Literatur

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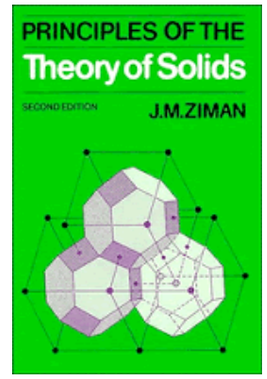
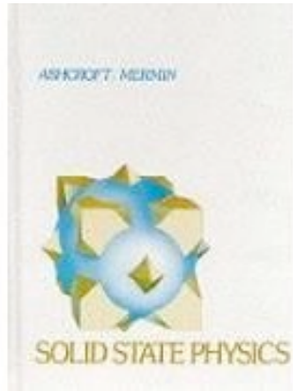
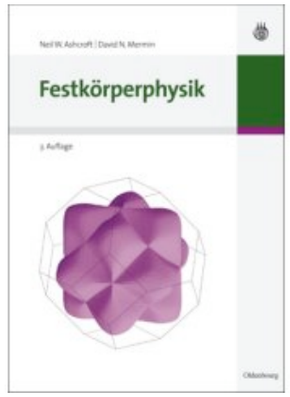
- John Ziman: *Principles of the Theory of Solids*
  Cambridge University Press, 1963
  Prinzipien der Festkörpertheorie
  Harri Deutsch



- Neil Ashcroft and David Mermin: *Solid State Physics*
  Holt, Rinehart and Winston, 1976
  Festkörperphysik
  Oldenbourg





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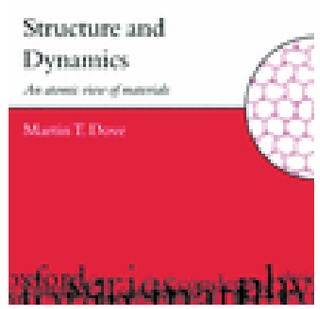
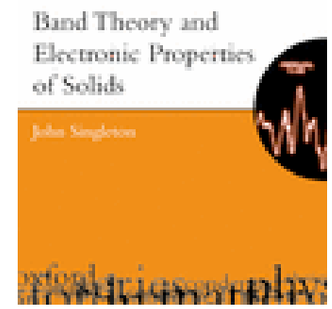
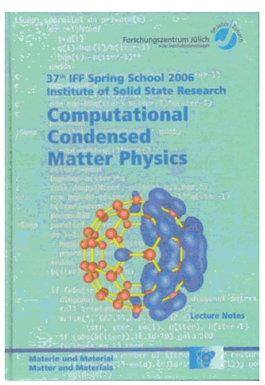
  Oxford University Press, 2003
  John Singleton:
  Band Theory and Electronic Properties of Solids
  Oxford University Press, 2001





- 37. IFF Ferienschule 2006
  Computational Condensed Matter Physics



Übungsaufgabe

gegeben
N_e Elektronen, N_i Atomkerne der Masse M_α und Kernladungszahl Z_α,
lösen Sie:

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N_e}\nabla_j^2 - \sum_{\alpha=1}^{N_i}\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \frac{1}{4\pi\epsilon_0}\sum_{j=1}^{N_e}\sum_{\alpha=1}^{N_i}\frac{Z_\alpha e^2}{|r_j - R_\alpha|} + \frac{1}{4\pi\epsilon_0}\sum_{j<k}^{N_e}\frac{e^2}{|r_j - r_k|} + \frac{1}{4\pi\epsilon_0}\sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|}$$

The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that exact applications of these laws lead to equations which are too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

P.M.A Dirac, *Proceedings of the Royal Society* **A123**, 714 (1929)

More is Different

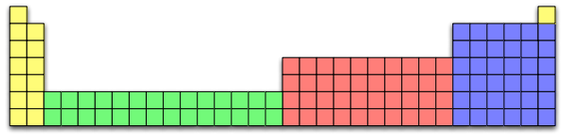
… the reductionist hypothesis does not by any means imply a ``constructionist'' one: The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe.

