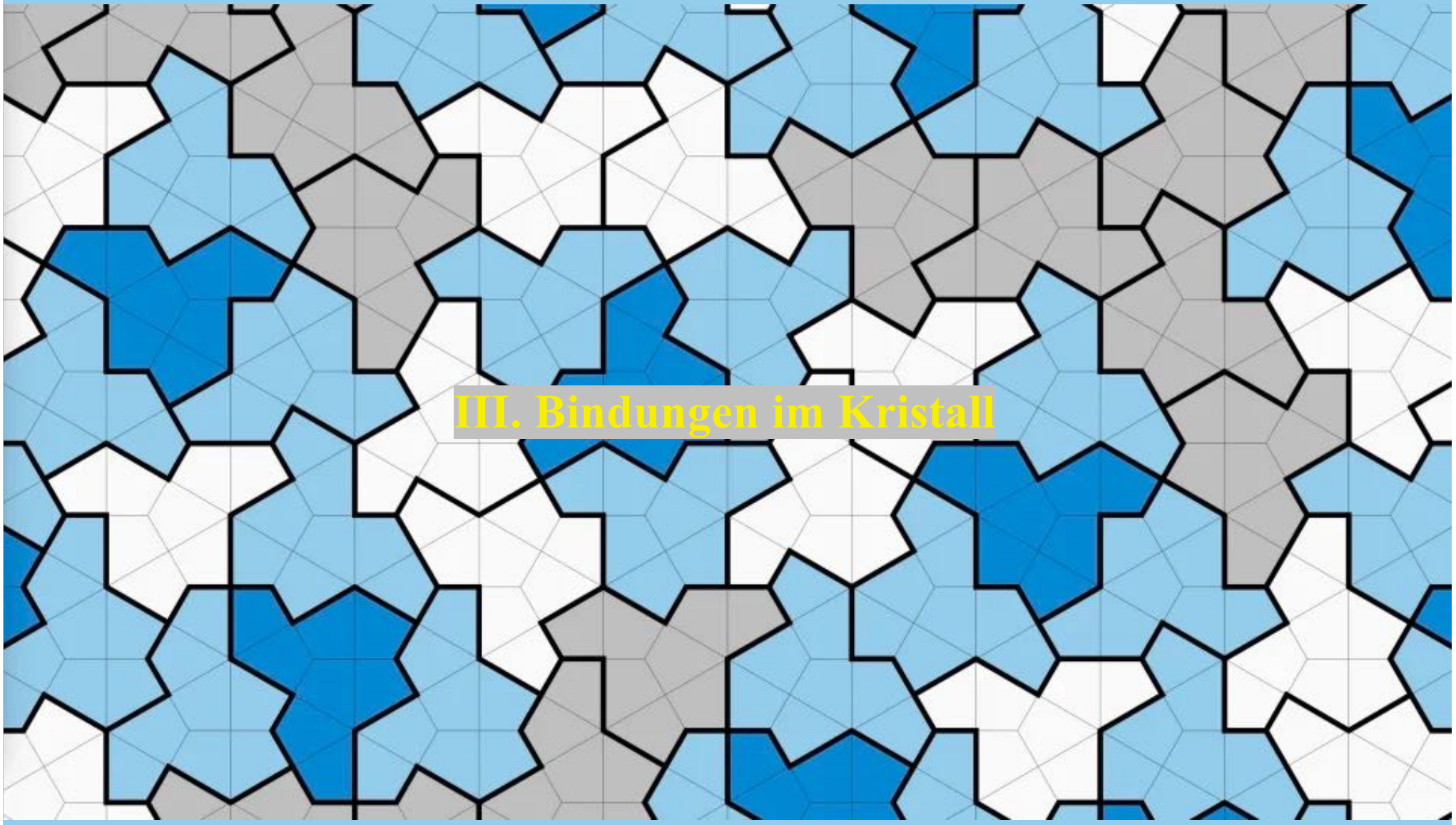
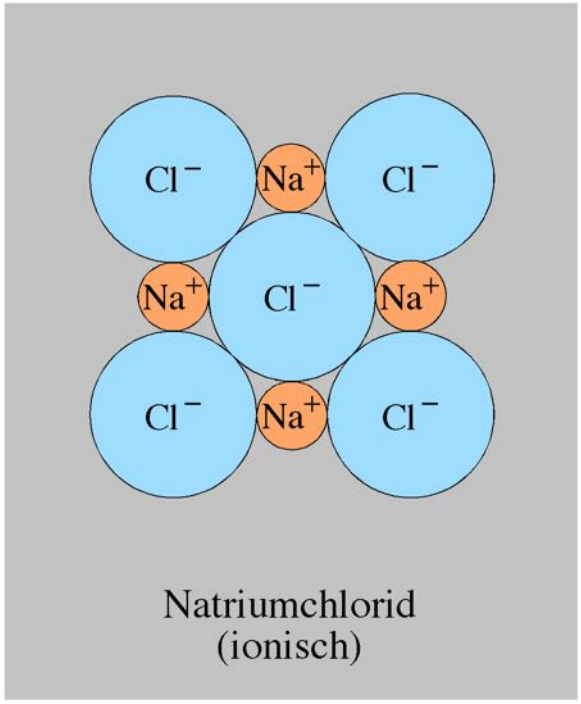
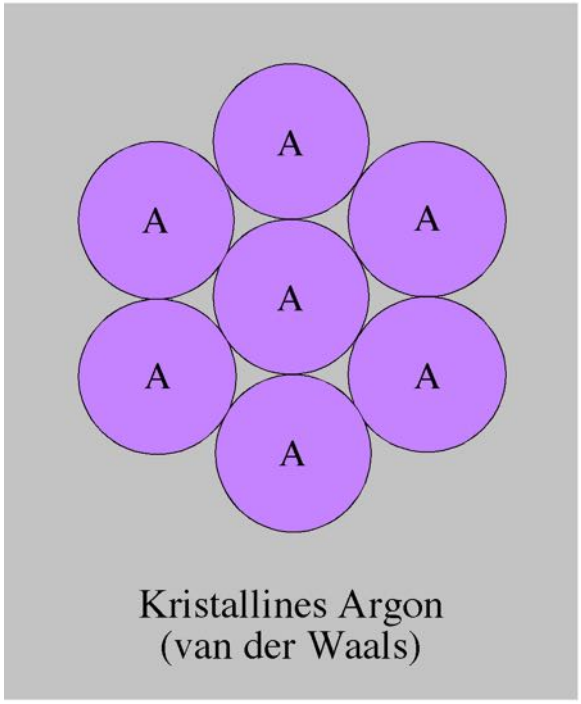


