

Lecture General Chemistry

Winter Term 2024/25

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

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Discovery of the periodic system: patterns

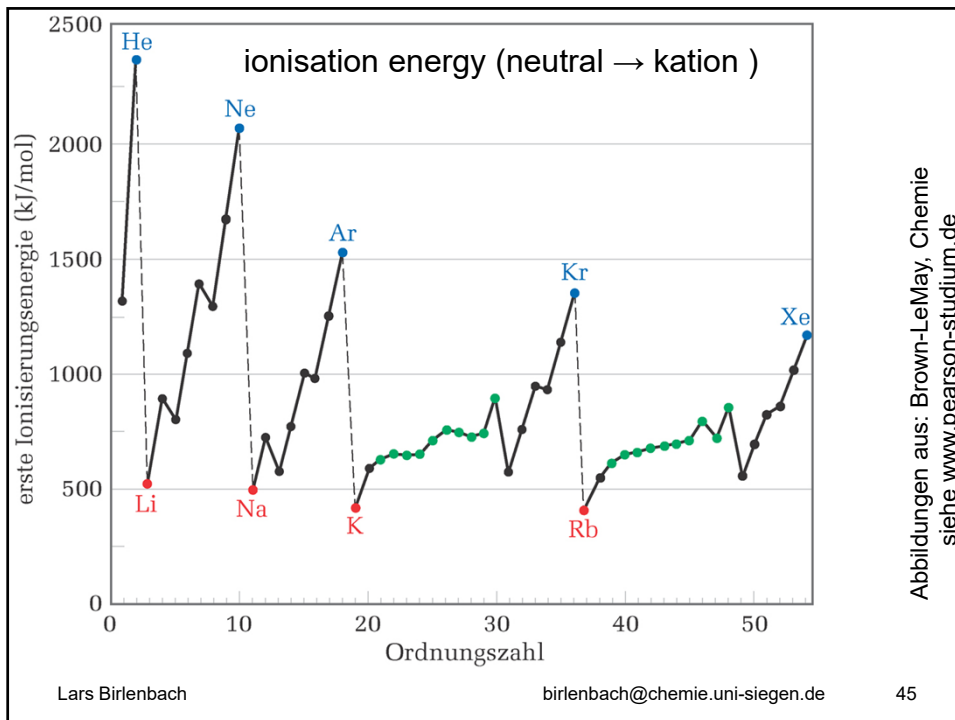
Ordnungs- zahl	1	2	3	4	9	10	11	12	17	18	19	20
Symbol	H	He	Li	Be	F	Ne	Na	Mg	Cl	Ar	K	Ca
	nicht- reaktives Gas	weiches, reaktives Metall	nicht- reaktives Gas	weiches, reaktives Metall	nicht- reaktives Gas	weiches, reaktives Metall	nicht- reaktives Gas	weiches, reaktives Metall				

