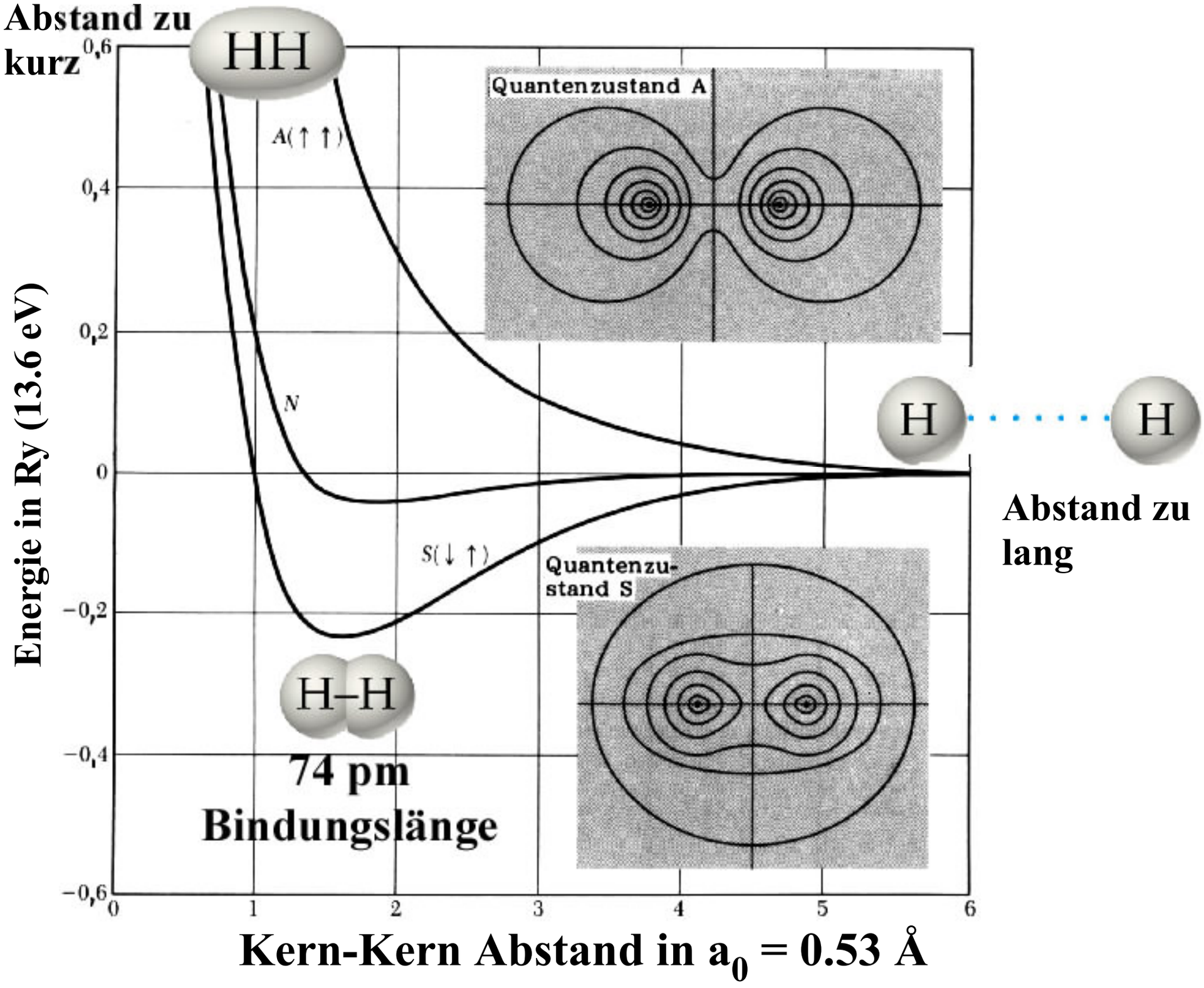
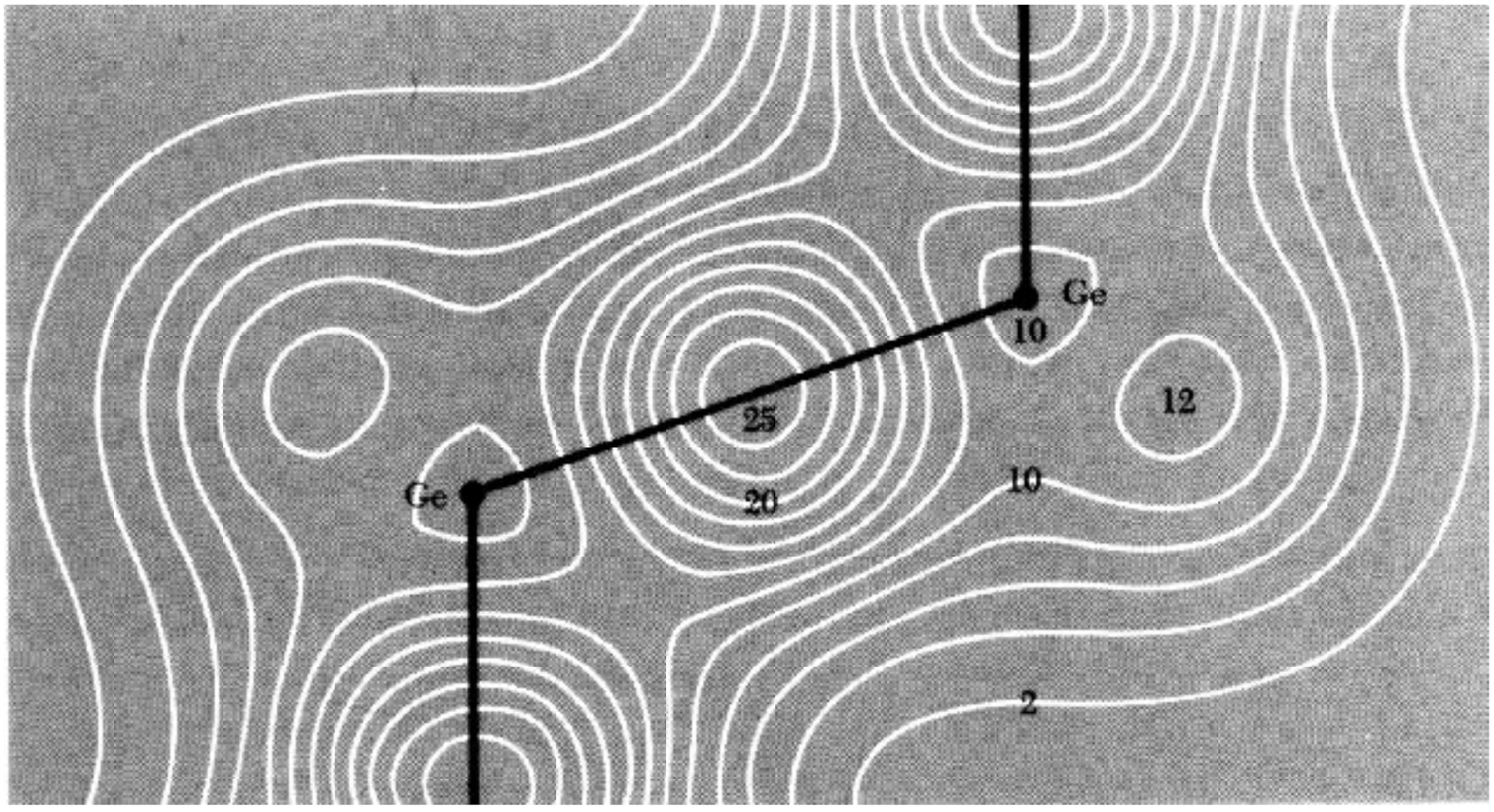
Potenzial

