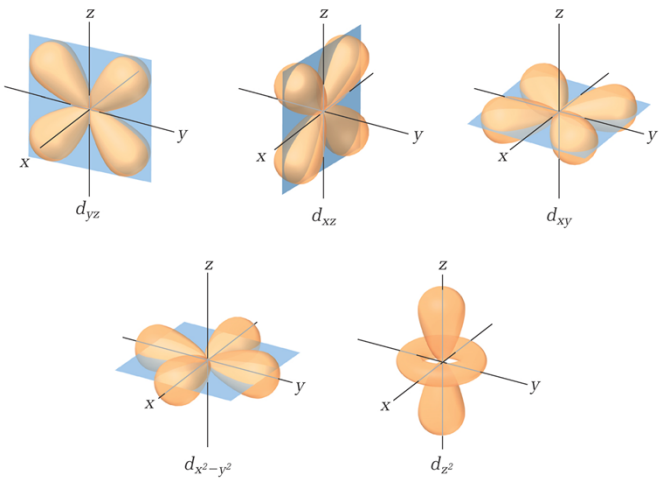
1 nodal plane
p-Orbitals

2 nodal planes
d-Orbitals

p-Orbitals



d-Orbitals



Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

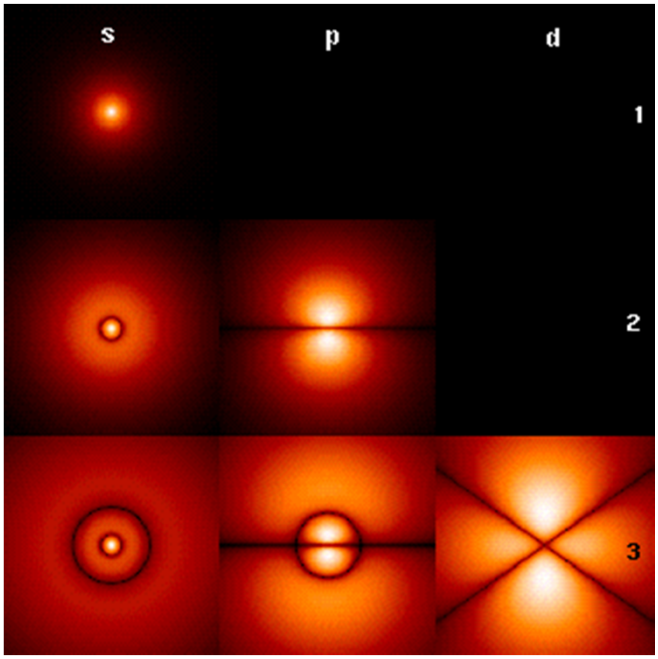


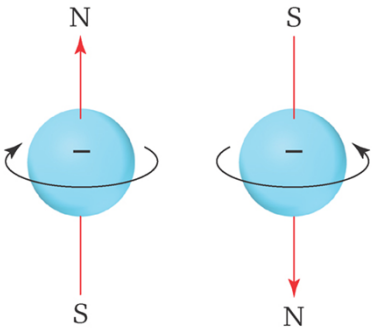
TABLE 6.5

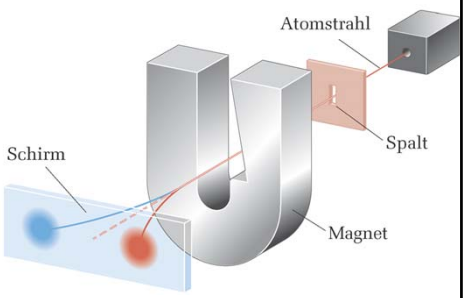
The complete hydrogenlike atomic wave functions for $n = 1$, 2, and 3. The quantity Z is the atomic number of the nucleus, and $\sigma = Zr/a_0$, where a_0 is the Bohr radius.