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Abbildungen aus: Brown-LeMay, Chemie
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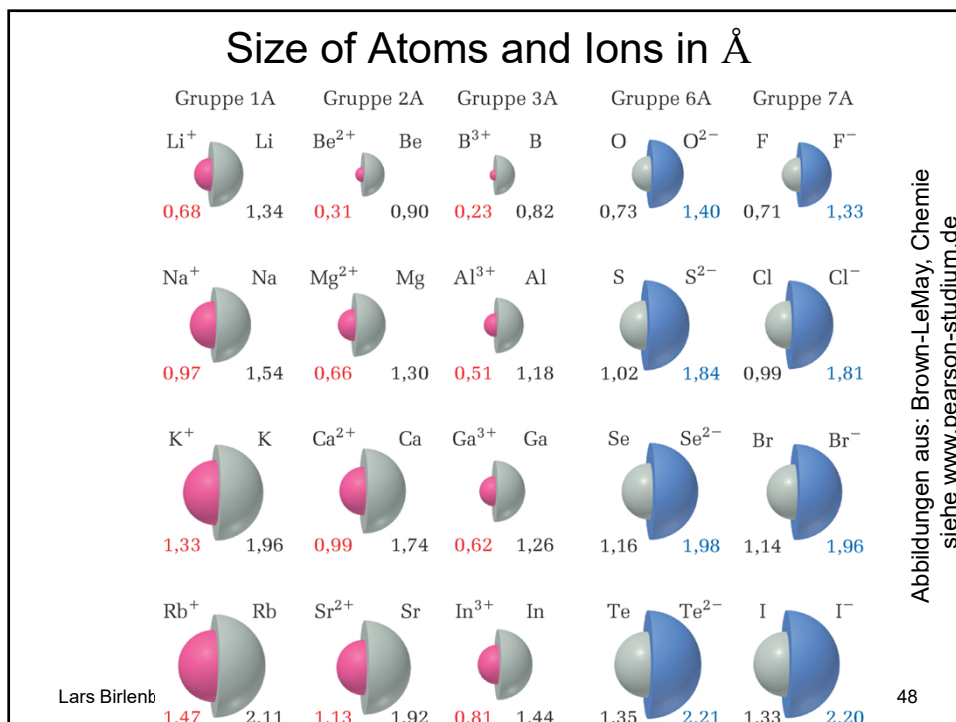
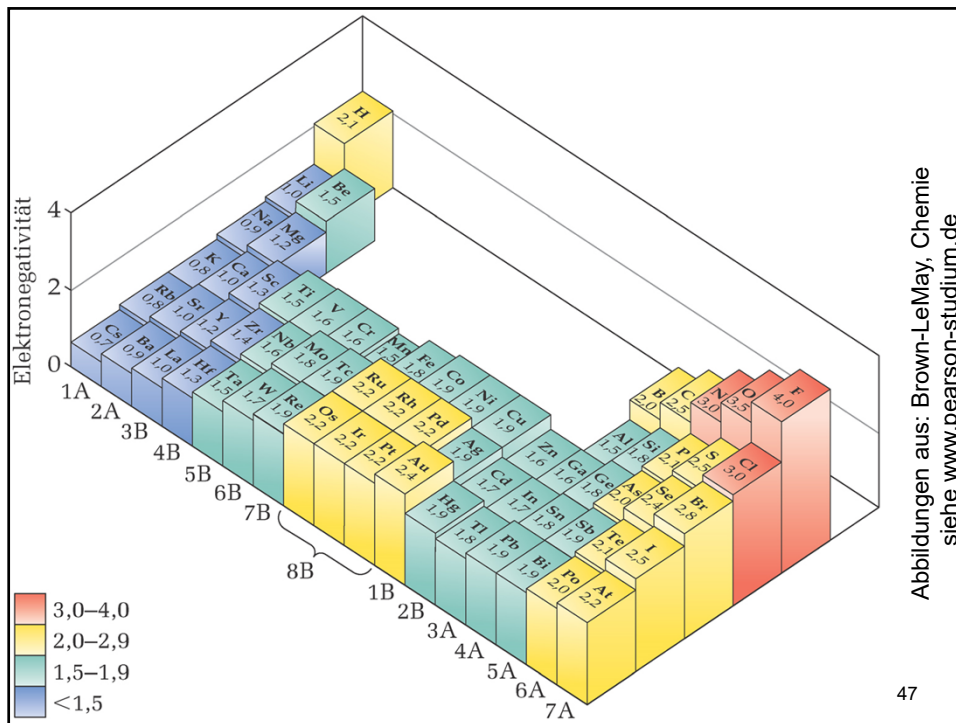
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Elektron affinities (neutral → Anion)

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
1A	2A	3A	4A	5A	6A	7A	8A

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Common ions

1A		2A		Transition elements										3A	4A	5A	6A	7A	8A		
H ⁺																					
Li ⁺														Al ³⁺			N ³⁻	O ²⁻	F ⁻		
Na ⁺	Mg ²⁺																P ³⁻	S ²⁻	Cl ⁻		
K ⁺	Ca ²⁺				Cr ³⁺	Mn ²⁺	Fe ²⁺ Fe ³⁺	Co ²⁺	Ni ²⁺	Cu ⁺ Cu ²⁺	Zn ²⁺								Se ²⁻	Br ⁻	
Rb ⁺	Sr ²⁺									Ag ⁺	Cd ²⁺								Te ²⁻	I ⁻	
Cs ⁺	Ba ²⁺								Pt ²⁺	Au ⁺ Au ³⁺	Hg ₂ ²⁺ Hg ²⁺										

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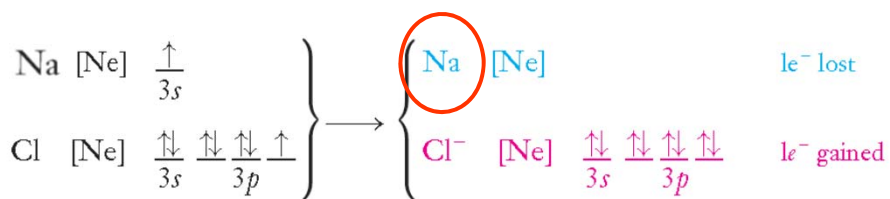
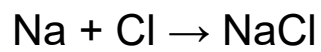
Valence electrons