Energie der Molekülorbitale als Funktion des Abstandes

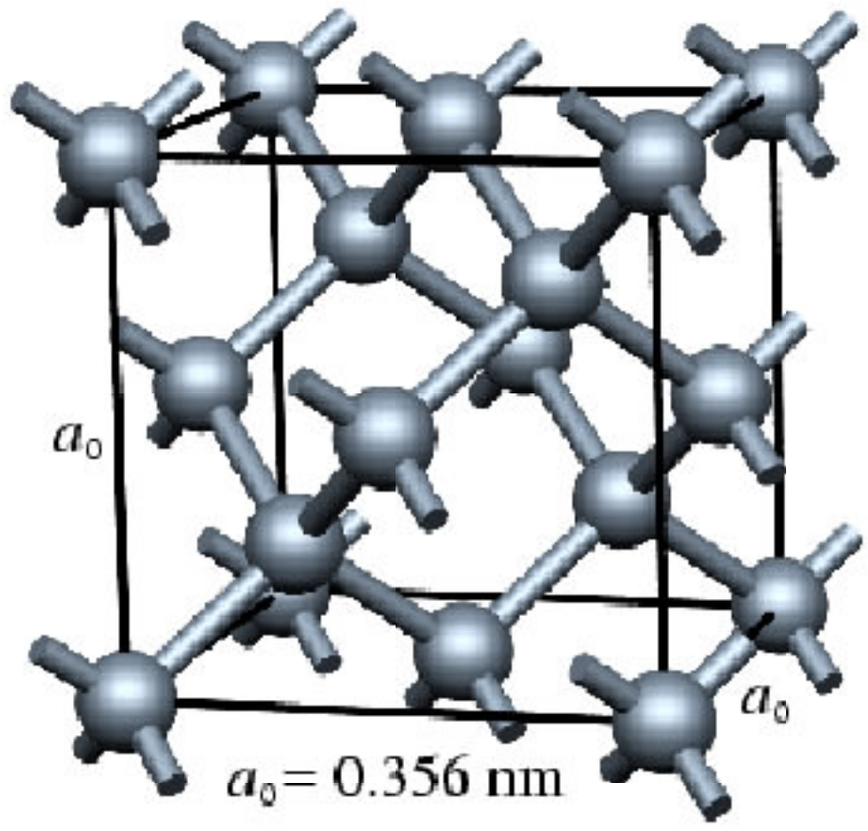


Kovalente Bindung

Elektronendichte in Germanium



Diamant



Elektronendichte nicht kugelsymmetrisch

Oft tetraedrische Koordination

Kovalente Festkörper sind i.A.

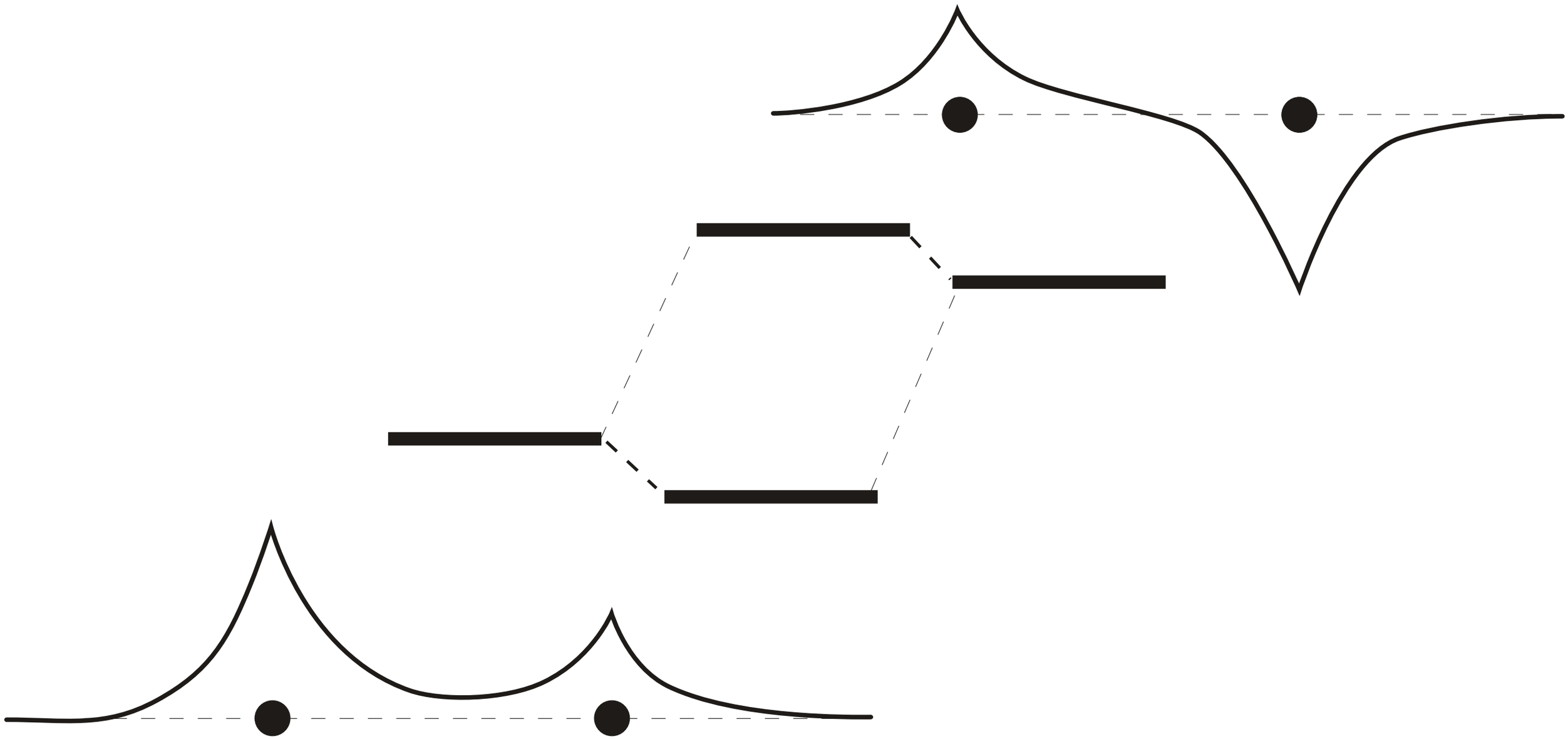
- **hart (z.B. Diamant)**
- **elektrische Isolatoren**
- **transparent für langwelliges Licht**

Beispiele:

- **Silizium**
- **InSb**
- **Mg2Sn**

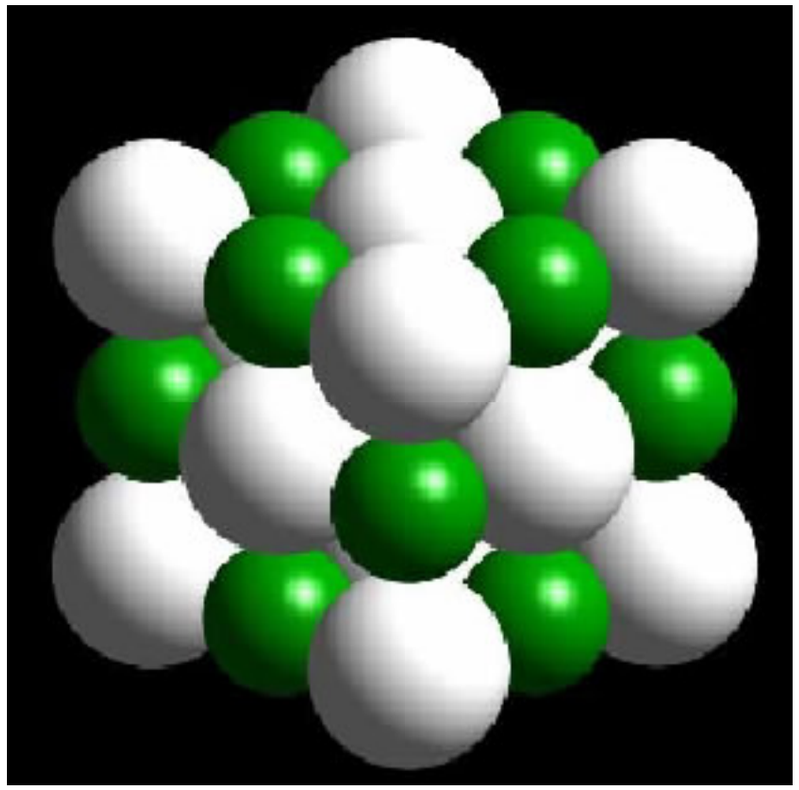
Asymmetrische Moleküle

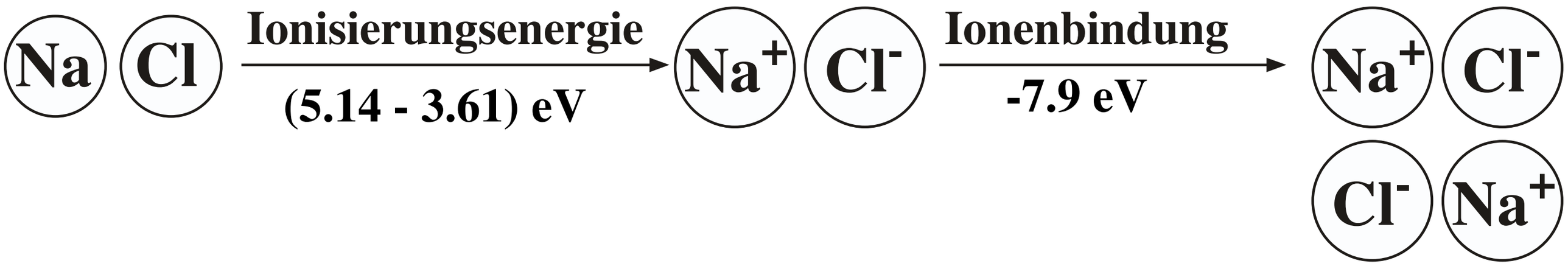
Molekülorbitale in AB



Ionische Bindung

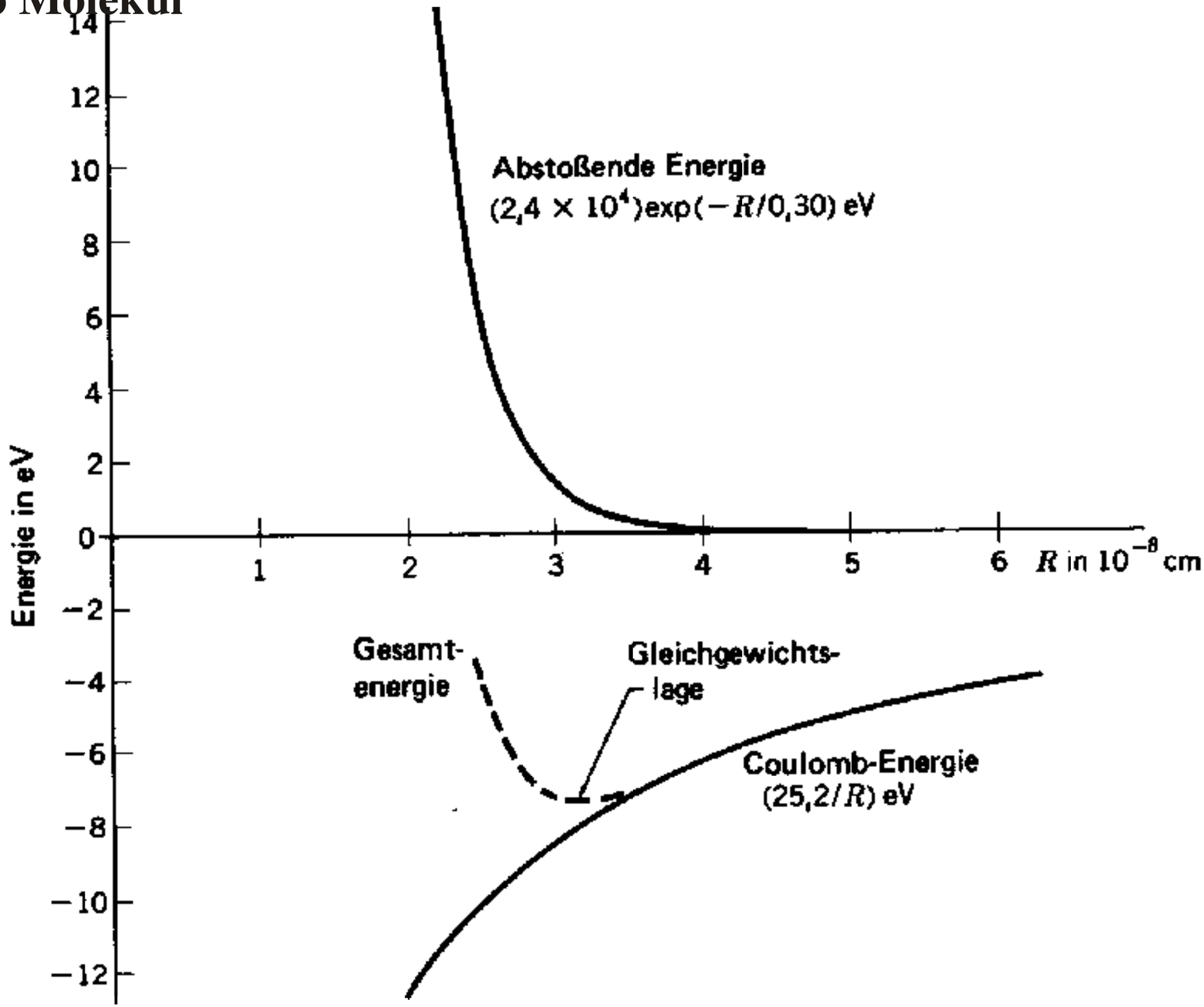
NaCl





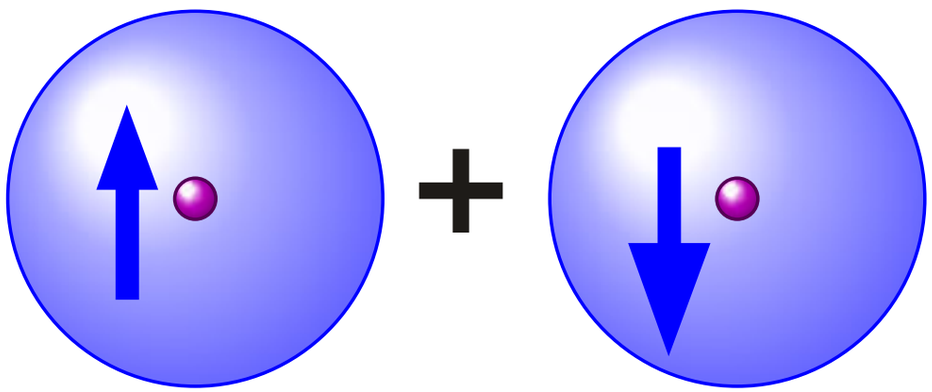
Potenzial eines KCl Kristalls

Energie pro Molekül



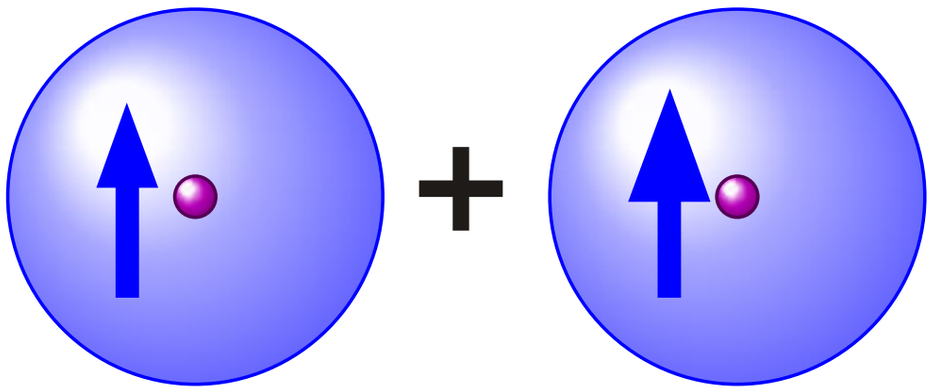
Pauli Prinzip

^{1}H ^{1}H ^{2}He



$1s\uparrow 1s\downarrow$

Gesamtspin 0
Elektronische Energie -80 eV



$1s\uparrow 2s\uparrow$

Gesamtspin 1
Elektronische Energie -59 eV

Atom- und Ionenradien

Einheit: Å

H 2.08																	He
Li 0.68 1.56	Be 0.35 1.06 1.13											B 0.23 0.88 0.98	C 0.15 0.77 0.92	N 1.71 0.70	O 1.40 0.66	F 1.36 0.64	Ne 1.58
Na 0.97 1.91	Mg 0.65 1.40 1.60	⟵ Standardradien für Ionen mit Edelgaskonfiguration (gefüllte Schale) ⟶ ⟵ Atomradien in tetraedisch-kovalenten Bindugen ⟶ ⟵ Ionenradien für Metalle in 12er Koordination ⟶										Al 0.50 1.26 1.43	Si 0.41 1.17 1.32	P 2.12 1.10	S 1.84 1.04	Cl 1.81 0.99	Ar 1.88