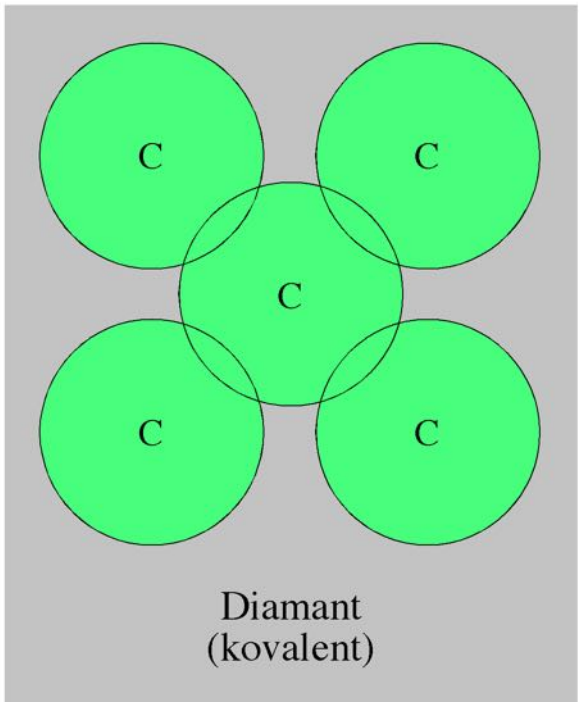
III. Bindungen im Kristall



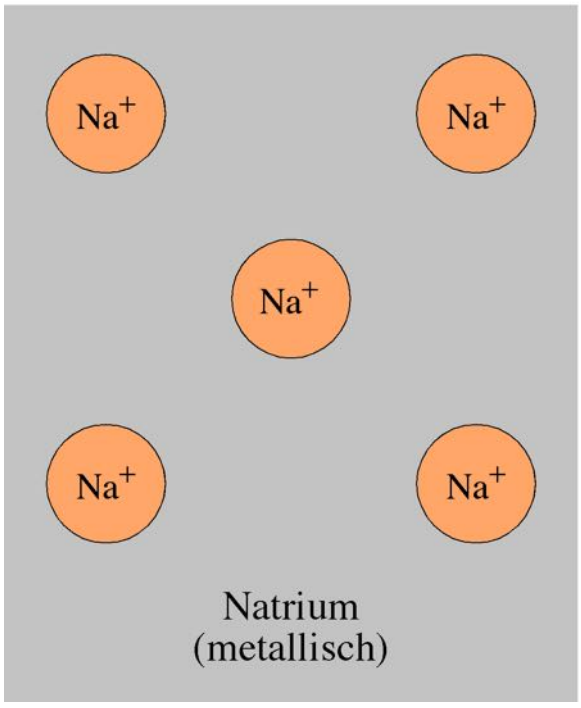
Natriumchlorid
(ionisch)



Kristallines Argon
(van der Waals)



Diamant
(kovalent)



Natrium
(metallisch)

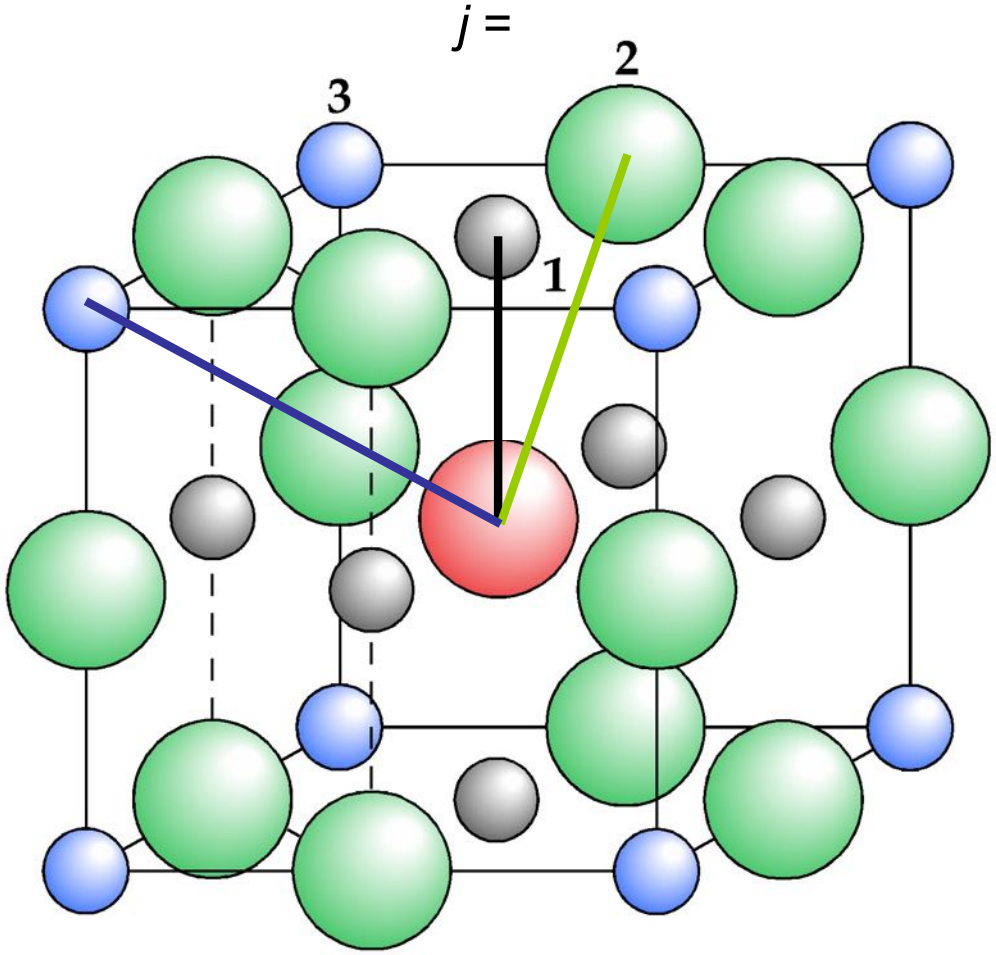
Bindungstyp	Beispiel	Bindungsenergie (eV)
Ionisch	NaCl LiF	8.23 10.92
Van-der-Waals	Ar Kr	0.080 0.116
Kovalent	Diamant Si	7.36 4.64
Metallisch	Na Fe W	1.13 4.29 8.66
Wasserstoff-Brücken	H_2O HF	0.52 0.30

Bindungsenergien

Angegeben ist die pro Atom notwendige Energie, um aus einem Festkörper bei 0 K und 1 atm freie, neutrale Atome in ihrem Grundzustand zu bilden. Die Daten wurden von Prof. Leo Brewer in der Einheit kcal/mol angegeben, nach dem LBL-Report 3720 vom 4.Mai 1977.