$n = 1,$	$l = 0,$	$m = 0$	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$
$n = 2,$	$l = 0,$	$m = 0$	$\psi_{200} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (2-\sigma)e^{-\sigma/2}$
	$l = 1,$	$m = 0$	$\psi_{210} = \frac{1}{\sqrt{32\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\cos\theta$
	$l = 1,$	$m = \pm 1$	$\psi_{21\pm1} = \frac{1}{\sqrt{64\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma e^{-\sigma/2}\sin\theta e^{\pm i\phi}$
$n = 3,$	$l = 0,$	$m = 0$	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (27-18\sigma+2\sigma^2)e^{-\sigma/3}$
	$l = 1,$	$m = 0$	$\psi_{310} = \frac{1}{81}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\cos\theta$
	$l = 1,$	$m = \pm 1$	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} (6\sigma-\sigma^2)e^{-\sigma/3}\sin\theta e^{\pm i\phi}$
	$l = 2,$	$m = 0$	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}(3\cos^2\theta - 1)$
	$l = 2,$	$m = \pm 1$	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\sin\theta\cos\theta e^{\pm i\phi}$
	$l = 2,$	$m = \pm 2$	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3}\sin^2\theta e^{\pm 2i\phi}$

aus: McQuarrie, Simon: Physical Chemistry. University Science Books

Electron spin





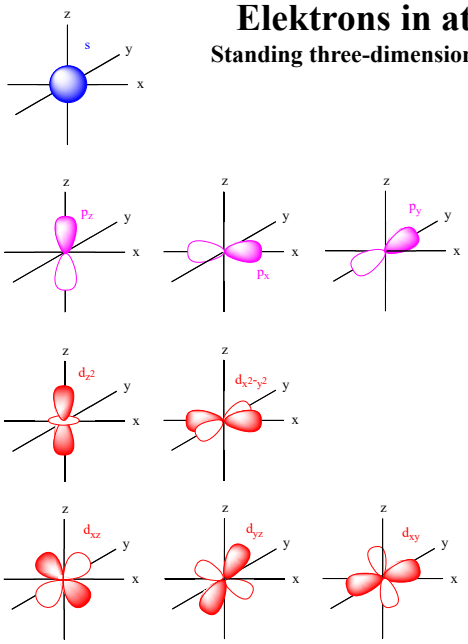
Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

Quantum numbers

- Main quantum number *n*: Size of wave function
  - $n = 1,2, ...$
- Azimutal quantum number *l*: number of nodal planes
  - $l = 0$ no nodal plane
  - $l = 1$ one nodal plane
  - $l = 2$, two nodal planes
  - $l = 0, 1, 2, ... n-1$
- Magnetic quantum number *m*: distribution in space
  - $m = -l, ... , 0, ... , +l$
- Spin quantum number *s*: angular momentum
  - $+½ , -½$

Elektrons in atoms

Standing three-dimensional waves



0 nodal planes

s-Orbitals

1 nodal plane

p-Orbitals

2 nodal planes

d-Orbitals

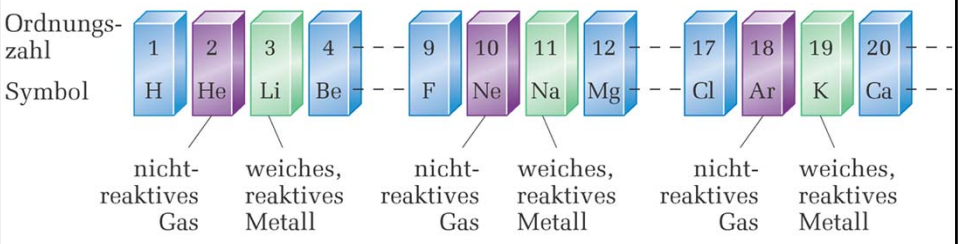
Electronic configuration for Chlorine

Electron	n	ℓ	m_ℓ	m_s	e^- Configuration
1, 2	1	0	0	$\pm\frac{1}{2}$	$1s^2$
3, 4	2	0	0	$\pm\frac{1}{2}$	$2s^2$
5–10	2	1	−1	$\pm\frac{1}{2}$	$2p^6$
	2	1	0	$\pm\frac{1}{2}$	
	2	1	+1	$\pm\frac{1}{2}$	
11, 12	3	0	0	$\pm\frac{1}{2}$	$3s^2$
13–17	3	1	−1	$\pm\frac{1}{2}$	$3p^5$
	3	1	0	$\pm\frac{1}{2}$	
	3	1	+1	$+\frac{1}{2}$ or $-\frac{1}{2}$*	