K 1.33 2.38	Ca 0.99 1.98	Sc 0.81 1.64	Ti 0.68 1.46	V 1.35	Cr 1.28	Mn 1.26	Fe 1.27	Co 1.25	Ni 1.25	Cu 1.35 1.28	Zn 0.74 1.31 1.39	Ga 0.62 1.26 1.41	Ge 0.53 1.22 1.37	As 2.22 1.18 1.39	Se 1.98 1.14	Br 1.95 1.11	Kr 2.00
Rb 1.48 2.55	Sr 1.13 2.15	Y 0.93 1.80	Zr 0.80 1.60	Nb 0.67 1.47	Mo 1.40	Tc 1.36	Ru 1.34	Rh 1.35	Pd 1.38	Ag 1.26 1.52 1.45	Cd 0.97 1.48 1.57	In 0.81 1.44 1.66	Sn 0.71 1.40 1.55	Sb 2.45 1.36 1.59	Te 2.21 1.32	I 2.16 1.28	Xe 2.17
Cs 1.67 2.73	Ba 1.35 2.24	La 1.15 1.88	Hf 1.58	Ta 1.47	W 1.41	Re 1.38	Os 1.35	Ir 1.36	Pt 1.39	Au 1.37 1.44	Hg 1.10 1.48 1.57	Tl 0.95 1.72	Pb 0.84 1.75	Bi 1.70	Po 1.76	At 	Rn
Fr 1.75	Ra 1.37	Ac 1.11															

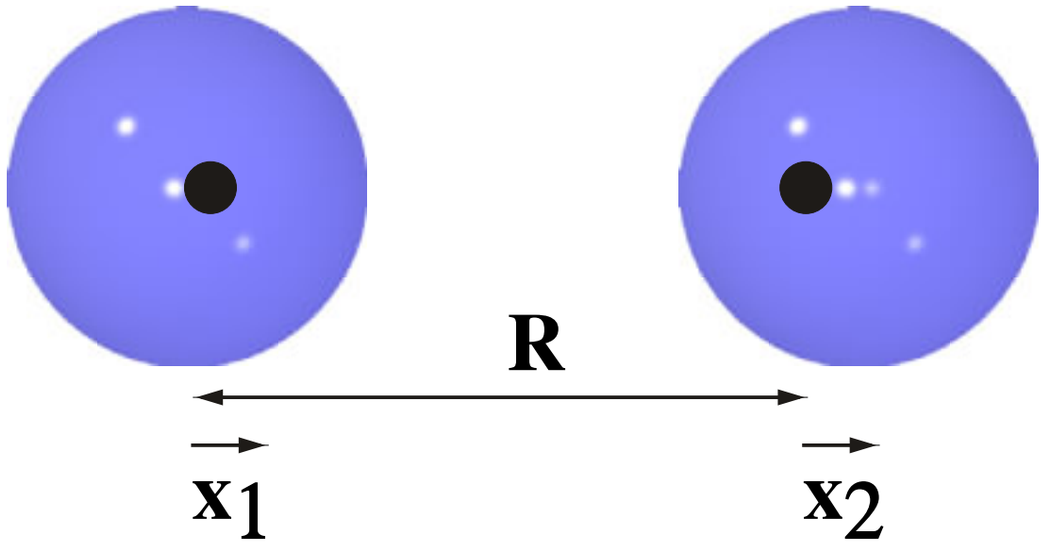
Ce 1.01 1.71– 1.82	Pr 1.83	Nd 1.82	Pm 1.81	Sm 1.80	Eu 2.04^{2+} 1.80^{3+}	Gd 1.80	Tb 1.78	Dy 1.77	Ho 1.77	Er 1.76	Tm 1.75	Yb 1.94^{2+} 1.74^{3+}	Lu
Th 0.99 1.80	Pa 0.90 1.63	U 0.83 1.56	Np 1.56	Pu 1.58– 1.64	Am 1.81	Cm 	Bk 	Cf 	Es 	Fm 	Md 	No 	Lr