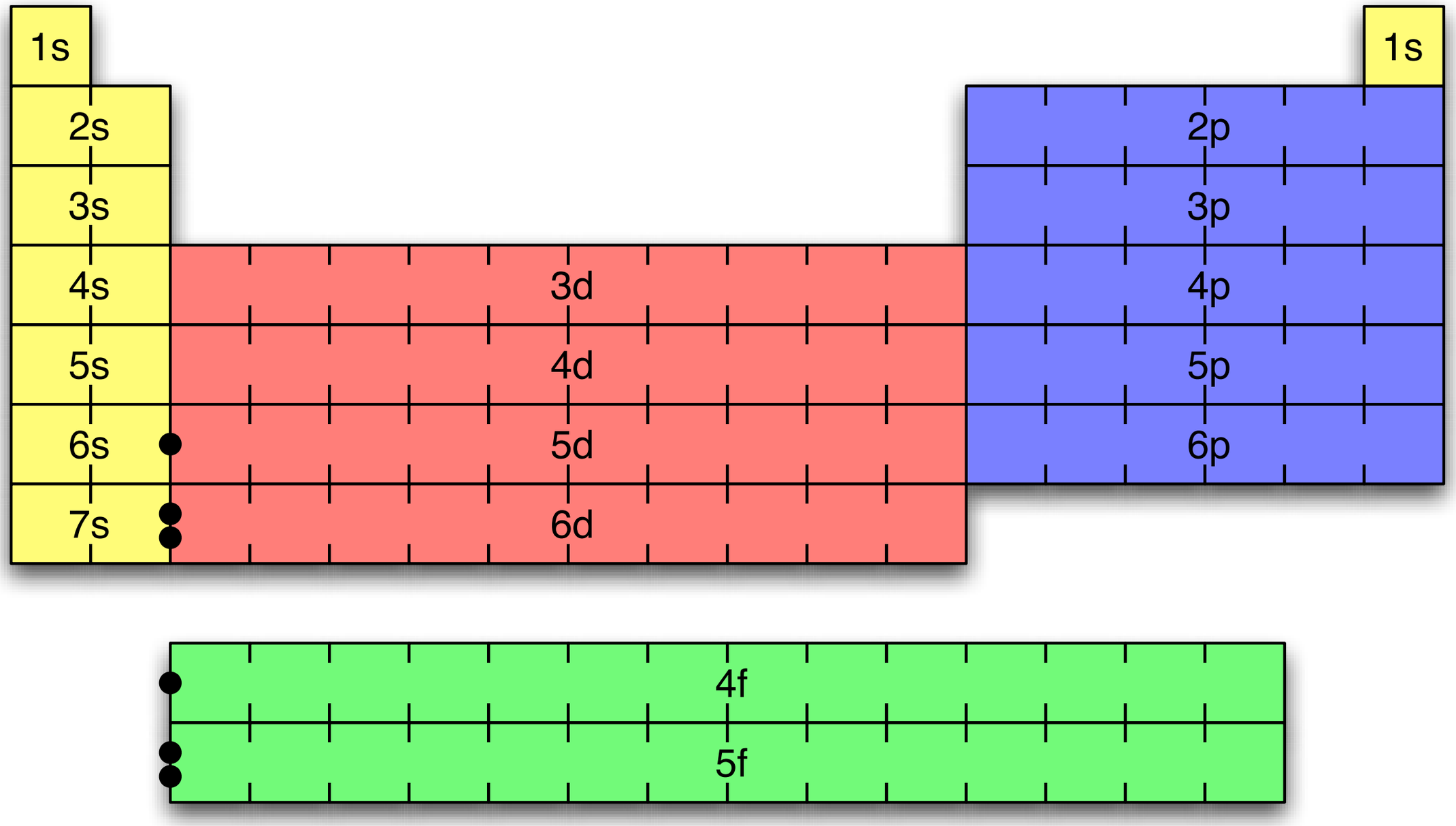
Sometimes, as in the case of superconductivity, the new symmetry — now called broken symmetry because the original symmetry is no longer evident — may be of an entirely unexpected kind and extremely difficult to visualize. In the case of superconductivity, 30 years elapsed between the time when physicists were in possession of every fundamental law necessary for explaining it and the time when it was actually done.

Thus with increasing complication at each stage, we go up the hierarchy of the sciences. We expect to encounter fascinating and, I believe, very fundamental questions at each stage in fitting together less complicated pieces into the more complicated system and understanding the the basically new types of behavior which can result.

P.W. Anderson: More is Different, *Science* **177**, 393 (1972)

Periodensystem





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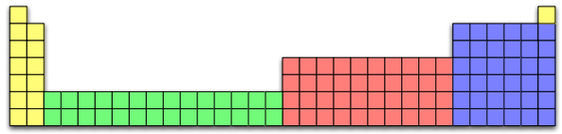