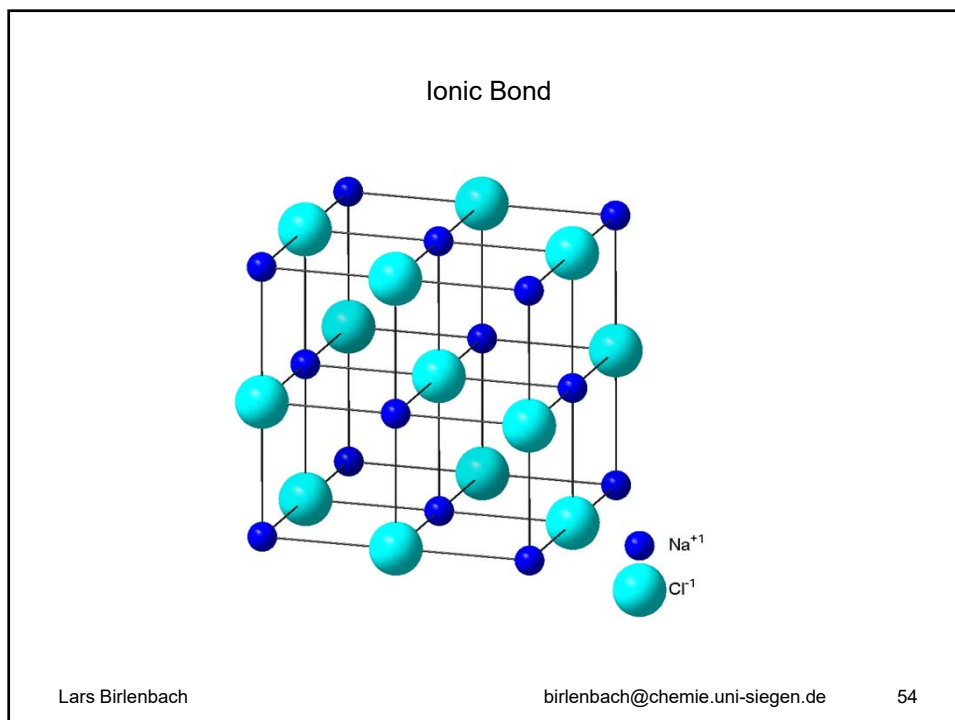
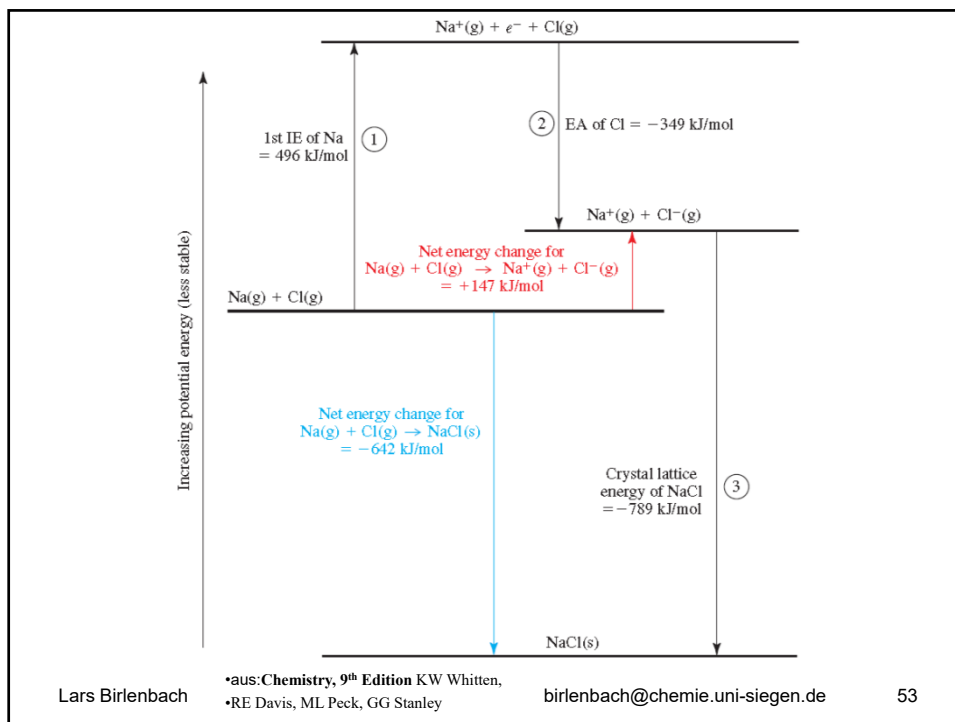
Group	1A	2A	3A	4A	5A	6A	7A	8A
<i>Number of electrons in valence shell</i>	1	2	3	4	5	6	7	8 (except He)
Period 1	H ·							He :
Period 2	Li ·	Be :	B ·	C ·	N ·	O :	F :	Ne :
Period 3	Na ·	Mg :	Al ·	Si ·	P ·	S :	Cl :	Ar :
Period 4	K ·	Ca :	Ga ·	Ge ·	As ·	Se :	Br :	Kr :
Period 5	Rb ·	Sr :	In ·	Sn ·	Sb ·	Te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