Electronic configurations

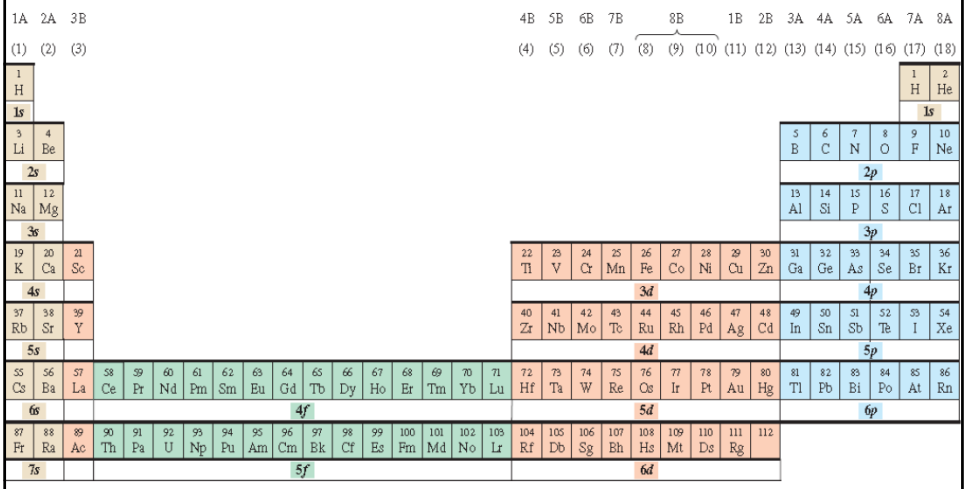
n	ℓ	m_ℓ	m_s	Electron Capacity of Subshell = $4\ell + 2$	Electron Capacity of Shell = $2n^2$
1	0(1*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	2
2	0(2*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	8
	1(2*p*)	$-1, 0, +1$	$\pm\frac{1}{2}$ for each value of m_ℓ	6	
3	0(3*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	18
	1(3*p*)	$-1, 0, +1$	$\pm\frac{1}{2}$ for each value of m_ℓ	6	
	2(3*d*)	$-2, -1, 0, +1, +2$	$\pm\frac{1}{2}$ for each value of m_ℓ	10	
4	0(4*s*)	0	$+\frac{1}{2}, -\frac{1}{2}$	2	32
	1(4*p*)	$-1, 0, +1$	$\pm\frac{1}{2}$ for each value of m_ℓ	6	
	2(4*d*)	$-2, -1, 0, +1, +2$	$\pm\frac{1}{2}$ for each value of m_ℓ	10	
	3(4*f*)	$-3, -2, -1, 0, +1, +2, +3$	$\pm\frac{1}{2}$ for each value of m_ℓ	14	