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt									

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

Atomradien

E. Clementi, D.L.Raimondi, and W.P. Reinhardt
J. Chem. Phys. 47, 1300 (1967)

dichteste Kugelpackung

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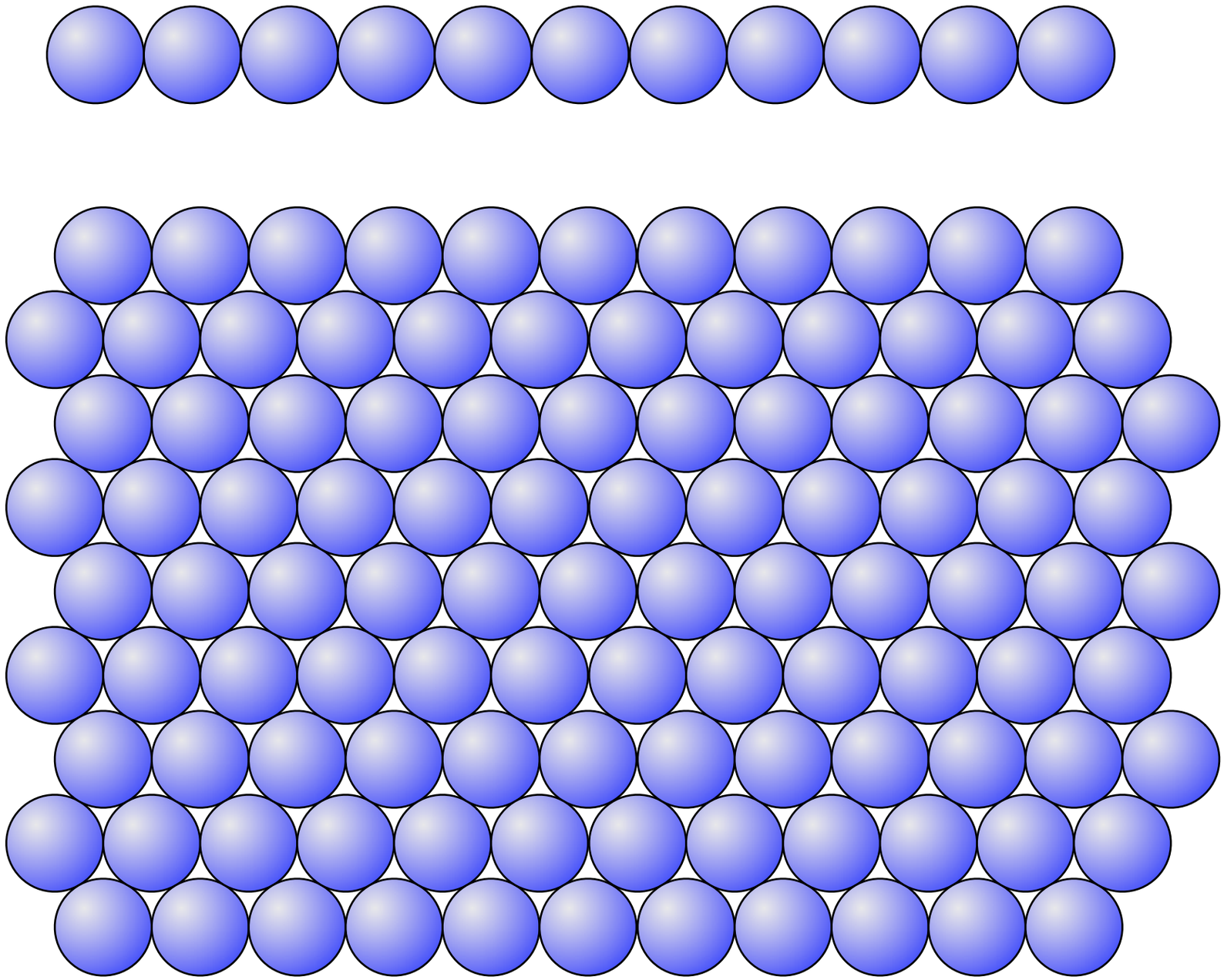
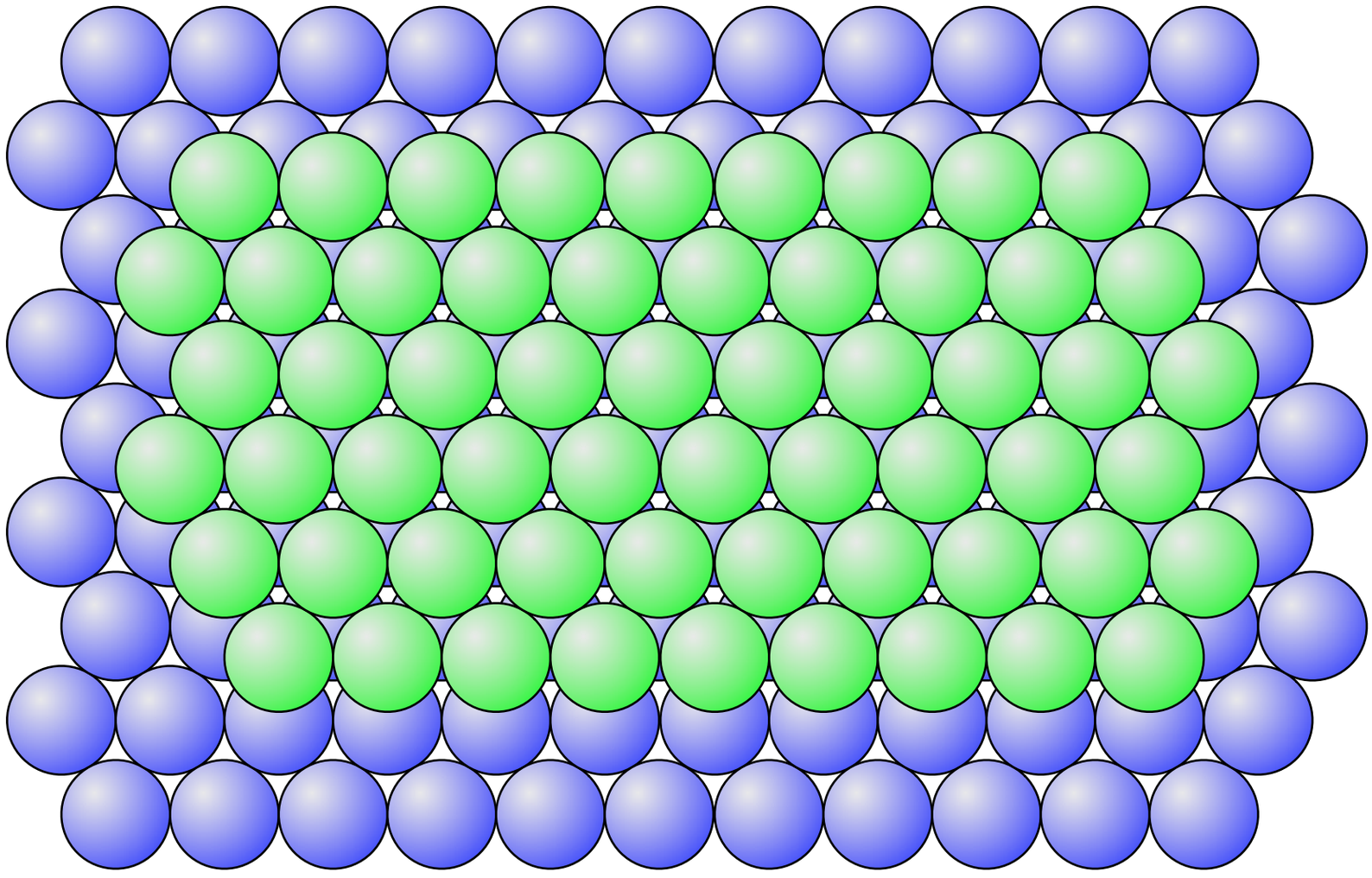