Li	**Be**											**B**	**C**	**N**	**O**	**F**	**Ne**
158.	320.											561	711.	474.	251.	81.0	1.92
1.63	3.32											5.81	7.37	4.92	2.60	0.84	0.020
37.7	76.5											134	170.	113.4	60.03	19.37	0.46
Na	**Mg**											**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
107.	145.	← kJ/mol →										327.	446.	331.	275.	135.	7.74
1.113	1.51	← eV/atom →										3.39	4.63	3.43	2.85	1.40	0.080
25.67	34.7	← kcal/mol →										78.1	106.7	79.16	65.75	32.2	1.85
K	**Ca**	**Sc**	**Ti**	**V**	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**	**Zn**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
90.1	178.	376	468.	512.	395.	282.	413.	424.	428.	336.	130	271.	372.	285.3	237	118.	11.2
0.934	1.84	3.90	4.85	5.31	4.10	2.92	4.28	4.39	4.44	3.49	1.35	2.81	3.85	2.96	2.46	1.22	0.116
21.54	42.5	89.9	111.8	122.4	94.5	67.4	98.7	101.3	102.4	80.4	31.04	64.8	88.8	68.2	56.7	28.18	2.68
Rb	**Sr**	**Y**	**Zr**	**Nb**	**Mo**	**Tc**	**Ru**	**Rh**	**Pd**	**Ag**	**Cd**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
82.2	166.	422.	603.	730.	658.	661.	650.	554.	376.	284.	112.	243.	303.	265.	211.	107.	15.9
0.852	1.72	4.37	6.25	7.57	6.82	6.85	6.74	5.75	3.89	2.95	1.16	2.52	3.14	2.75	2.19	1.11	0.16
19.64	39.7	100.8	144.2	174.5	157.2	158.	155.4	132.5	89.8	68.0	26.73	58.1	72.4	63.4	50.34	25.62	3.80
Cs	**Ba**	**La**	**Hf**	**Ta**	**W**	**Re**	**Os**	**Ir**	**Pt**	**Au**	**Hg**	**Tl**	**Pb**	**Bi**	**Po**	**At**	**Rn**
77.6	183.	431.	621.	782.	859.	775.	788.	670.	564.	368.	65.	182.	196.	210.	144.		19.5
0.804	1.90	4.47	6.44	8.10	8.90	8.03	8.17	6.94	5.84	3.81	0.67	1.88	2.03	2.18	1.50		0.202
18.54	43.7	103.1	148.4	186.9	205.2	185.2	188.4	160.1	134.7	87.96	15.5	43.4	46.78	50.2	34.5		4.66
Fr	**Ra**	**Ac**															
	160.	410.															
	1.66	4.25															
	38.2	98.															

Ce	**Pr**	**Nd**	**Pm**	**Sm**	**Eu**	**Gd**	**Tb**	**Dy**	**Ho**	**Er**	**Tm**	**Yb**	**Lu**
417.	357.	328.		206.	179.	400.	391.	294.	302.	317.	233.	154.	428.
4.32	3.70	3.40		2.14	1.86	4.14	4.05	3.04	3.14	3.29	2.42	1.60	4.43
99.7	85.3	78.5		49.3	42.8	95.5	93.4	70.2	72.3	75.8	55.8	37.1	102.2
Th	**Pa**	**U**	**Np**	**Pu**	**Am**	**Cm**	**Bk**	**Cf**	**Es**	**Fm**	**Md**	**No**	**Lr**
598.		536.	456	347.	264.	385							
6.20		5.55	4.73	3.60	2.73	3.99							
142.9		128.	109.	83.0	63.	92.1							

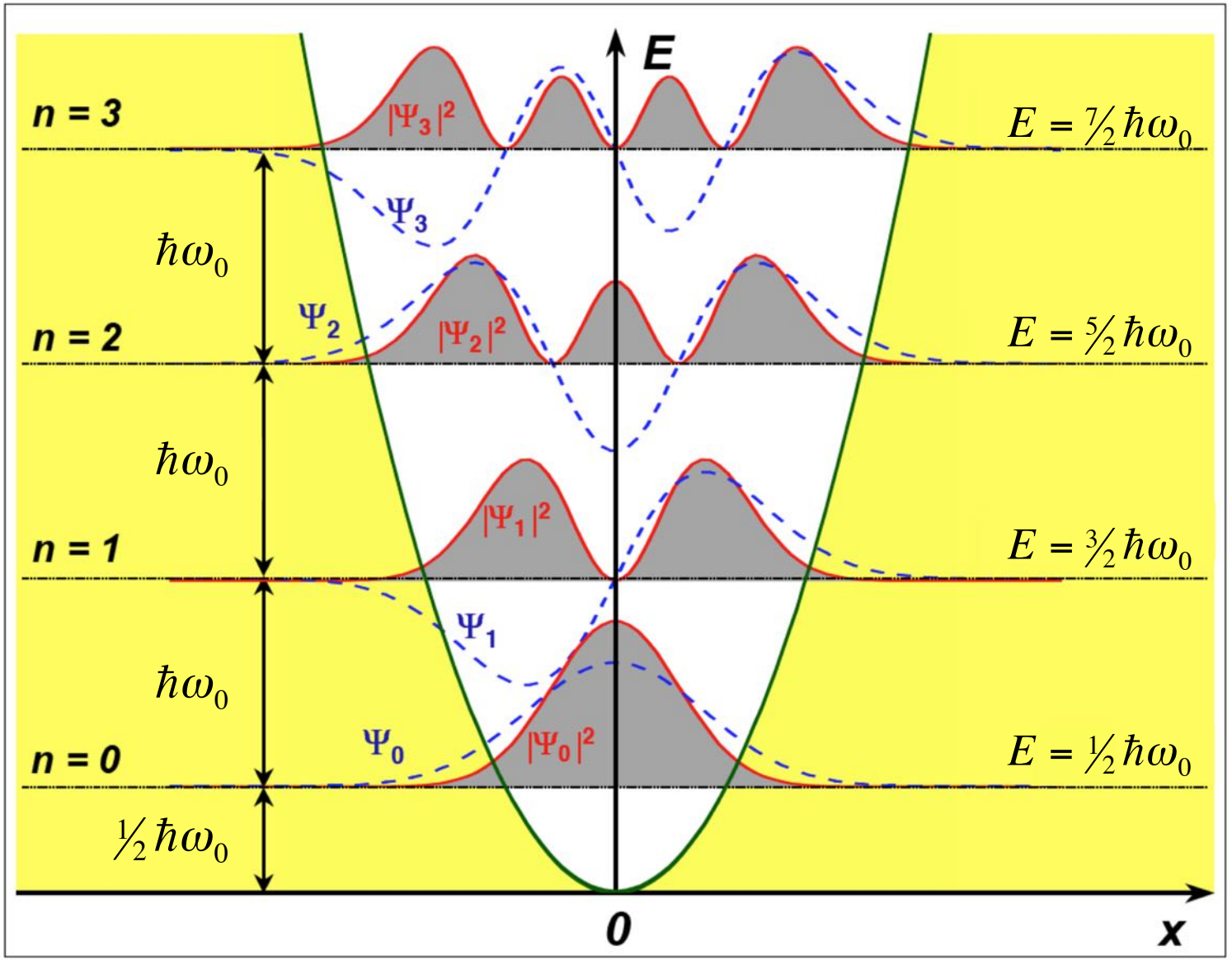


NaCl Struktur mit nächsten, übernächsten und über-übernächsten Nachbarn

$$\alpha = -\sum_j \frac{\pm 1}{p_j} = \frac{6}{1} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \ldots = 1.748$$