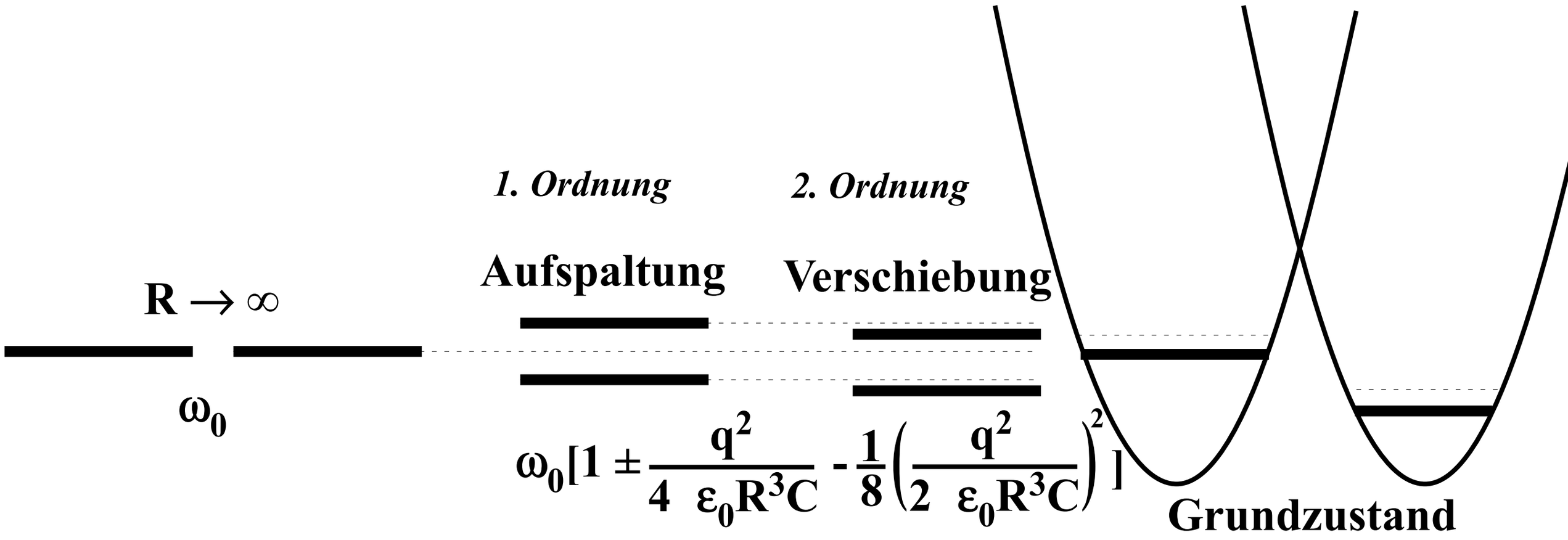
Ionisierungsenergien

H 13,595																	He 24,58 78,98
Li 5,39 81,01	Be 9,32 27,53											B 8,30 33,45	C 11,26 35,64	N 14,54 44,14	O 13,61 48,76	F 17,42 52,40	Ne 21,56 62,63
Na 5,14 52,43	Mg 7,64 22,67	← Energie zur Entfernung eines Elektrons, in eV. → ← Energie zur Entfernung zweier Elektronen, in eV. →										Al 5,98 24,80	Si 8,15 24,49	P 10,55 30,20	S 10,36 34,0	Cl 13,01 36,81	Ar 15,76 43,38
K 4,34 36,15	Ca 6,11 17,98	Sc 6,56 19,45	Ti 6,83 20,46	V 6,74 21,39	Cr 6,76 23,25	Mn 7,43 23,07	Fe 7,90 24,08	Co 7,86 24,91	Ni 7,63 25,78	Cu 7,72 27,93	Zn 9,39 27,35	Ga 6,00 26,51	Ge 7,88 23,81	As 9,81 30,0	Se 9,75 31,2	Br 11,84 33,4	Kr 14,00 38,56
Rb 4,18 31,7	Sr 5,69 16,72	Y 6,5 18,9	Zr 6,95 20,98	Nb 6,77 21,22	Mo 7,18 23,25	Tc 7,28 22,54	Ru 7,36 24,12	Rh 7,46 25,53	Pd 8,33 27,75	Ag 7,57 29,05	Cd 8,99 25,89	In 5,78 24,64	Sn 7,34 21,97	Sb 8,64 25,1	Te 9,01 27,6	I 10,45 29,54	Xe 12,13 33,3
Cs 3,89 29,0	Ba 5,21 15,21	La 5,61 17,04	Hf 7, 22,	Ta 7,88 24,1	W 7,98 25,7	Re 7,87 24,5	Os 8.7 26,	Ir 9,	Pt 8,96 27,52	Au 9,22 29,7	Hg 10,43 29,18	Tl 6,11 26,53	Pb 7,41 22,44	Bi 7,29 23,97	Po 8,43	At	Rn 10,74
Fr	Ra 5,28 15,42	Ac 6,9 19,0															

Ce 6,91	Pr 5,76	Nd 6,31	Pm	Sm 5,6	Eu 5,67	Gd 6,16	Tb 6,74	Dy 6,82	Ho	Er	Tm	Yb 6,2	Lu 5,0
Th	Pa	U 4	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

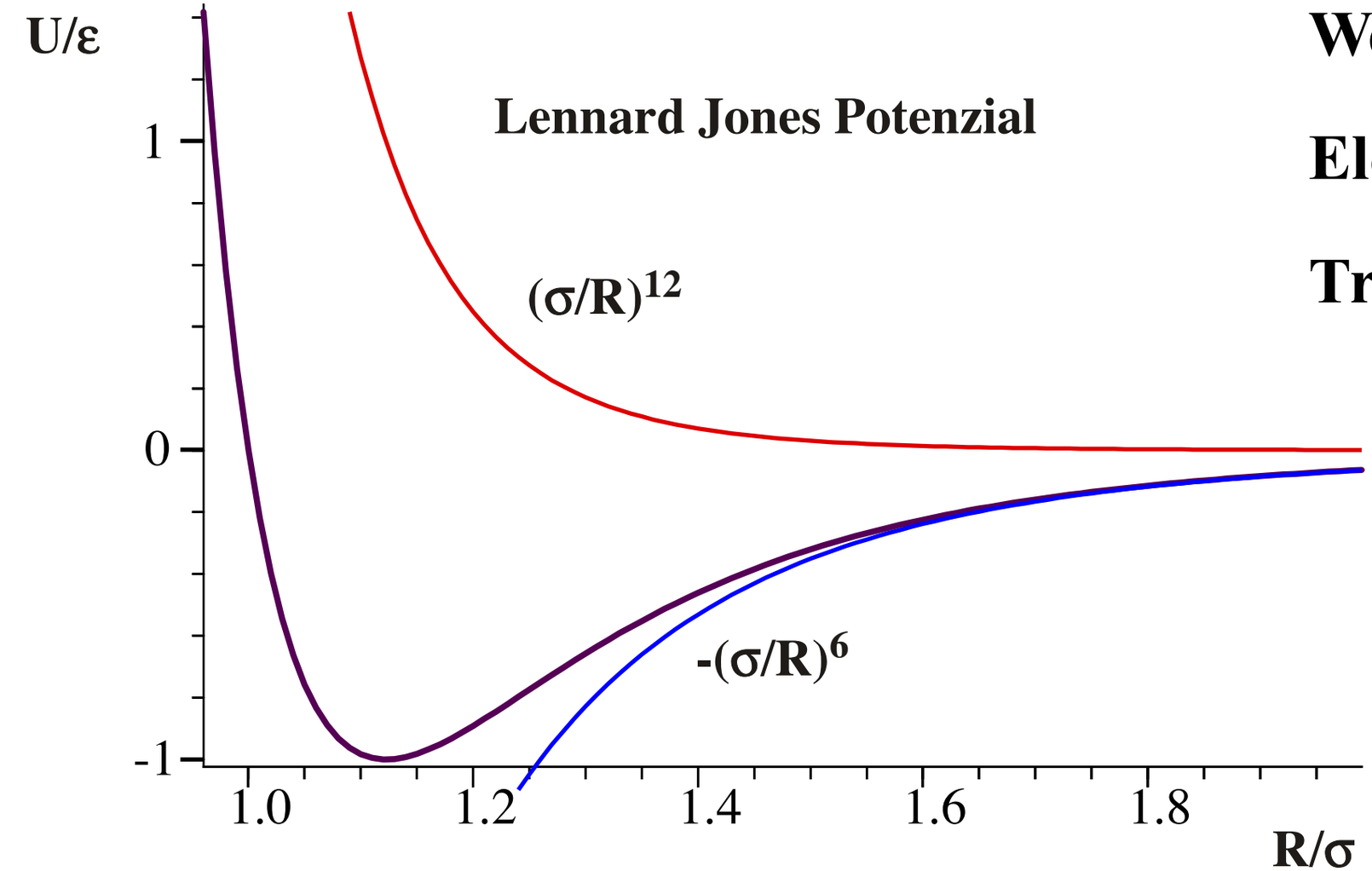
Van der Waals Bindung





Lennard-Jones Potenzial

Sir John Edward Lennard-Jones 1894-1954



Materialien:

- **Edelgase (z.B. Argon)**
- **Moleküle: Cl_2, H_2**

Bindungsenergie: 0.01 .. 0.1 eV

Nachbar-Abstände: ~ 4 Å

Weich, niedriger Schmelzpunkt

Elektrische Isolatoren

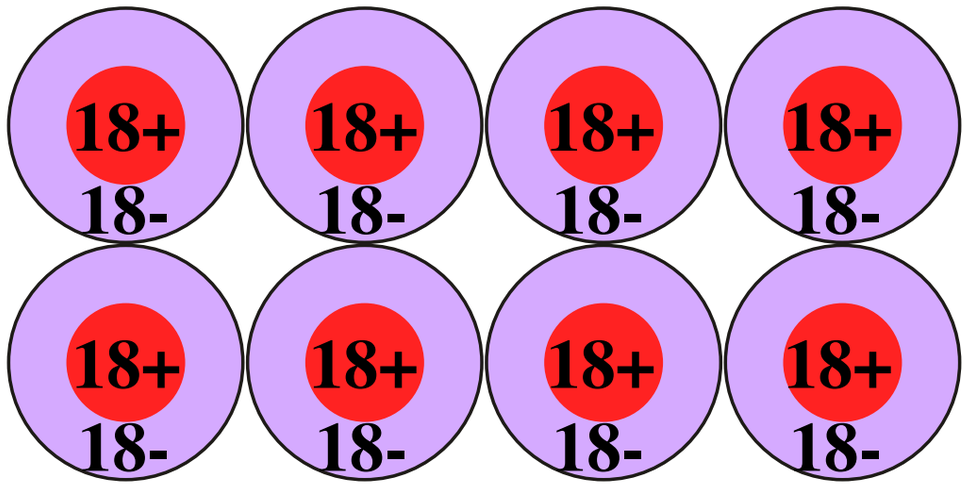
Transparent

Eigenschaften von Edelgaskristallen

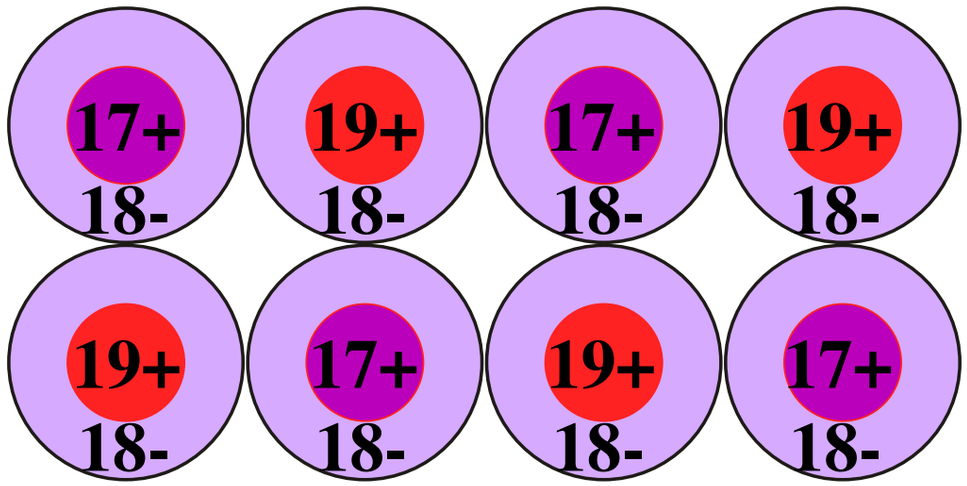
extrapoliert auf 0 K und 0 atm

Abstand zwischen nächsten Nachbarn, in Å	Bindungsenergie,		Schmelzpunkt, K	Ionisierungsenergie des freien Atoms, eV	Parameter im Lennard-Jones-Potential der Gleichung (10)	
	kJ/Mol	eV/Atom			ϵ, in 10^{-16} · erg	σ, in Å
He	**flüssig bei 0 atm.**			**24,58**	**14**	**2,56**
Ne 3,13	1,88	0,02	24	21,56	50	2,74
Ar 3,76	7,74	0,080	84	15,76	167	3,40
Kr 4,01	11,2	0,116	117	14,00	225	3,65
Xe 4,35	16,0	0,17	161	12,13	320	3,98