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The chemical bond

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





Elementary cells in cubic crystal lattice

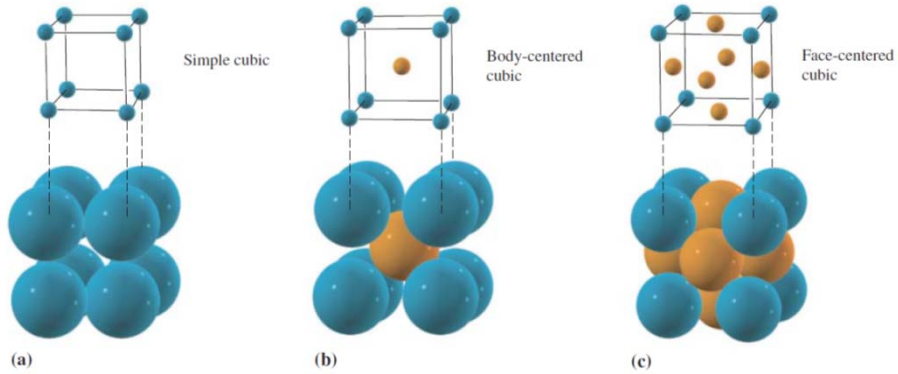
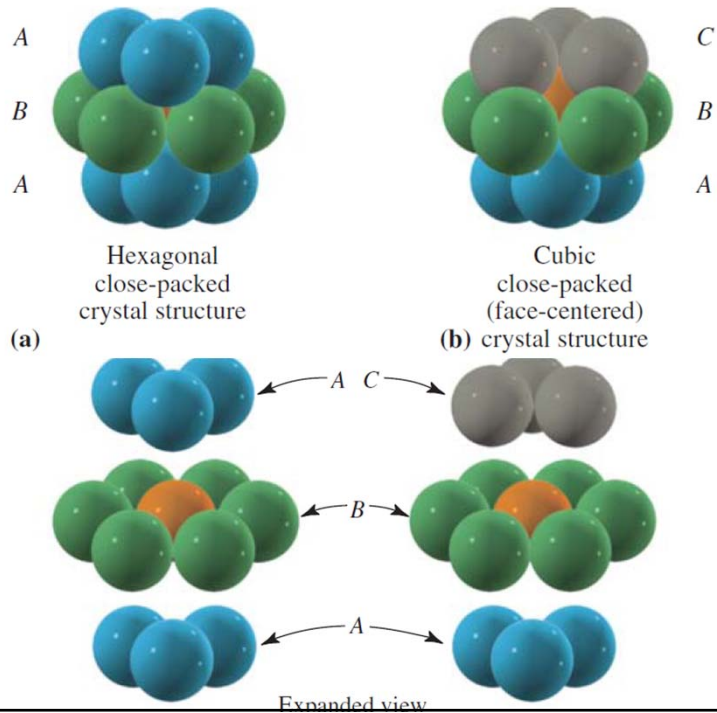


Figure 13-25 Unit cells for (a) simple cubic, (b) body-centered cubic, and (c) face-centered cubic. The spheres in each figure represent *identical* atoms or ions; different colors are shown *only* to help you visualize the spheres in the center of the cube in body-centered cubic (b) and in face-centered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

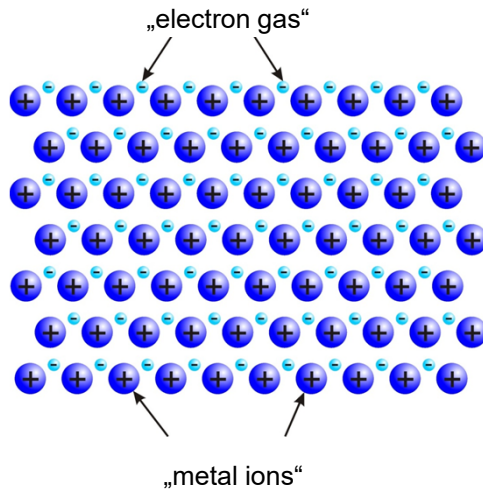
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Chemical bonds: metallic