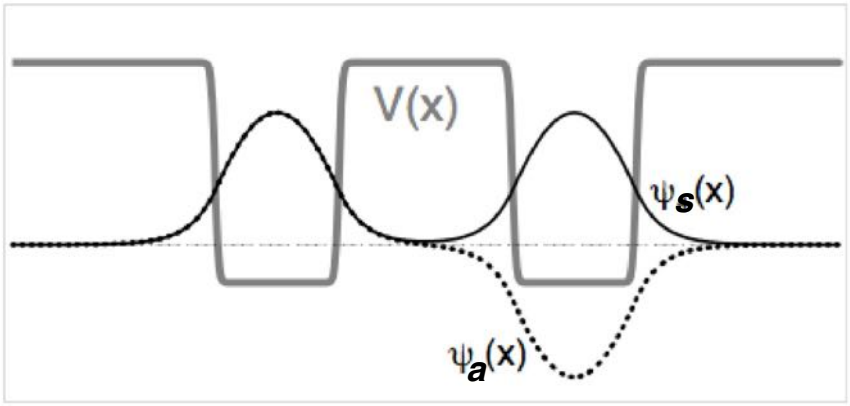
Strukturtyp	Beispiel	α
NaCl	NaCl, AgBr, EuS	1.748
CsCl	CsCl, CsBr, TlBr	1.763
Zinkblende ZnS	ZnS, CuCl, GaAs	1.638
Fluorit CaF_2	CaF_2, LaH_2, VO_2	5.039
Korund Al_2O_3	Al_2O_3, V_2O_3 , Cr_2O_3	25.031
Perovskit $CaTiO_3$	$CaTiO_3$, $BaTiO_3$	12.377

1D- quantenmechanischer harmonischer Oszillator mit ω_0



"Topfmolekül"

a)



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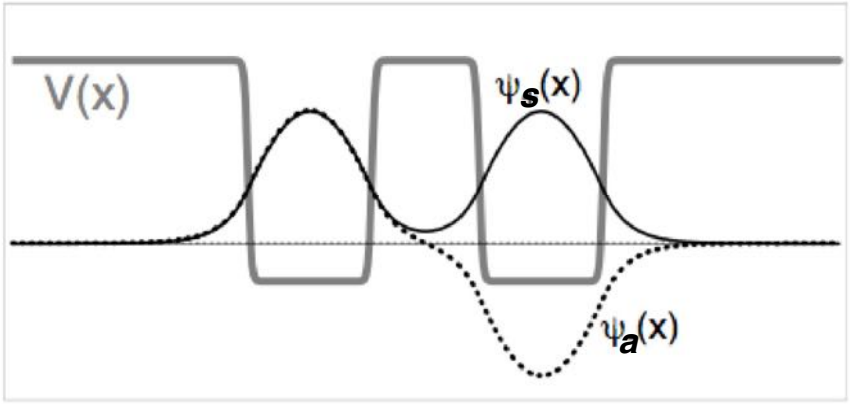

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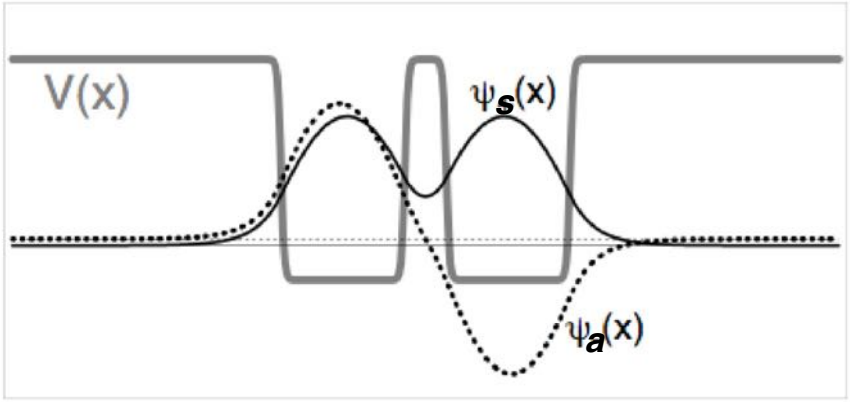
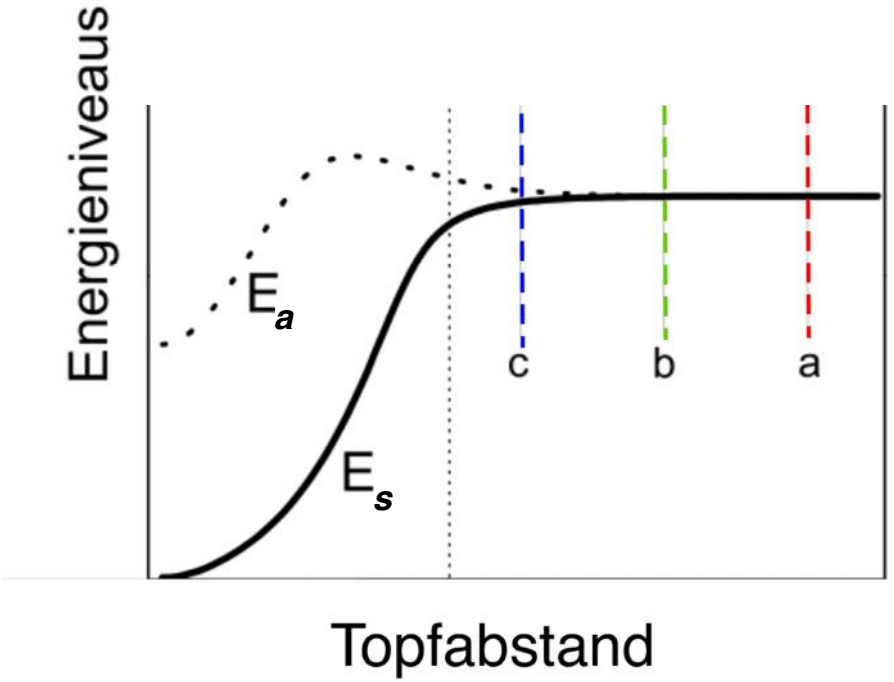
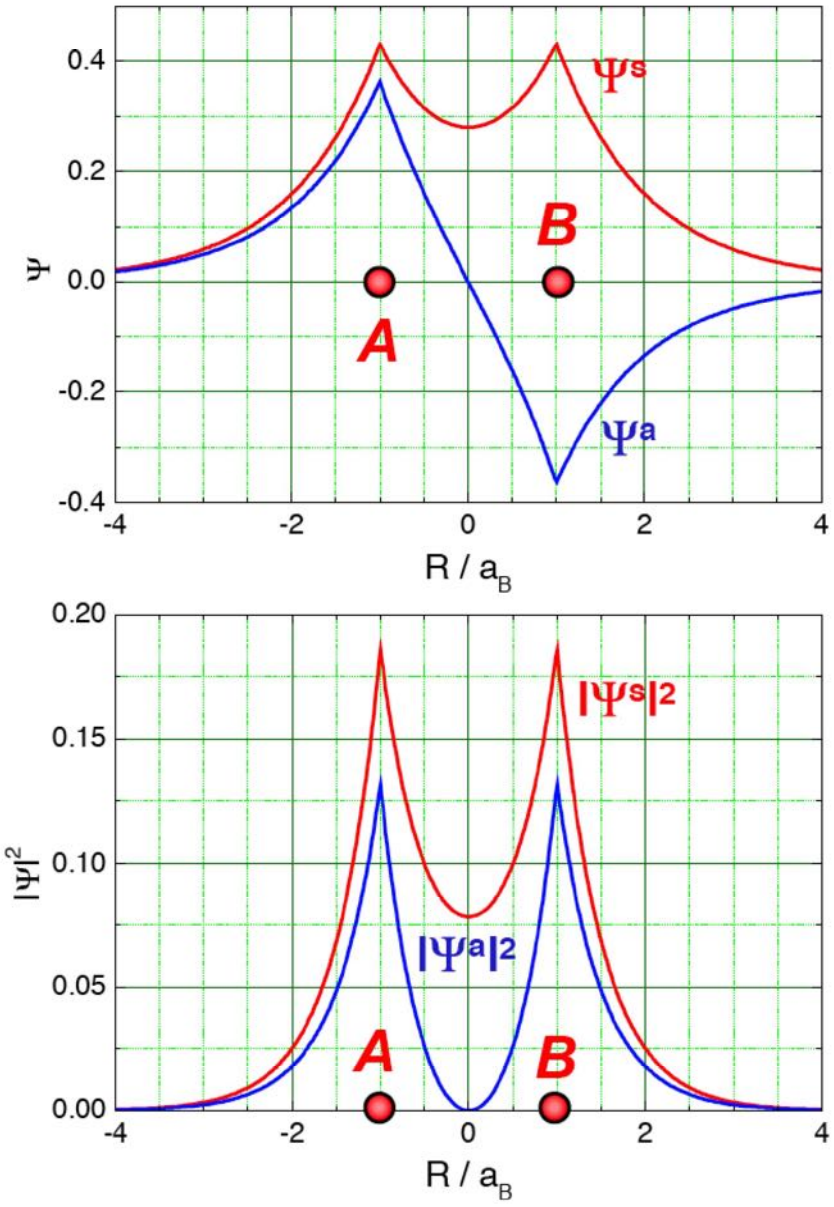
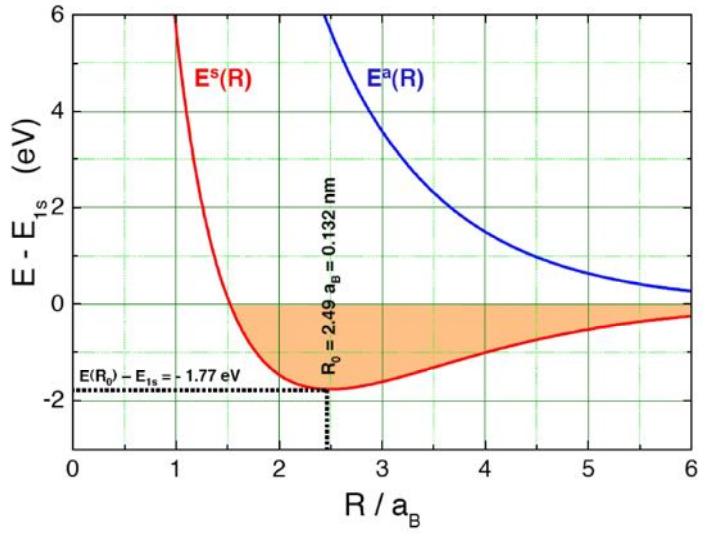