Discovery of the periodic system: patterns

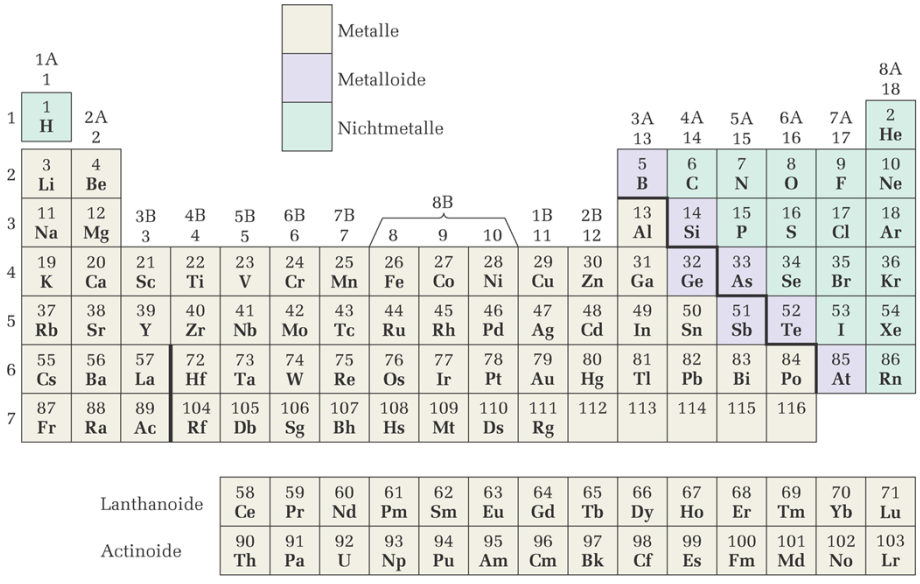


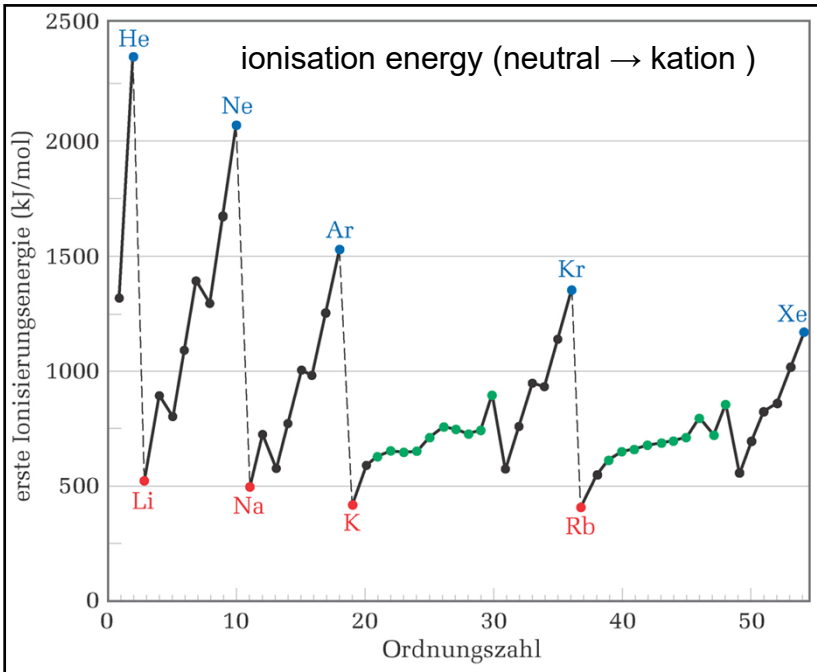
 Abbildungen aus: Brown-LeMay, Chemie siehe www.pearson-studium.de