d=2

Dreiecksgitter

dichteste Kugelpackung

d=3



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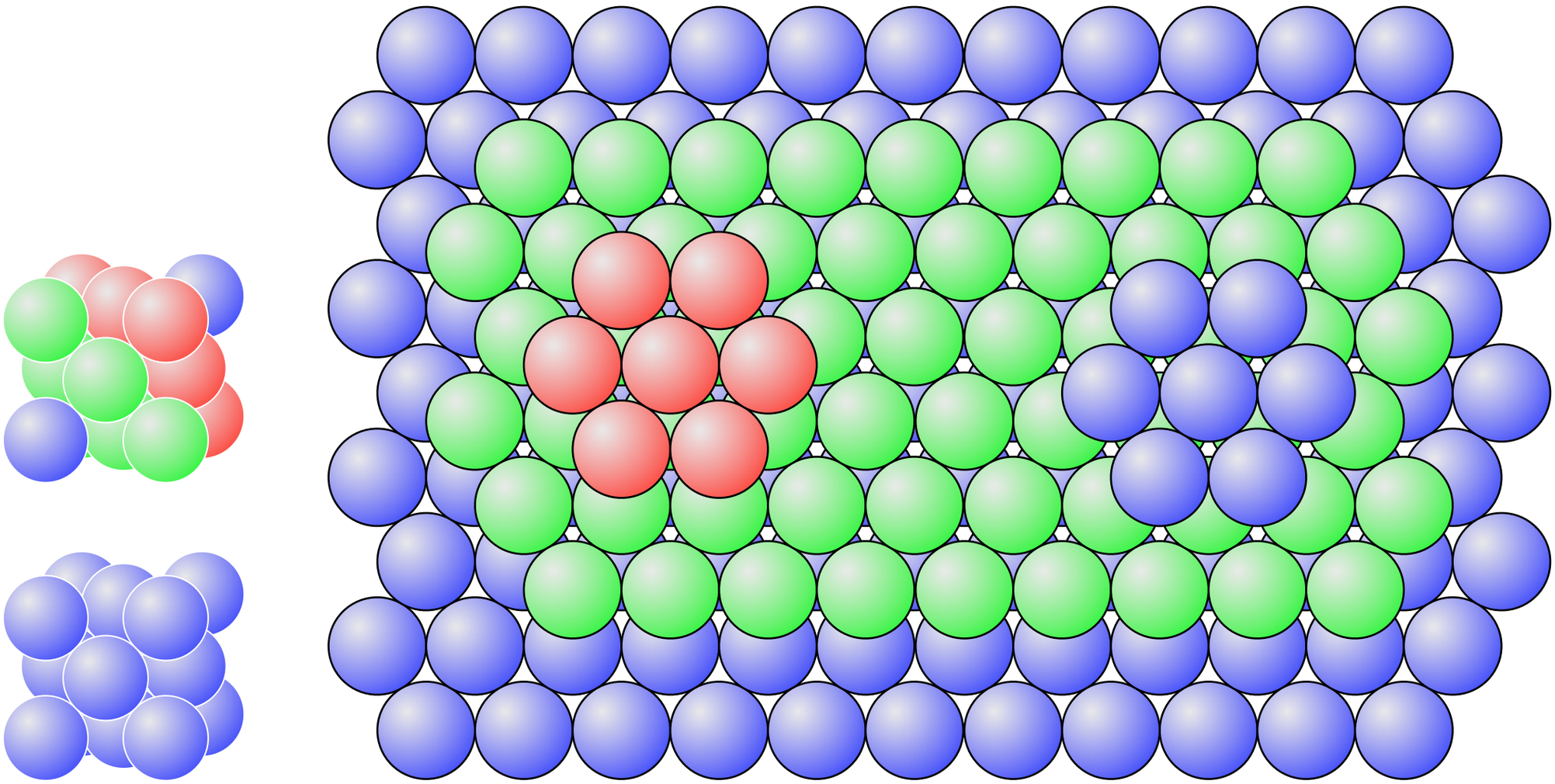
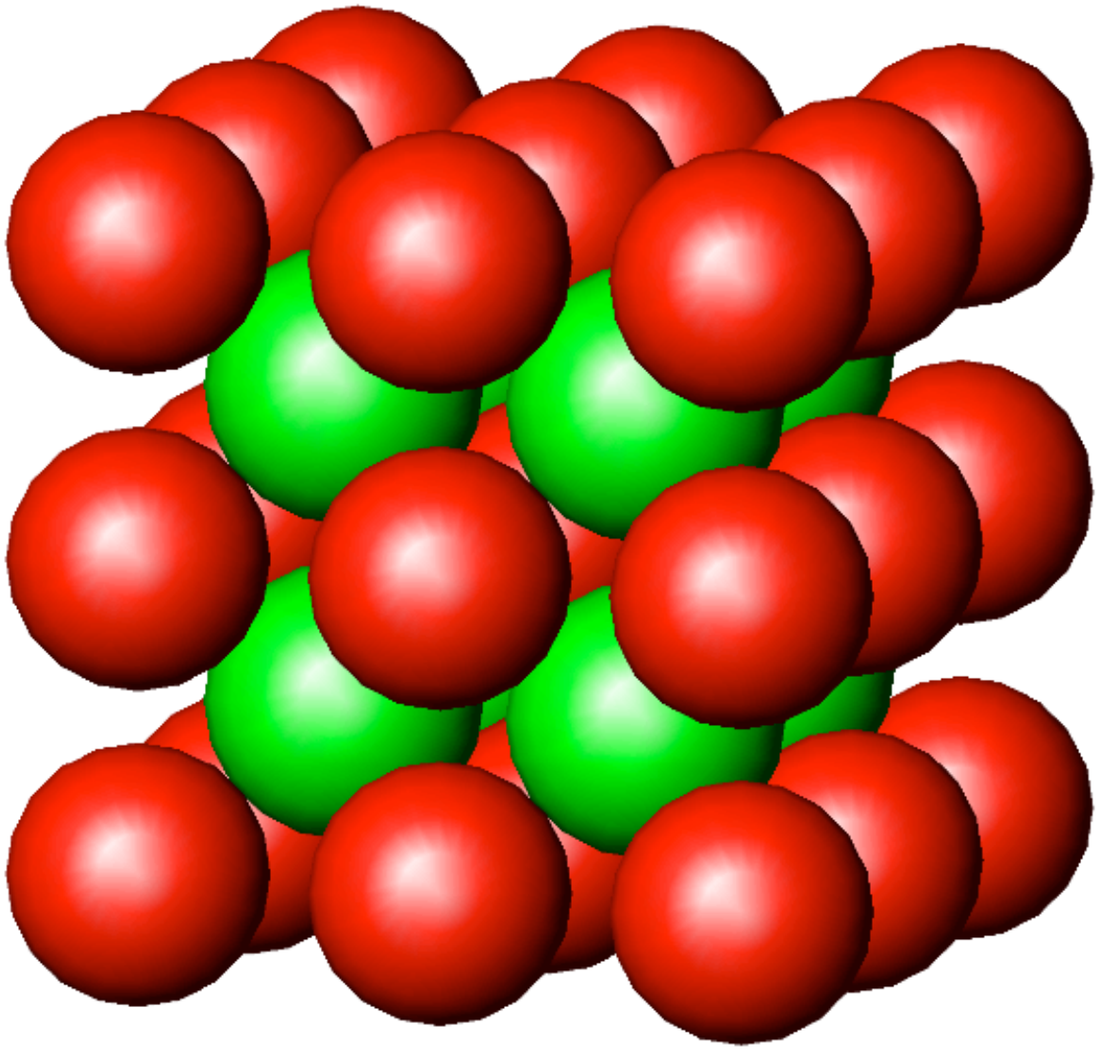
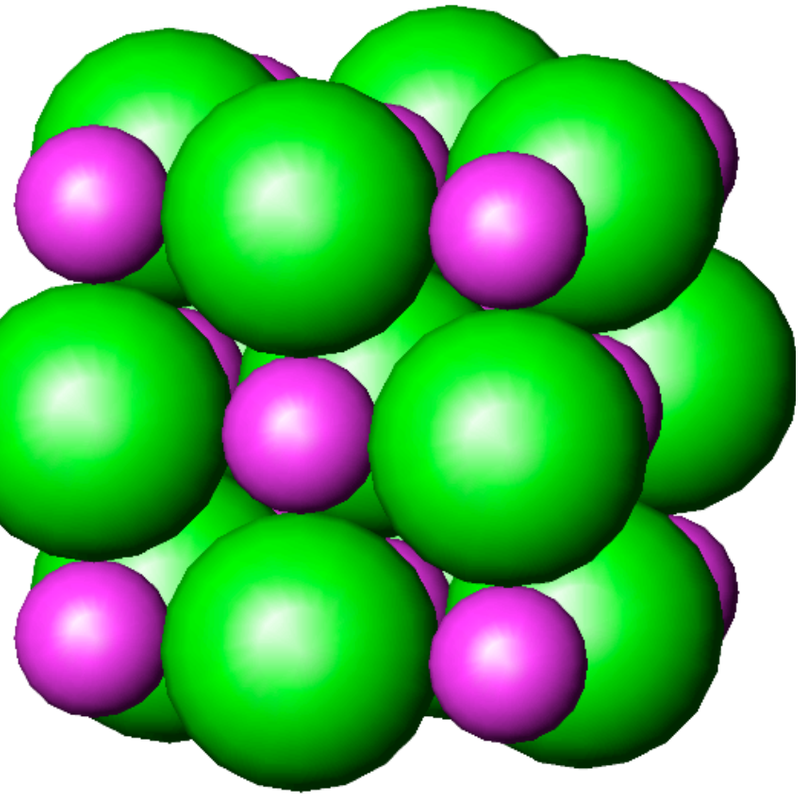