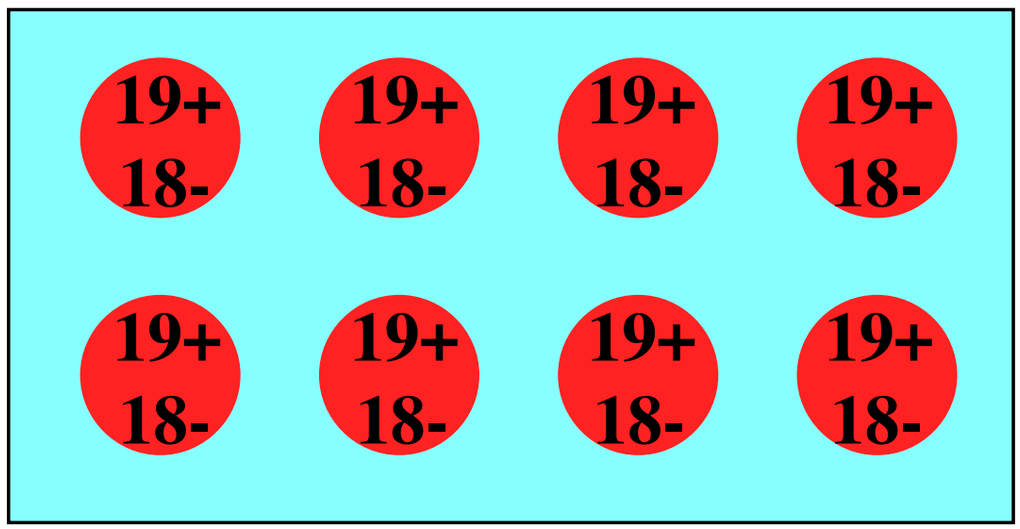
Bindungsarten



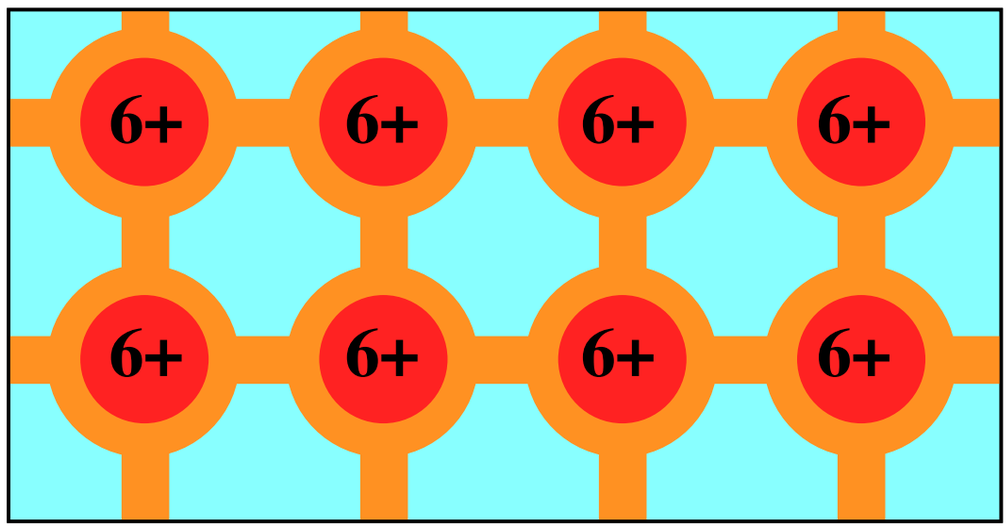
Van der Waals



Ionisch

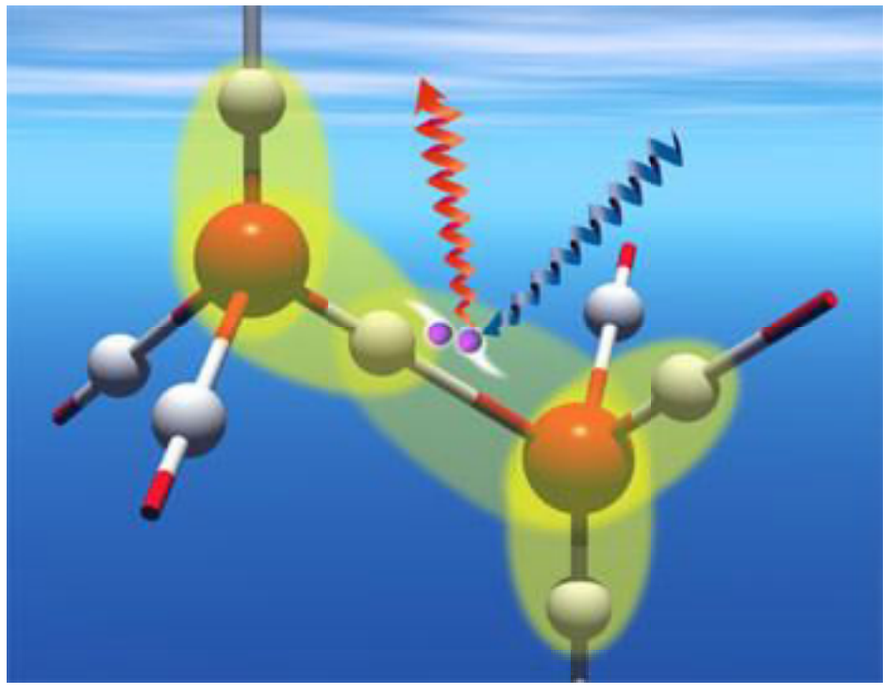


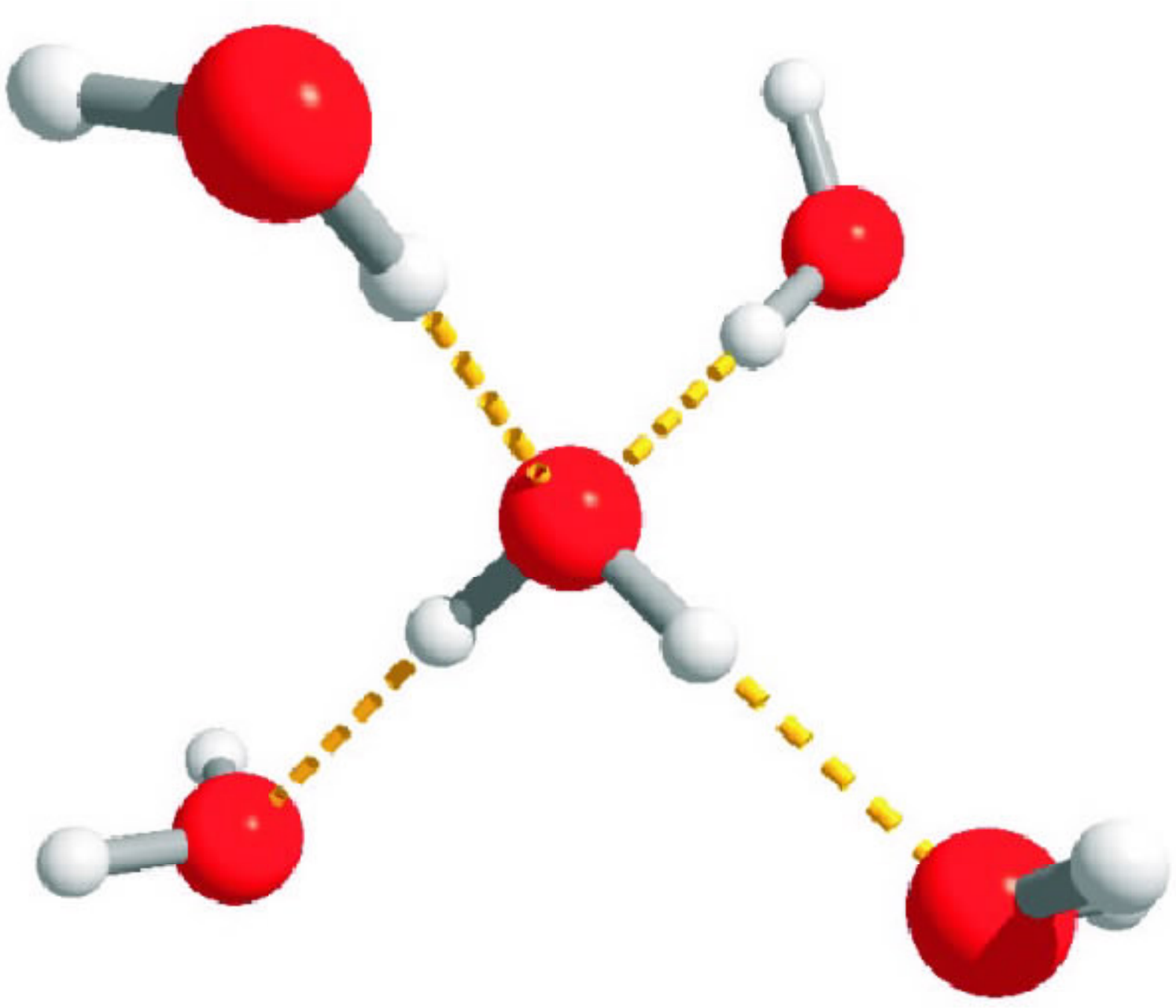
Metallisch