PSE and Orbitals



PSE and chemical properties



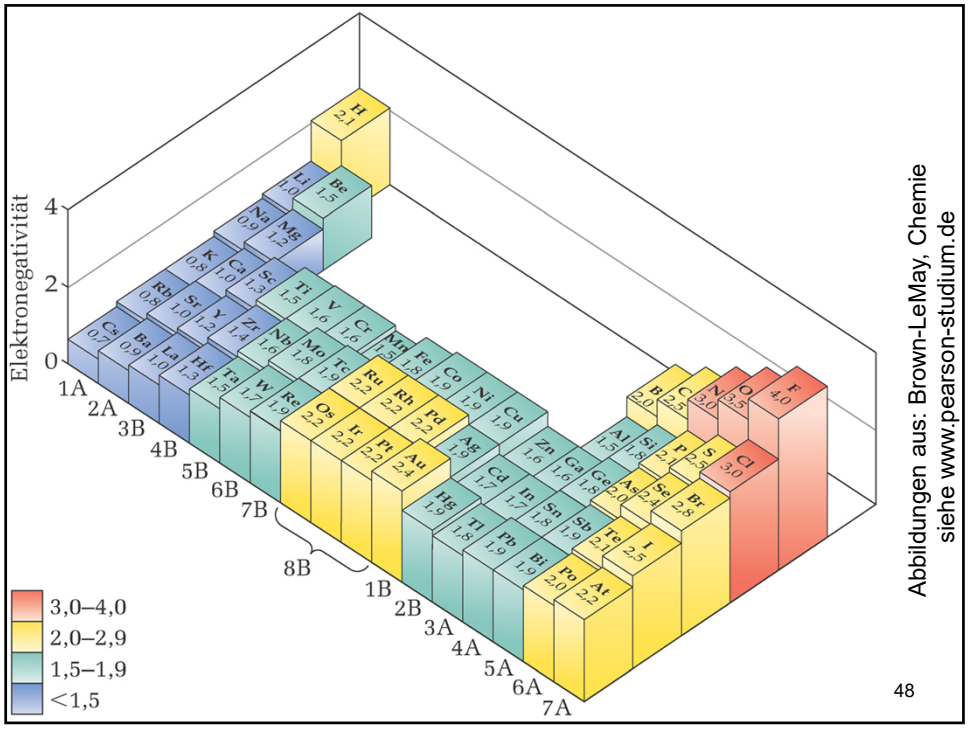


Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

Elektron affinities (neutral → Anion)

1A	2A	3A	4A	5A	6A	7A	8A
H −73							He > 0
Li −60	Be > 0	B −27	C −122	N > 0	O −141	F −328	Ne > 0
Na −53	Mg > 0	Al −43	Si −134	P −72	S −200	Cl −349	Ar > 0
K −48	Ca −2	Ga −30	Ge −119	As −78	Se −195	Br −325	Kr > 0
Rb −47	Sr −5	In −30	Sn −107	Sb −103	Te −190	I −295	Xe > 0

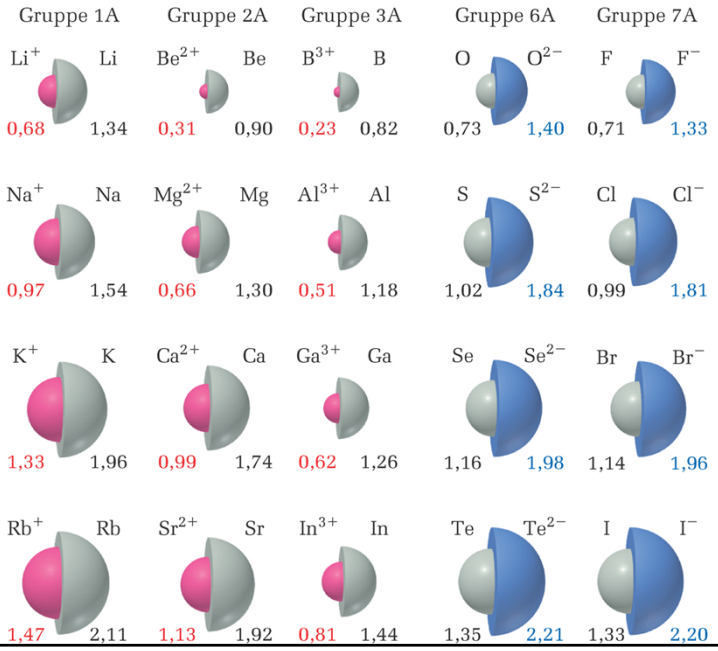
Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de



Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

48

Size of Atoms and Ions in Å



Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

Lars Birlenb

49

Common ions

1A	2A										3A	4A	5A	6A	7A	8A
H^+																
Li^+													N^{3-}	O^{2-}	F^-	E
Na^+	Mg^{2+}	Transition elements									Al^{3+}		P^{3-}	S^{2-}	Cl^-	D
K^+	Ca^{2+}				Cr^{3+}	Mn^{2+}	Fe^{2+} Fe^{3+}	Co^{2+}	Ni^{2+}	Cu^+ Cu^{2+}	Zn^{2+}			Se^{2-}	Br^-	E
Rb^+	Sr^{2+}									Ag^+	Cd^{2+}		Sn^{2+}	Te^{2-}	I^-	L
Cs^+	Ba^{2+}								Pt^{2+}	Au^+ Au^{3+}	Hg_2^{2+} Hg^{2+}		Pb^{2+}	Bi^{3+}		G
																A
																S
																E