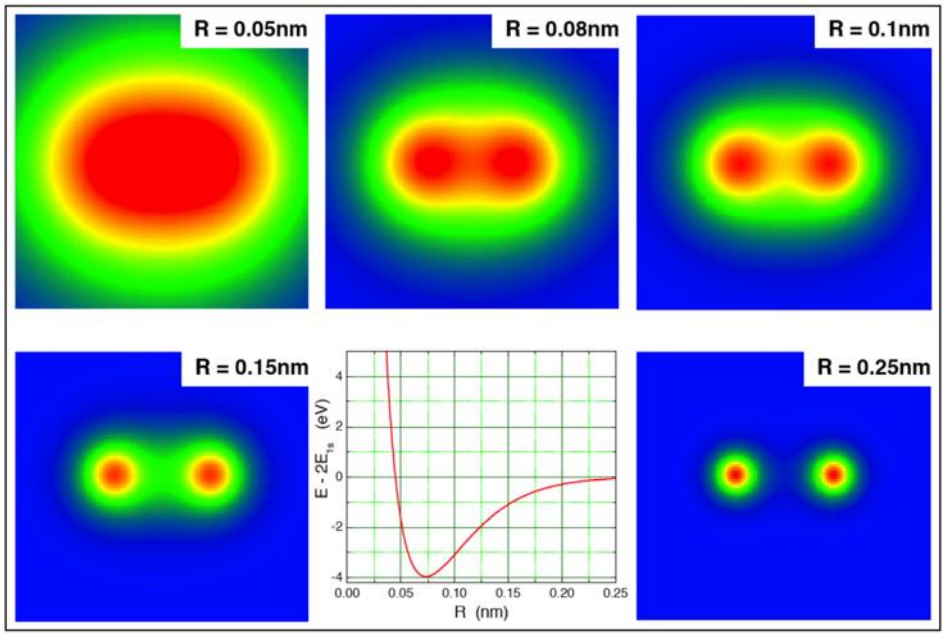
H_2^+ Ion

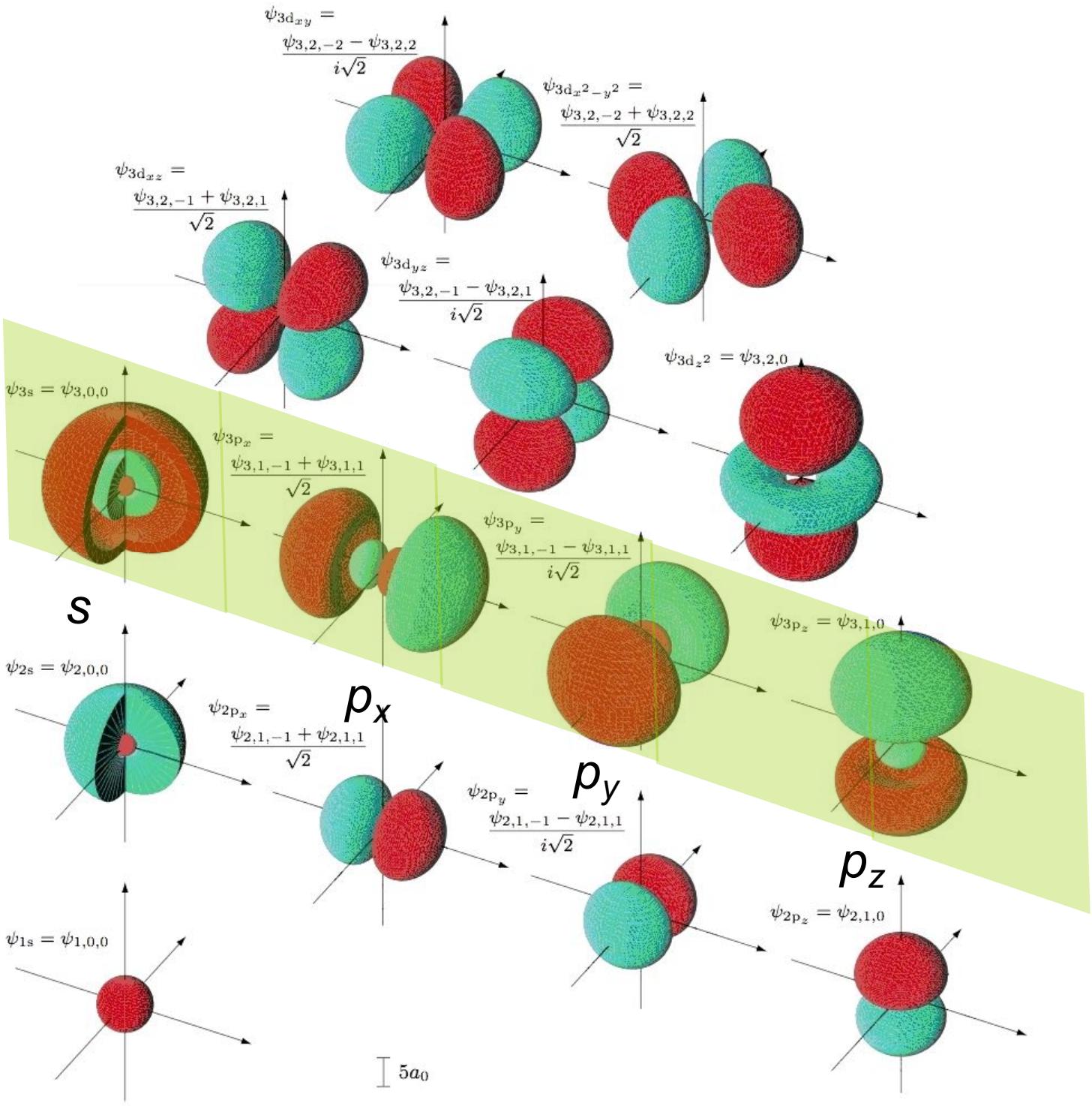

0.4
0.2
0.0
-0.2
-0.4
Ψ
Ψs
Ψa
A
B
-4
-2
0
2
4
R / a_B
0.20
0.15
0.10
0.05
0.00
|Ψ|2
|Ψs|2
|Ψa|2
A
B
-4
-2
0
2
4
R / a_B

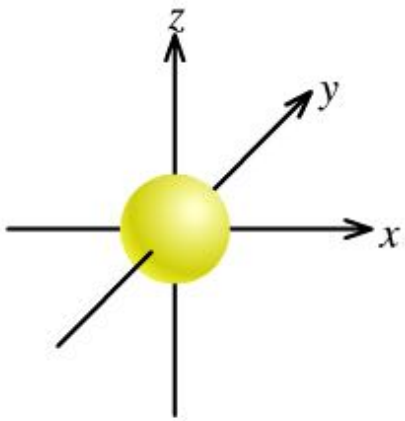
H_2^+-Molekül



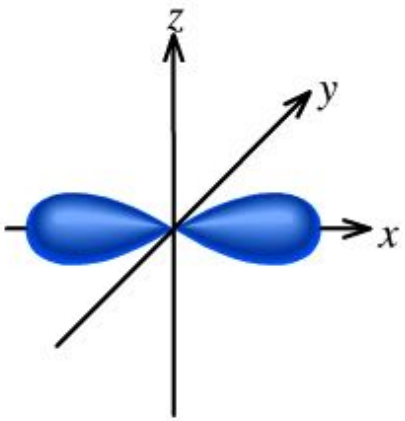
H_2-Molekül



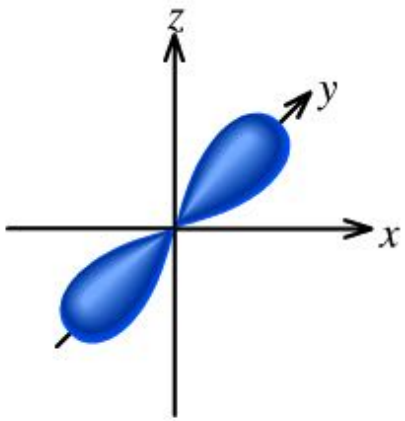

$\psi_{3d_{xy}} = \frac{\psi_{3,2,-2} - \psi_{3,2,2}}{i\sqrt{2}}$
$\psi_{3d_{x^2-y^2}} = \frac{\psi_{3,2,-2} + \psi_{3,2,2}}{\sqrt{2}}$
$\psi_{3d_{xz}} = \frac{\psi_{3,2,-1} + \psi_{3,2,1}}{\sqrt{2}}$
$\psi_{3d_{yz}} = \frac{\psi_{3,2,-1} - \psi_{3,2,1}}{i\sqrt{2}}$
$\psi_{3d_{z^2}} = \psi_{3,2,0}$
$\psi_{3s} = \psi_{3,0,0}$
$\psi_{3p_x} = \frac{\psi_{3,1,-1} + \psi_{3,1,1}}{\sqrt{2}}$
$\psi_{3p_y} = \frac{\psi_{3,1,-1} - \psi_{3,1,1}}{i\sqrt{2}}$
$\psi_{3p_z} = \psi_{3,1,0}$
s
$\psi_{2s} = \psi_{2,0,0}$
$\psi_{2p_x} = \frac{\psi_{2,1,-1} + \psi_{2,1,1}}{\sqrt{2}}$
p_x
$\psi_{2p_y} = \frac{\psi_{2,1,-1} - \psi_{2,1,1}}{i\sqrt{2}}$
p_y
p_z
$\psi_{2p_z} = \psi_{2,1,0}$
$\psi_{1s} = \psi_{1,0,0}$
$5a_0$