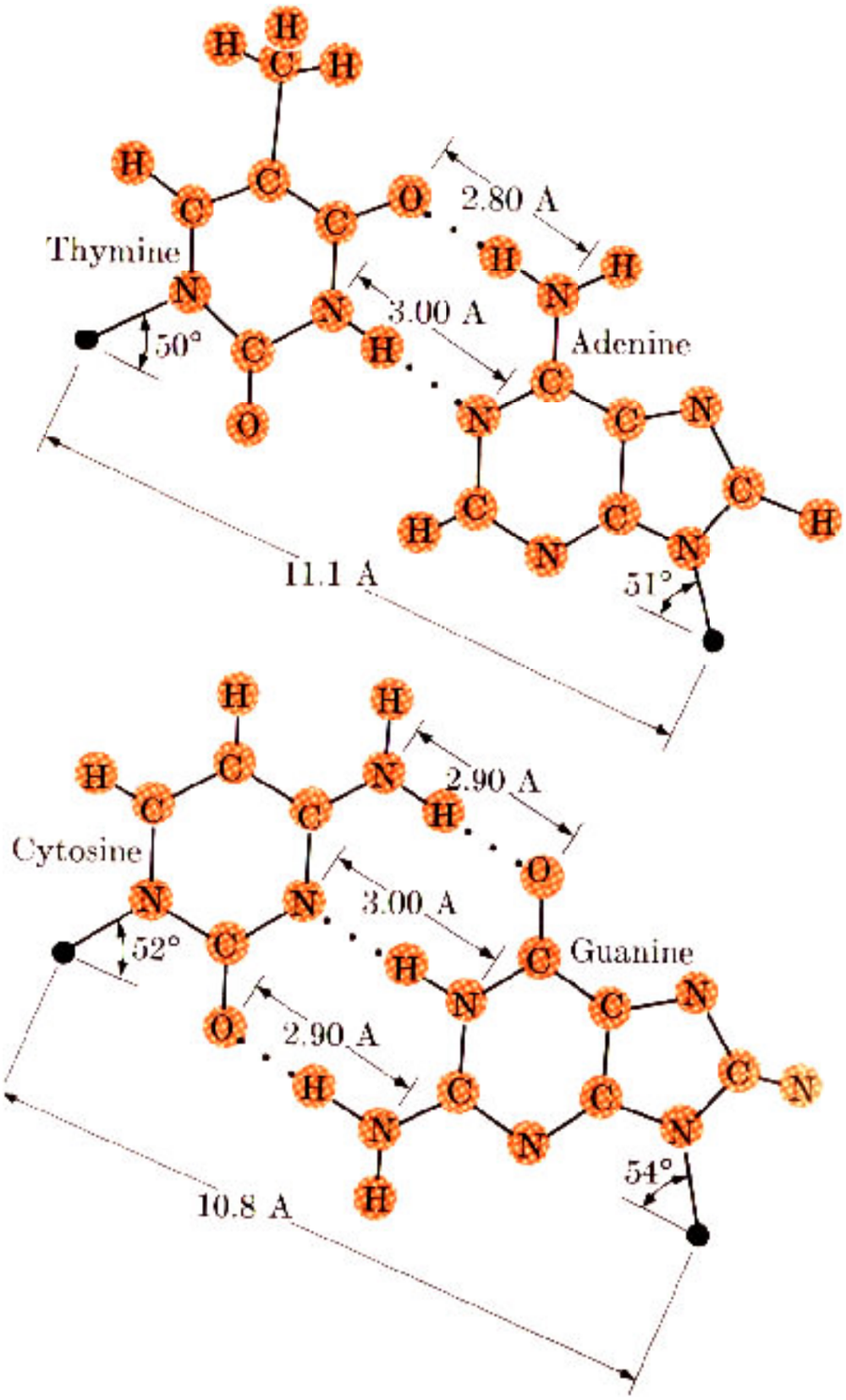
Kovalent

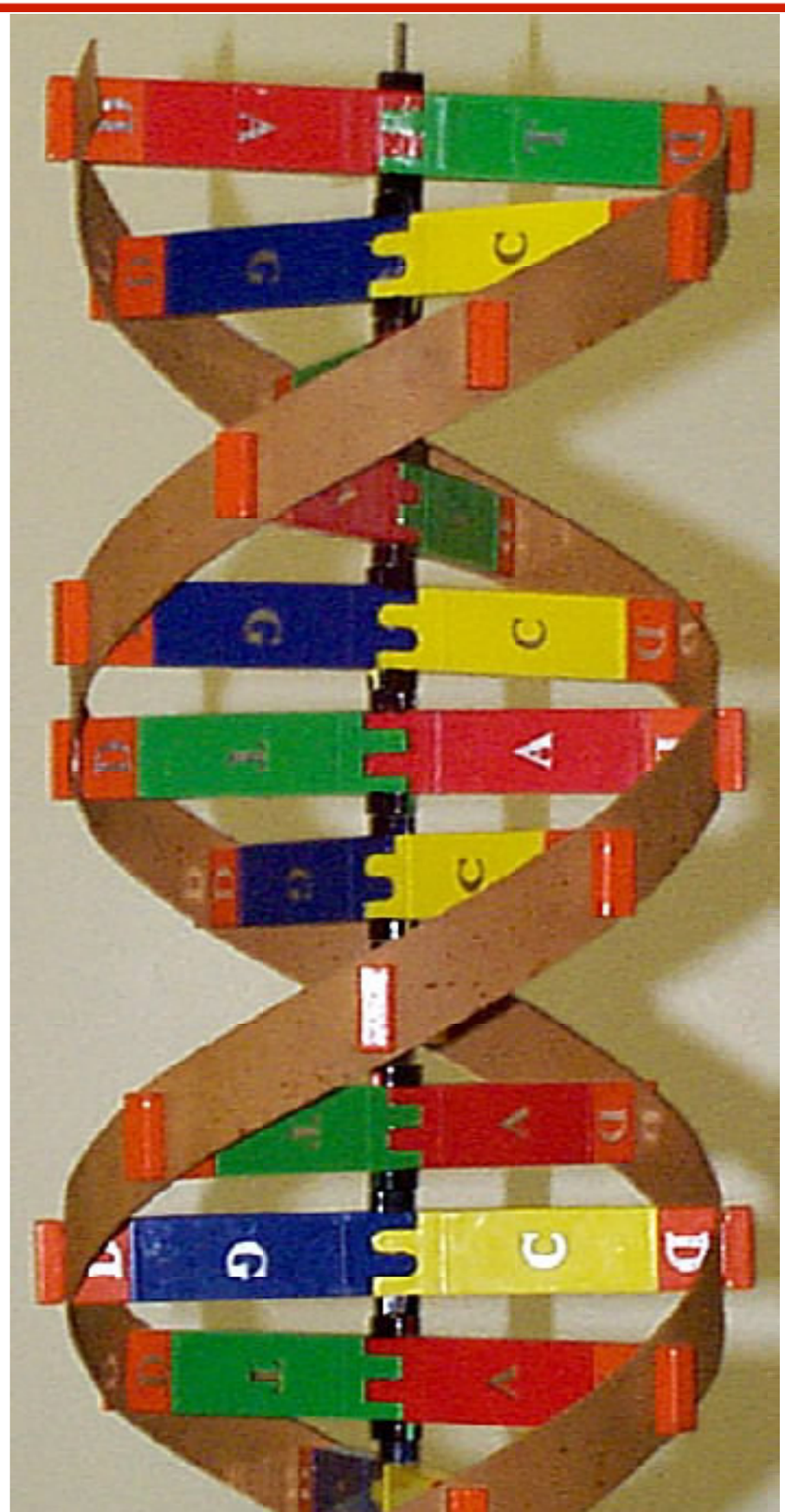
Wasserstoffbrücken



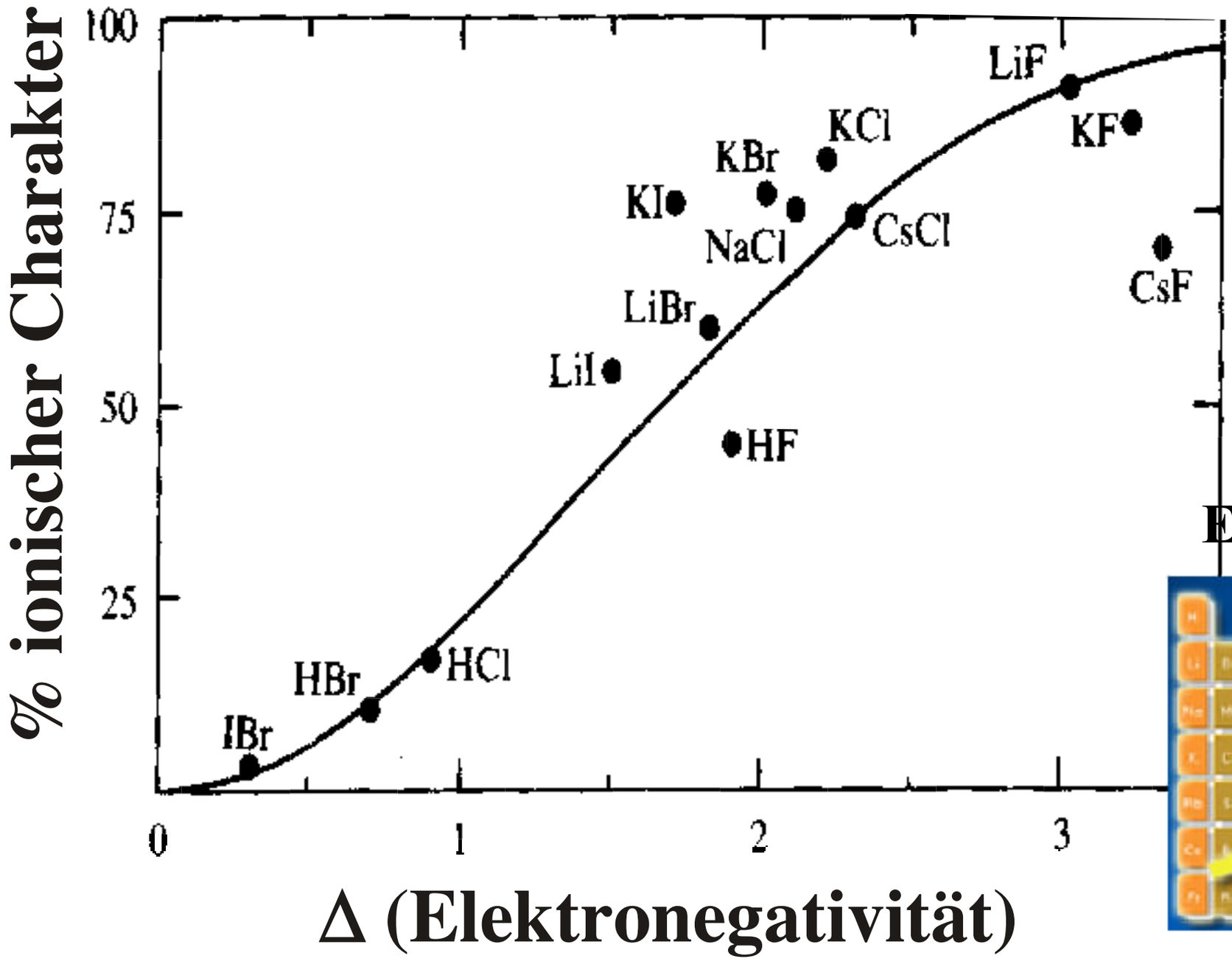


Wasserstoffbrücken in Nukleinsäuren





Ionisch vs. kovalent



Elektronegativität : Trend