Abbildungen aus: Brown-LeMay, Chemie
siehe www.pearson-studium.de

Valence electrons

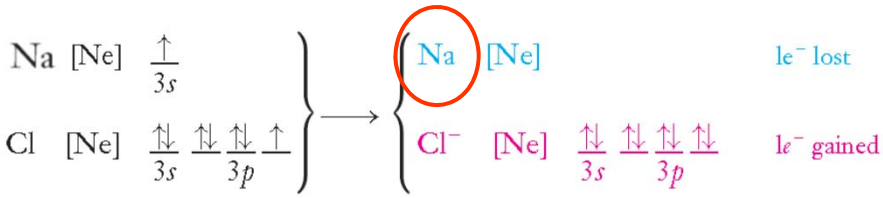
Group	1A	2A	3A	4A	5A	6A	7A	8A
Number of electrons in valence shell	1	2	3	4	5	6	7	8 *(except He)*
Period 1	H·							He:
Period 2	Li·	Be:	·B·	·C·	·N·	·O:	·F:	:Ne:
Period 3	Na·	Mg:	Al·	Si·	·P·	·S:	:Cl:	:Ar:
Period 4	K·	Ca:	Ga·	Ge·	·As·	·Se:	:Br:	:Kr:
Period 5	Rb·	Sr:	In·	Sn·	·Sb·	·Te:	:I:	:Xe:
Period 6	Cs·	Ba:	Tl·	Pb·	·Bi·	·Po:	:At:	:Rn:
Period 7	Fr·	Ra:						

•aus: **Chemistry, 9th Edition** KW Whitten,
•RE Davis, ML Peck, GG Stanley

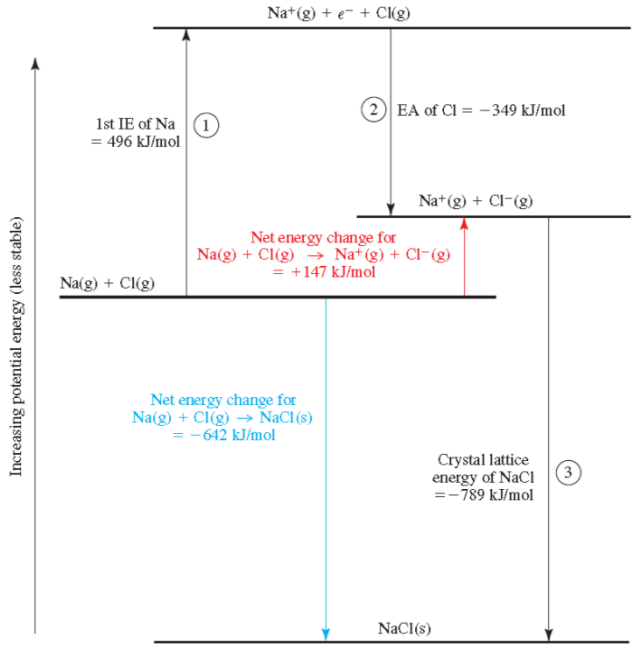
The chemical bond

- ionic bond
- metallic bond
- covalent bond (molecules)