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Band model

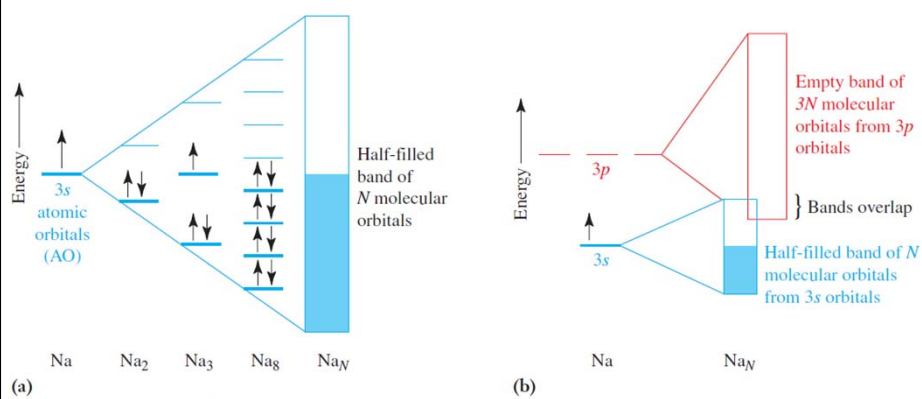


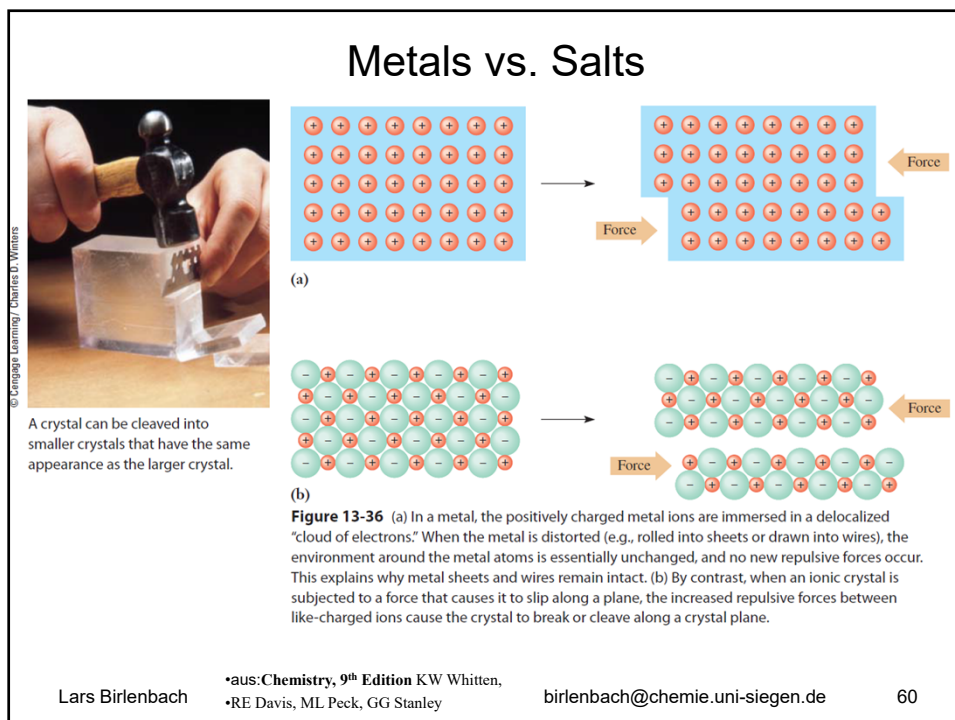
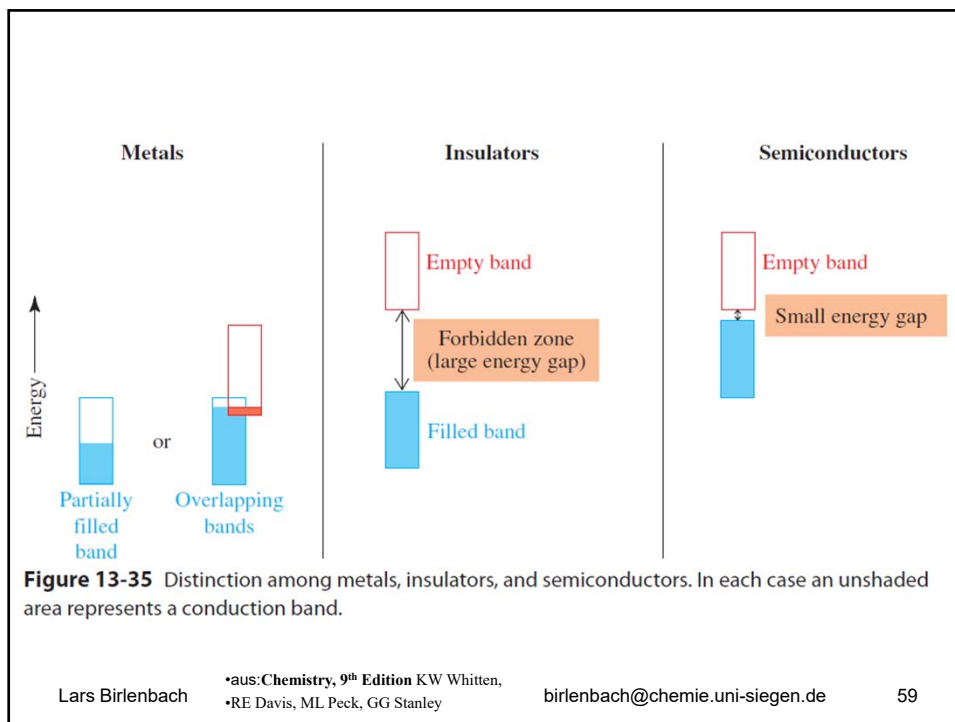
Figure 13-33 (a) The band of orbitals resulting from interaction of the $3s$ orbitals in a crystal of sodium. (b) Overlapping of a half-filled " $3s$ " band (blue) with an empty " $3p$ " band (red) of Na_N crystal.