Stapelfolge: ABCABC (fcc) oder ABABAB (hcp)

Ionenkristalle

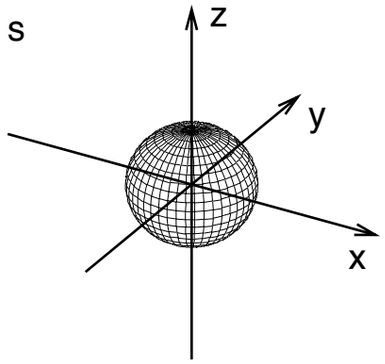


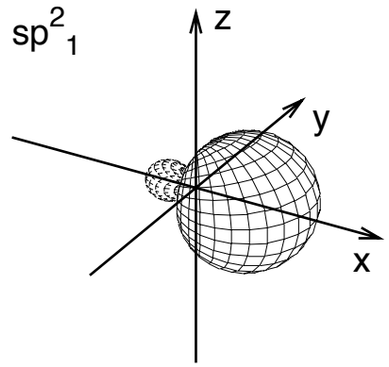
CsCl

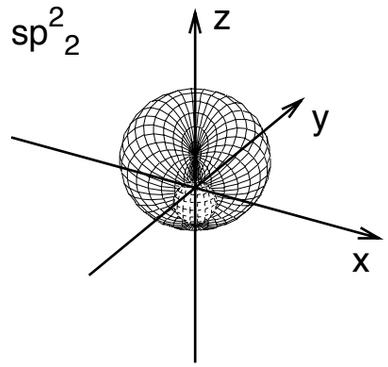


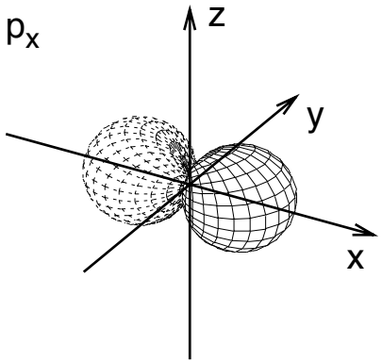
NaCl

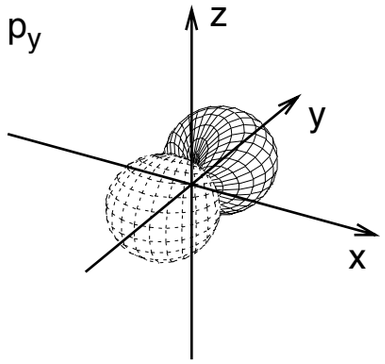
Atom- und Hybrid-Orbitale

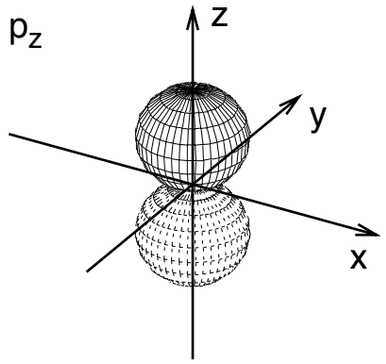


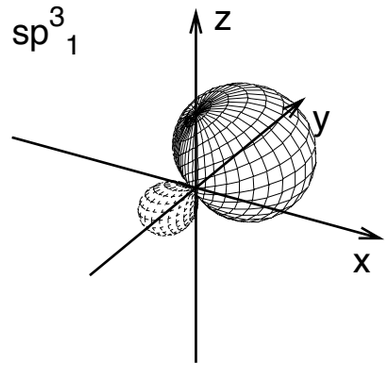


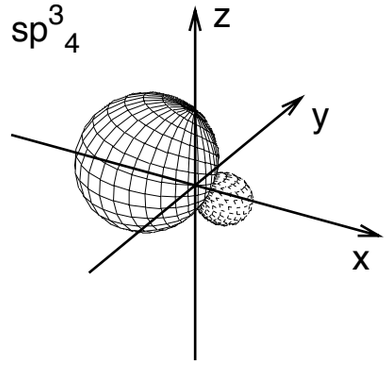