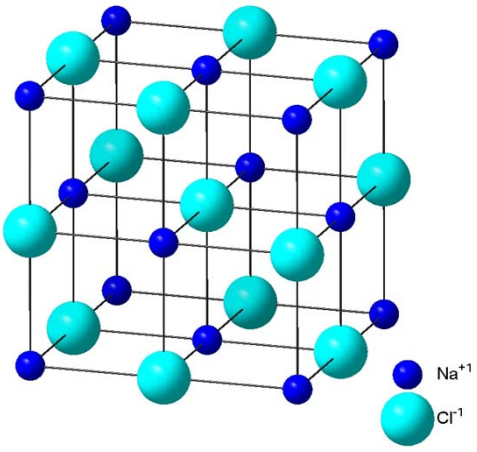
Na + Cl → NaCl



•aus: **Chemistry, 9th Edition** KW Whitten,
•RE Davis, ML Peck, GG Stanley


Na⁺(g) + e⁻ + Cl(g)
1st IE of Na = 496 kJ/mol
1
2
EA of Cl = −349 kJ/mol
Na⁺(g) + Cl⁻(g)
Net energy change for Na(g) + Cl(g) → Na⁺(g) + Cl⁻(g) = +147 kJ/mol
Na(g) + Cl(g)
Increasing potential energy (less stable)
Net energy change for Na(g) + Cl(g) → NaCl(s) = −642 kJ/mol
Crystal lattice energy of NaCl = −789 kJ/mol
3
NaCl(s)

Ionic Bond


Na+1
Cl-1

Elementary cells in cubic crystal lattice

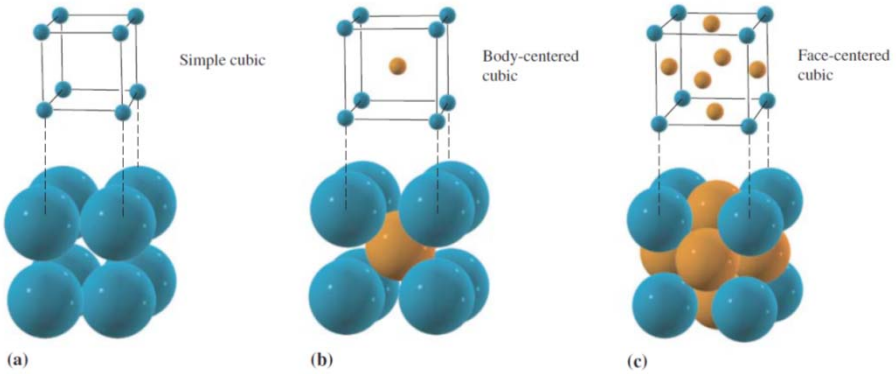
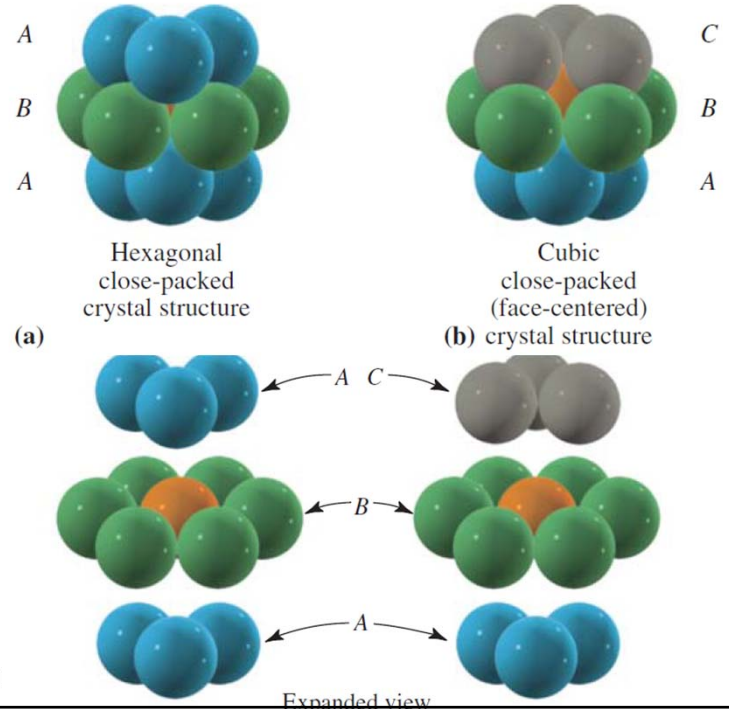
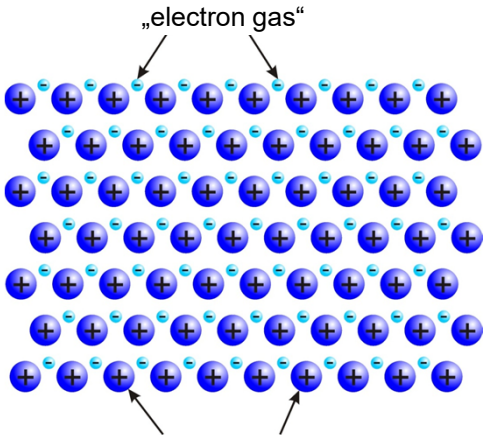