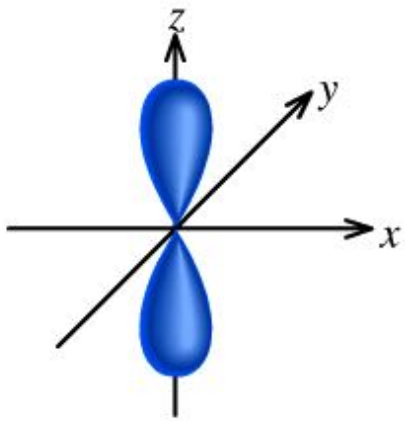
ψ_s



ψ_{px}



ψ_{py}



ψ_{pz}

ψsp^3_1

ψsp^3_2

ψsp^3_3

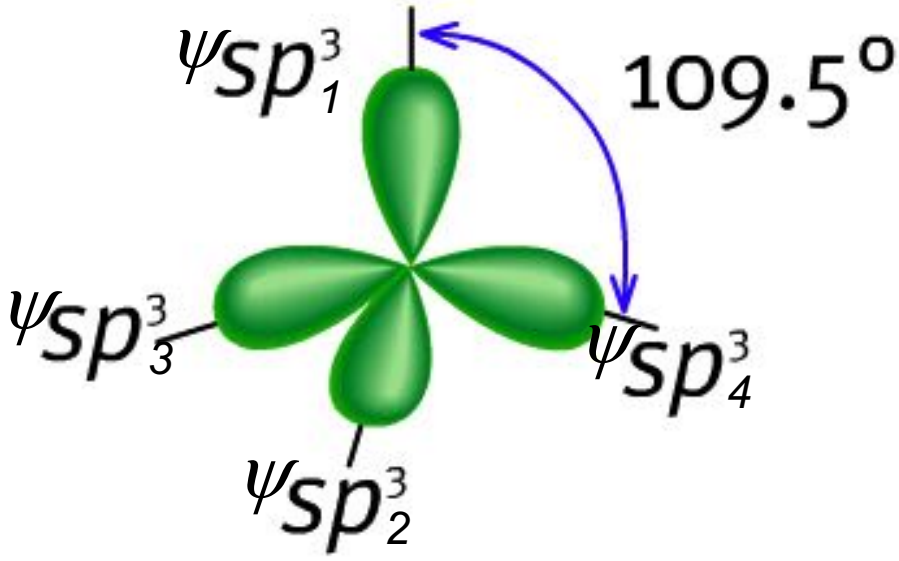
ψsp^3_4

$1/2(\psi_s + \psi_{px} + \psi_{py} + \psi_{pz})$

$1/2(\psi_s + \psi_{px} - \psi_{py} - \psi_{pz})$

$1/2(\psi_s - \psi_{px} + \psi_{py} - \psi_{pz})$

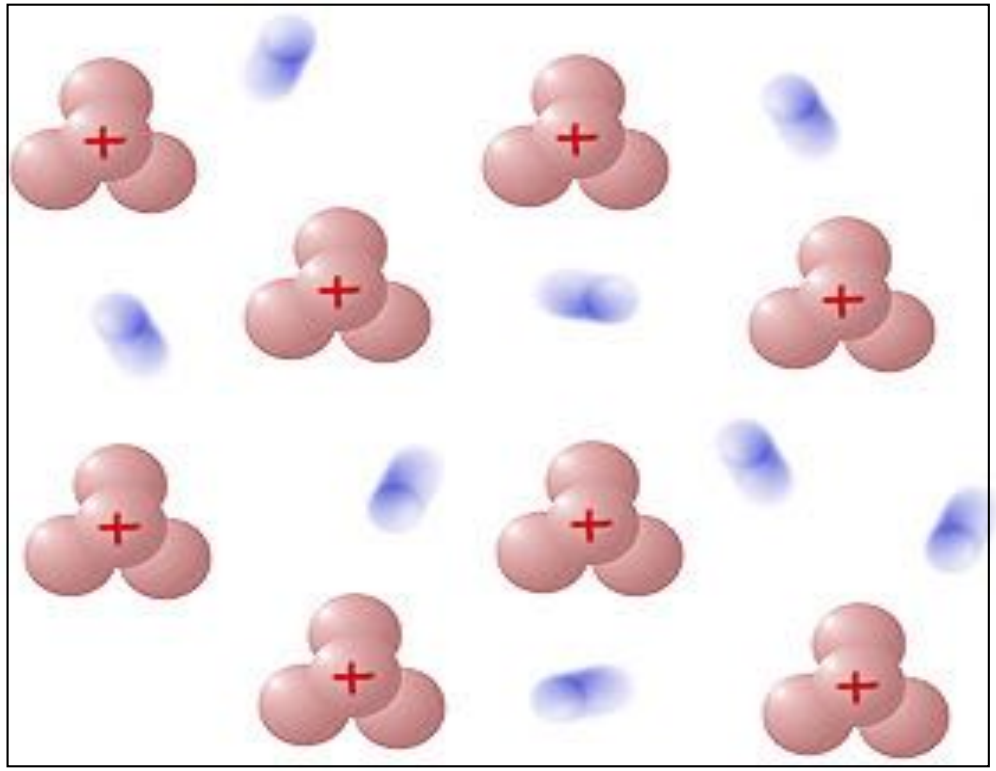
$1/2(\psi_s - \psi_{px} - \psi_{py} + \psi_{pz})$