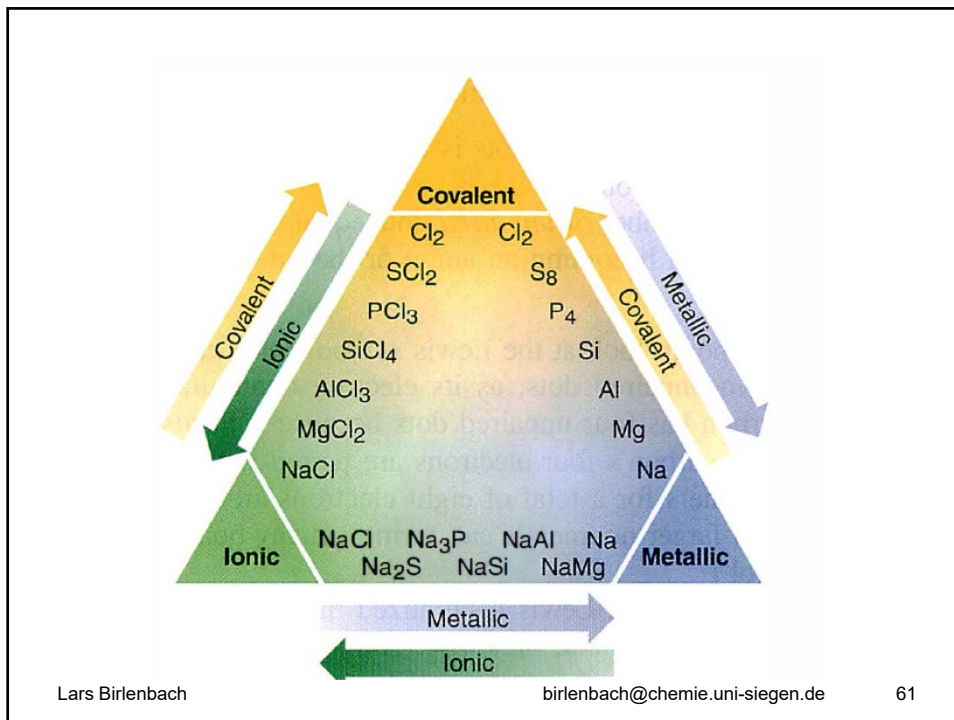
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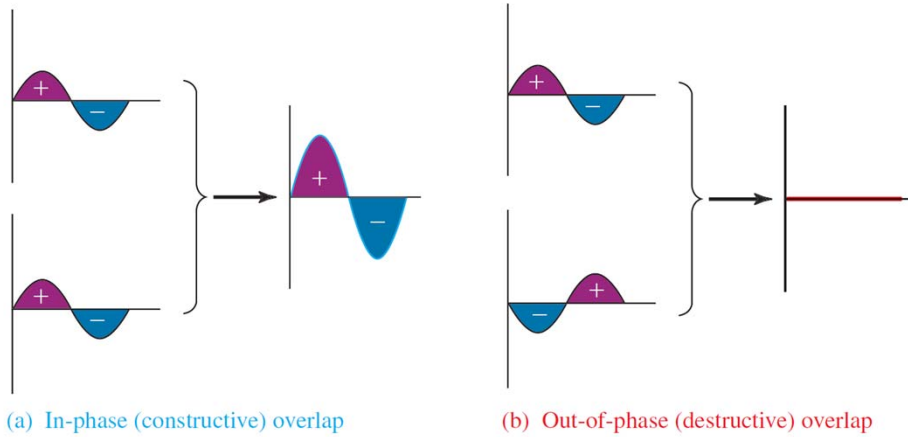


The covalent bond

The covalent bond

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Superposition of wave functions



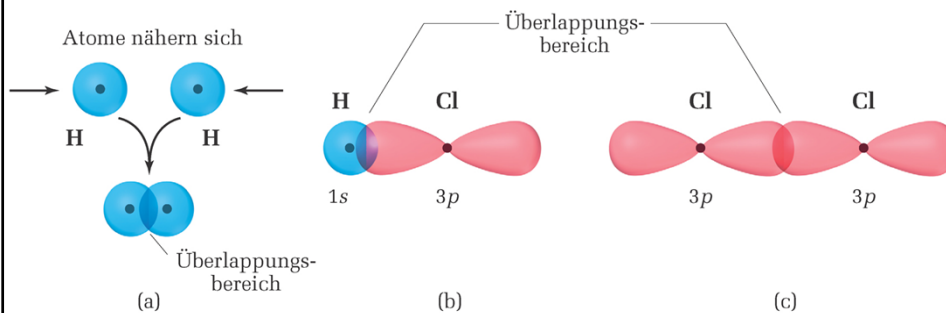
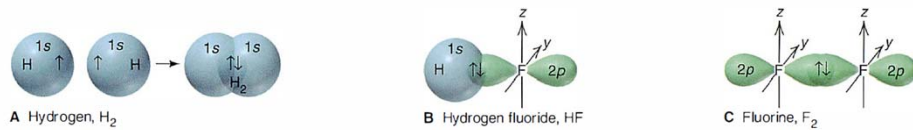
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Covalent bond