Figure 13-25 Unit cells for (a) simple cubic, (b) body-centered cubic, and (c) face-centered cubic. The spheres in each figure represent *identical* atoms or ions; different colors are shown *only* to help you visualize the spheres in the center of the cube in body-centered cubic (b) and in face-centered cubic (c) forms.



Chemical bonds: metallic



Band model

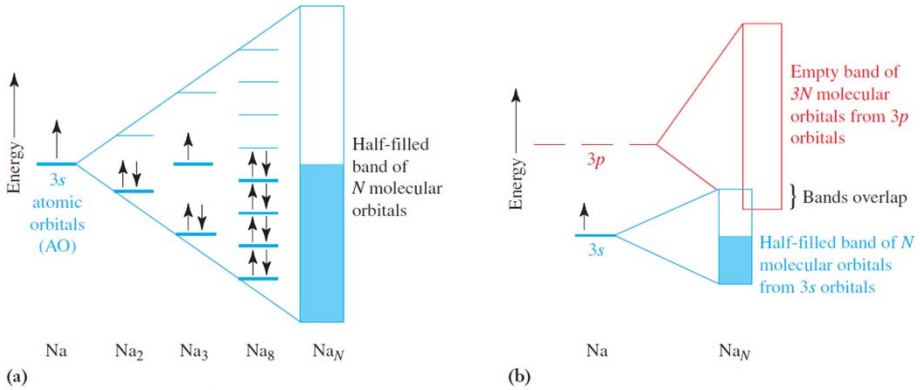


Figure 13-33 (a) The band of orbitals resulting from interaction of the 3*s* orbitals in a crystal of sodium. (b) Overlapping of a half-filled "3*s*" band (*blue*) with an empty "3*p*" band (*red*) of Na_N crystal.

•aus: **Chemistry, 9th Edition** KW Whitten,
•RE Davis, ML Peck, GG Stanley

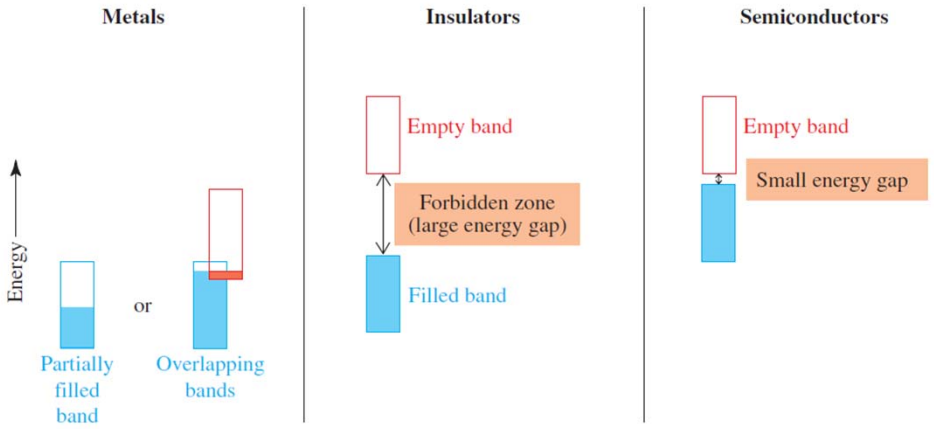


Figure 13-35 Distinction among metals, insulators, and semiconductors. In each case an unshaded area represents a conduction band.