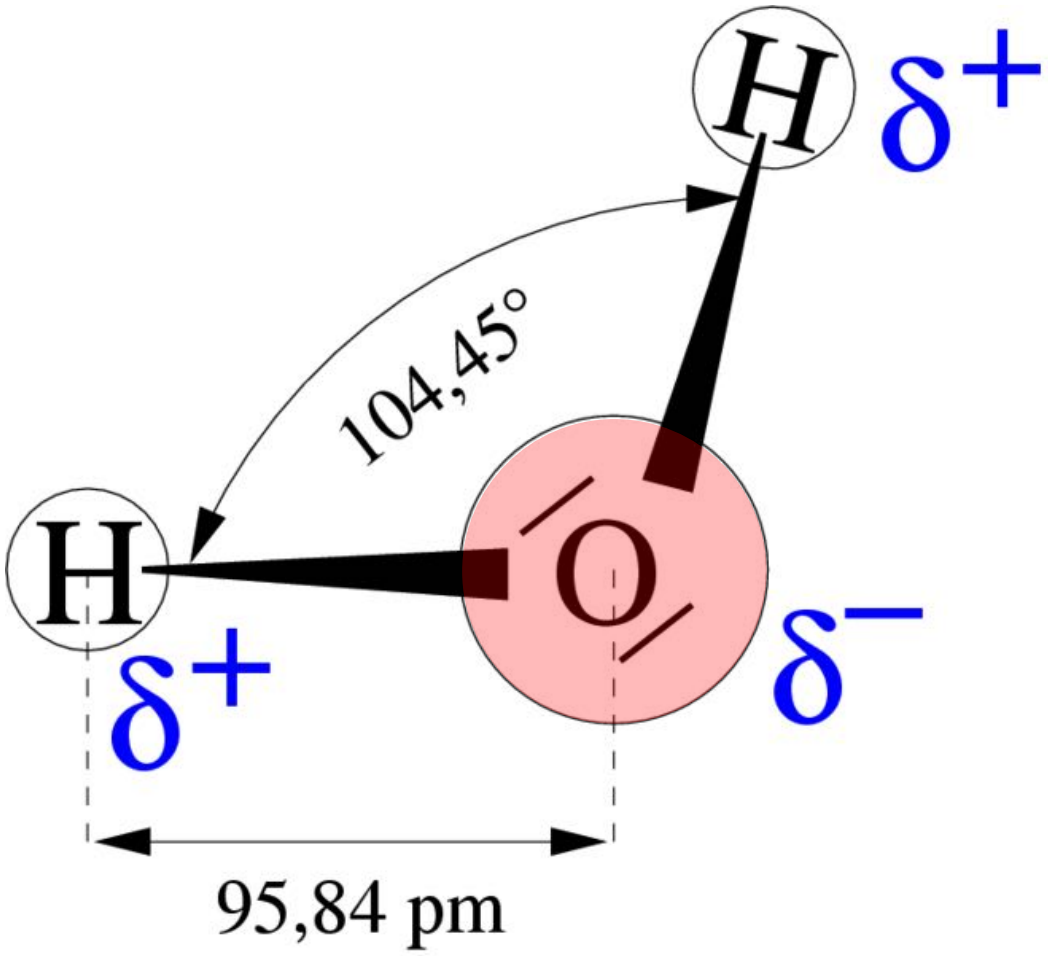
Tetraeder

Einfaches Modell eines Metalles

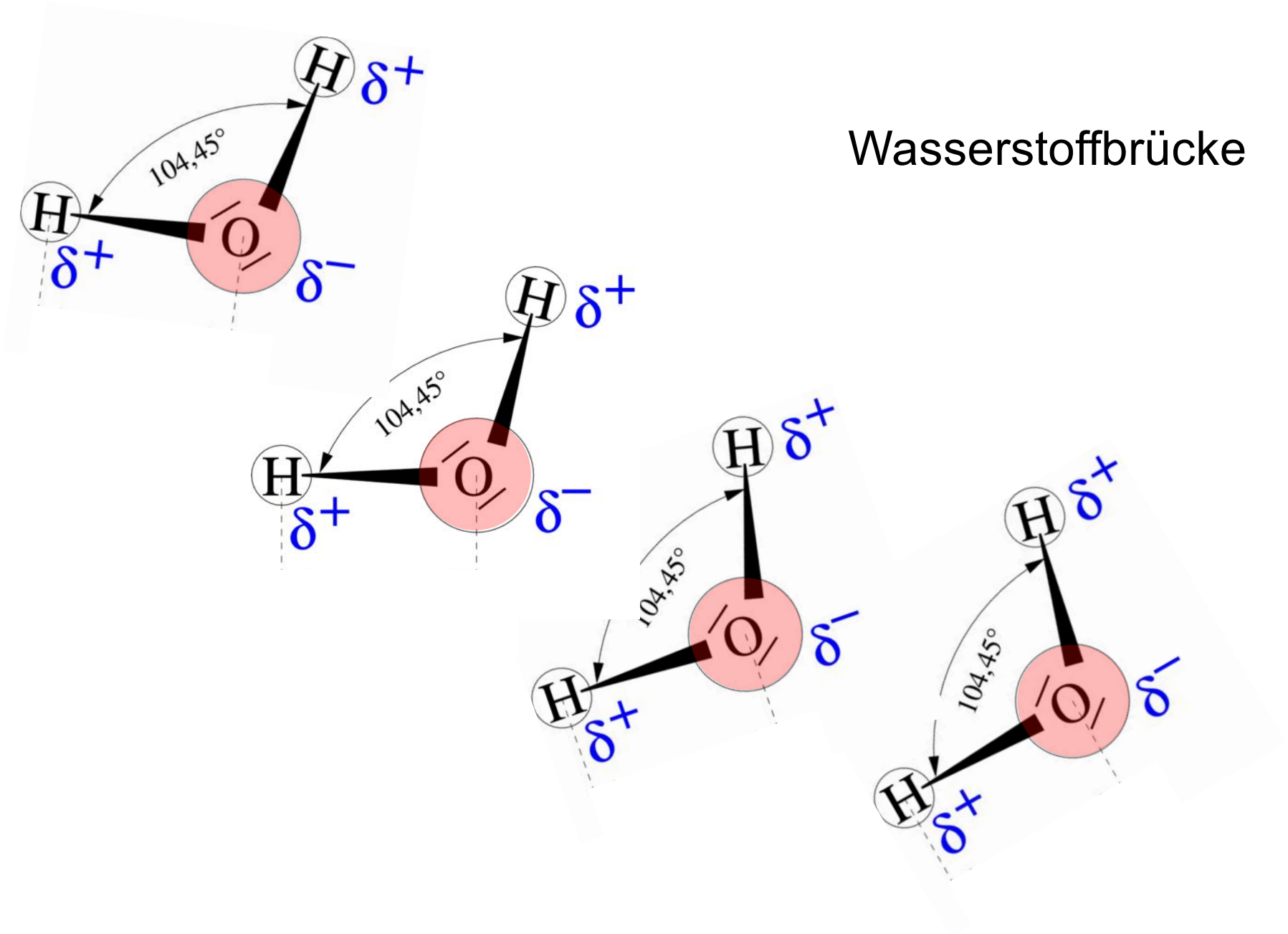
Atomrümpfe