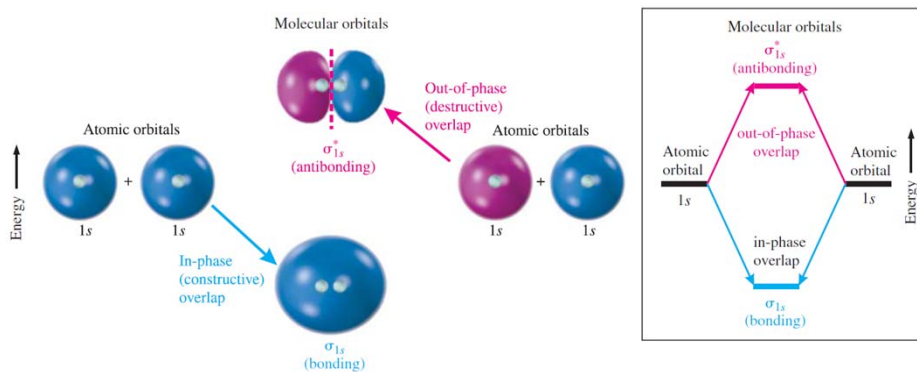


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σ -1s-Molecular orbitals



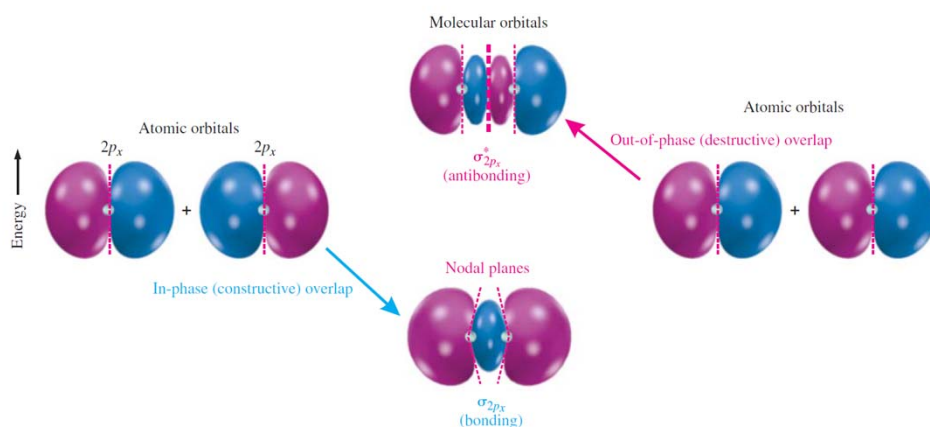
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σ -2p-Molecular orbitals