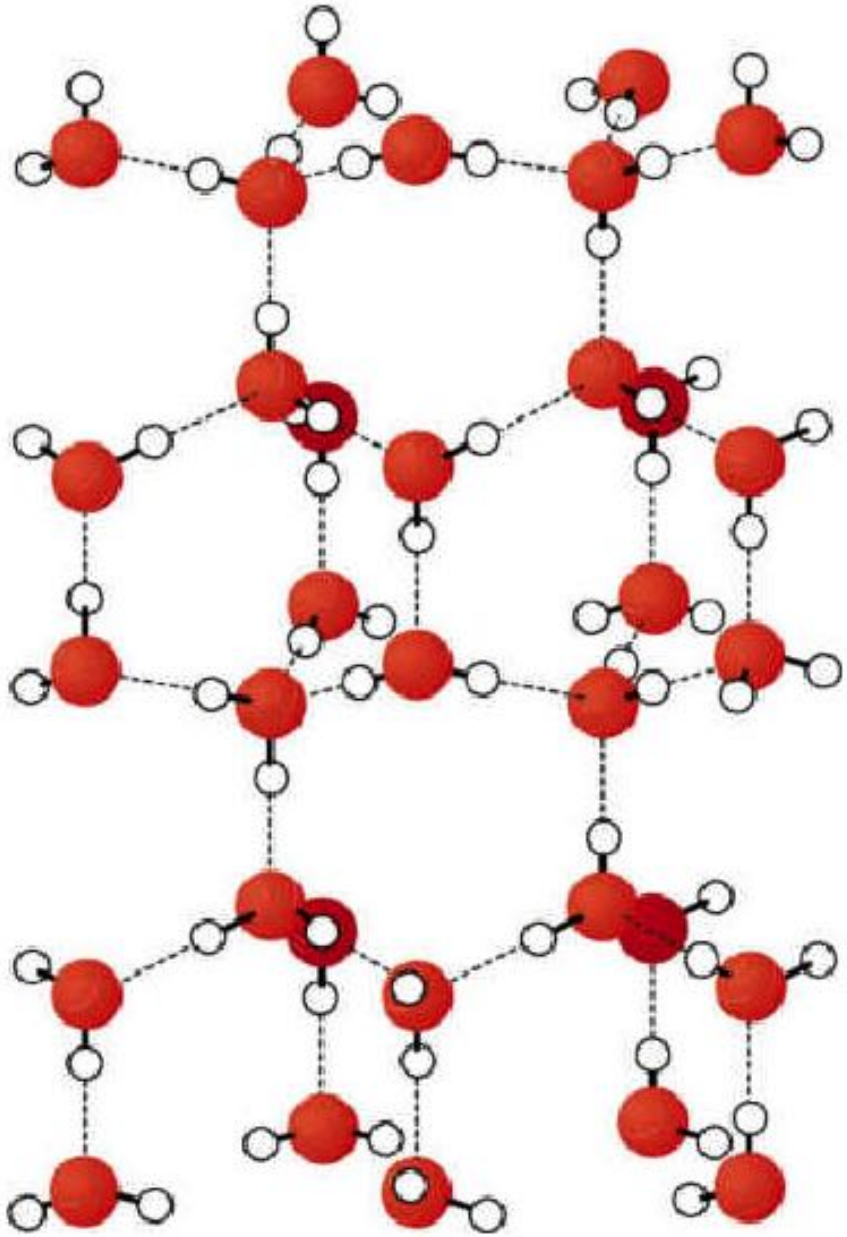


delokalisierte
äussere Elektronen


H
δ+
104,45°
H
O
δ+
δ−
95,84 pm

Wasserstoffbrücke





Wassereis