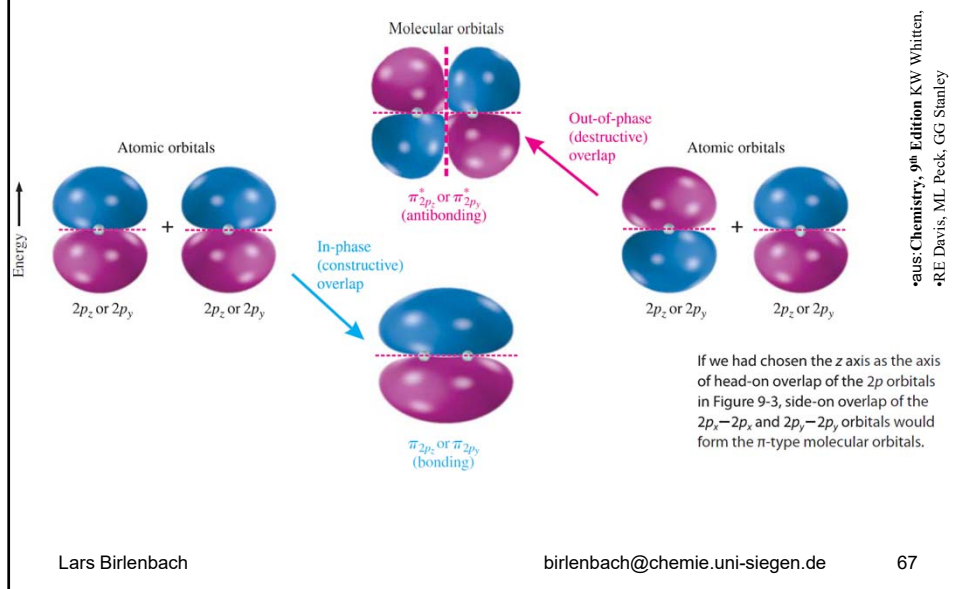
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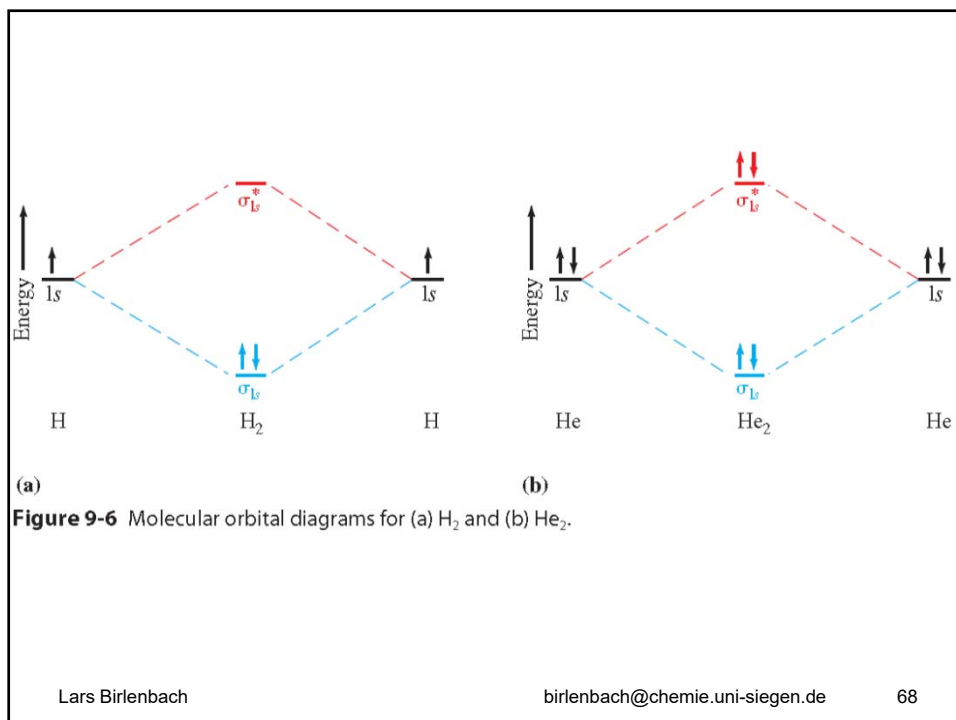
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Π -2p-Molecular orbitals



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	H ₂	He ₂ ^c	Li ₂ ^b	Be ₂ ^c	B ₂ ^b	C ₂ ^b	N ₂	
Increasing energy (not to scale)	σ_{2p}^*	—	—	—	—	—	—	
	$\pi_{2p_y}^*, \pi_{2p_z}^*$	—	—	—	—	—	—	
	σ_{2p}	—	—	—	—	—	$\uparrow\downarrow$	
	π_{2p_y}, π_{2p_z}	—	—	—	—	$\uparrow \uparrow$	$\uparrow\downarrow \uparrow\downarrow$	
	σ_{2s}^*	—	—	—	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
	σ_{2s}	—	—	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
	σ_{1s}^*	—	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
	σ_{1s}	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
Paramagnetic?	no	no	no	no	yes	no	no	
Bond order	1	0	1	0	1	2	3	
Observed bond length (Å)	0.74	—	2.67	—	1.59	1.31	1.09	
Observed bond energy (kJ/mol)	436	—	110	9	≈ 270	602	945	
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	O ₂	F ₂	Ne ₂ ^c	
	—	—	$\uparrow\downarrow$	
	$\uparrow \uparrow$	$\uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow$	
	π_{2p_y}, π_{2p_z}	$\uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow$
	σ_{2p}	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$
	yes	no	no	
	2	1	0	
	1.21	1.43	—	
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	H ₂	He ₂ ⁺	Li ₂ ⁺	Be ₂ ⁺	B ₂ ⁺	C ₂ ⁺	N ₂	O ₂	F ₂	Ne ₂ ⁺
Increasing energy (not to scale)	σ_{2p}^*	—	—	—	—	—	—	—	—	↑↓
	π_{2py}^*, π_{2pz}^*	—	—	—	—	—	—	↑ ↑	↑↓ ↑↓	↑↓ ↑↓
	σ_{2p}	—	—	—	—	—	↑↓	π_{2py}, π_{2pz}	↑↓ ↑↓	↑↓ ↑↓
	π_{2py}, π_{2pz}	—	—	—	—	↑ ↑	↑↓ ↑↓	σ_{2p}	↑↓	↑↓
	σ_{2z}^*	—	—	—	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓
	σ_{2z}	—	—	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓
	σ_{1z}^*	—	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓
	σ_{1z}	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓
Paramagnetic?	no	no	no	no	yes	no	no	yes	no	no
Bond order	1	0	1	0	1	2	3	2	1	0
Observed bond length (Å)	0.74	—	2.67	—	1.59	1.31	1.09	1.21	1.43	—
Observed bond energy (kJ/mol)	436	—	110	9	≈ 270	602	945	498	155	—

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