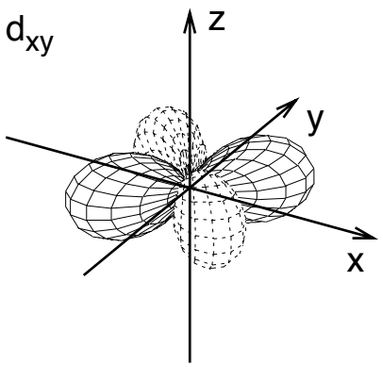


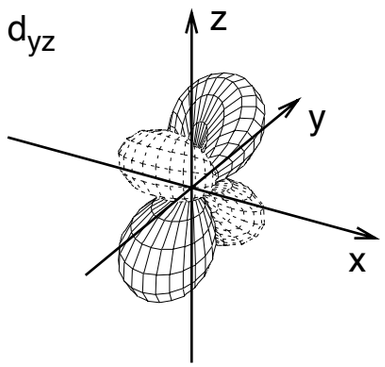


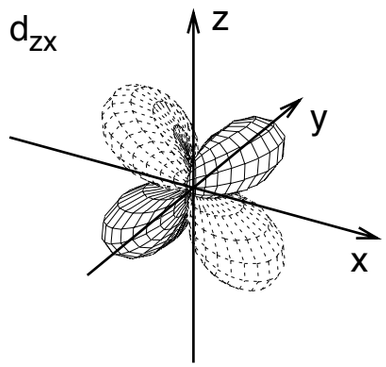


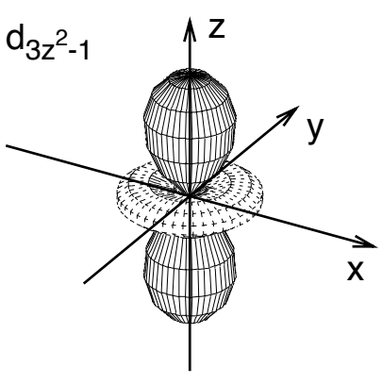


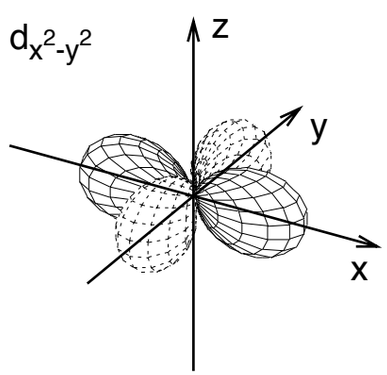




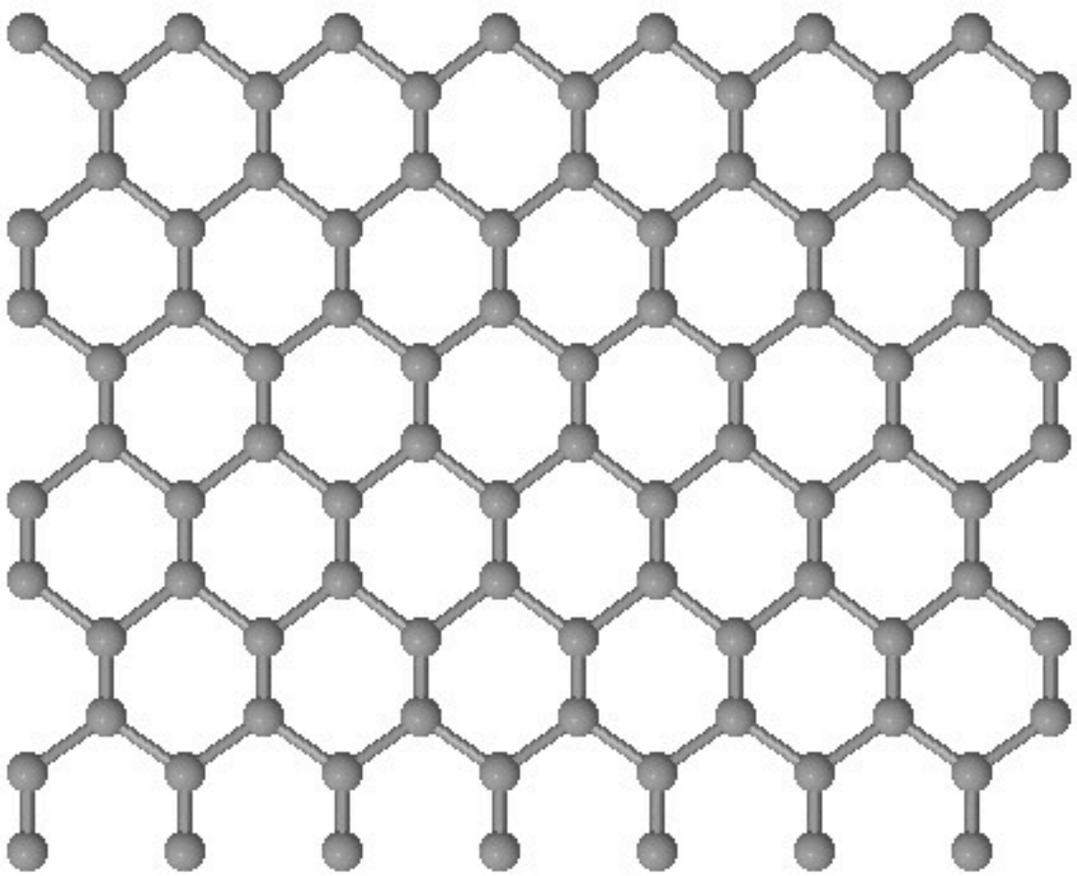








kovalente Kristalle: sp^2



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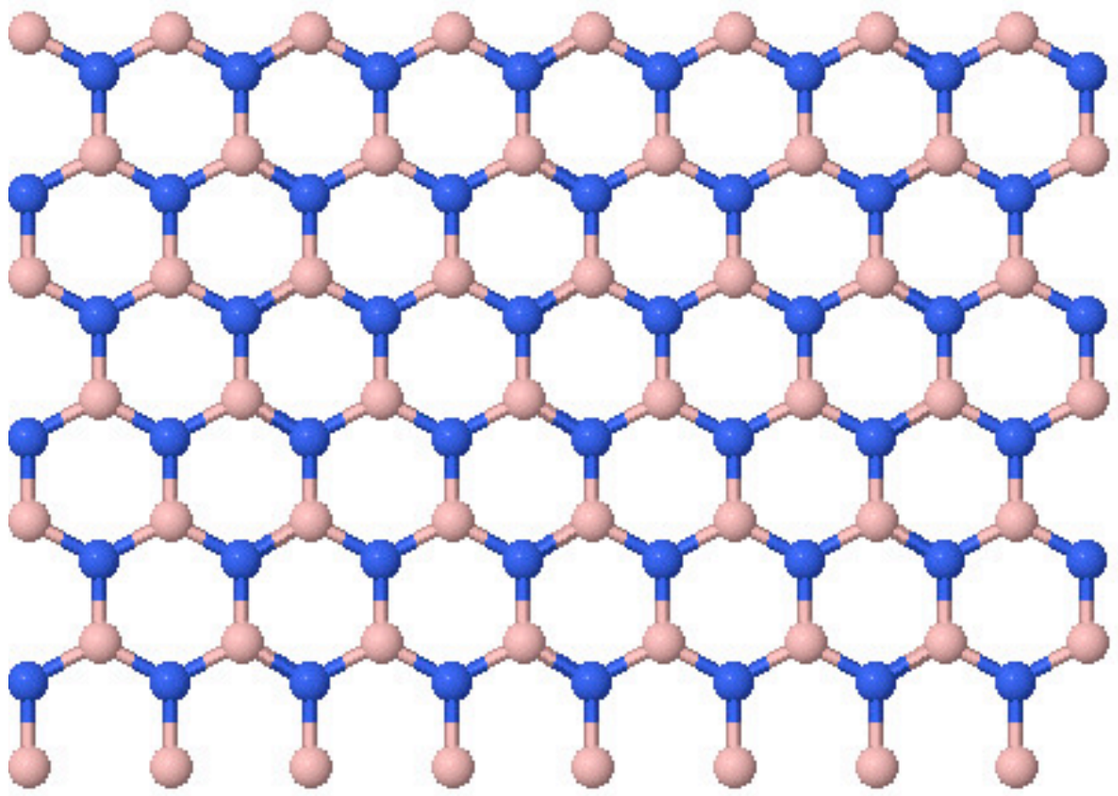

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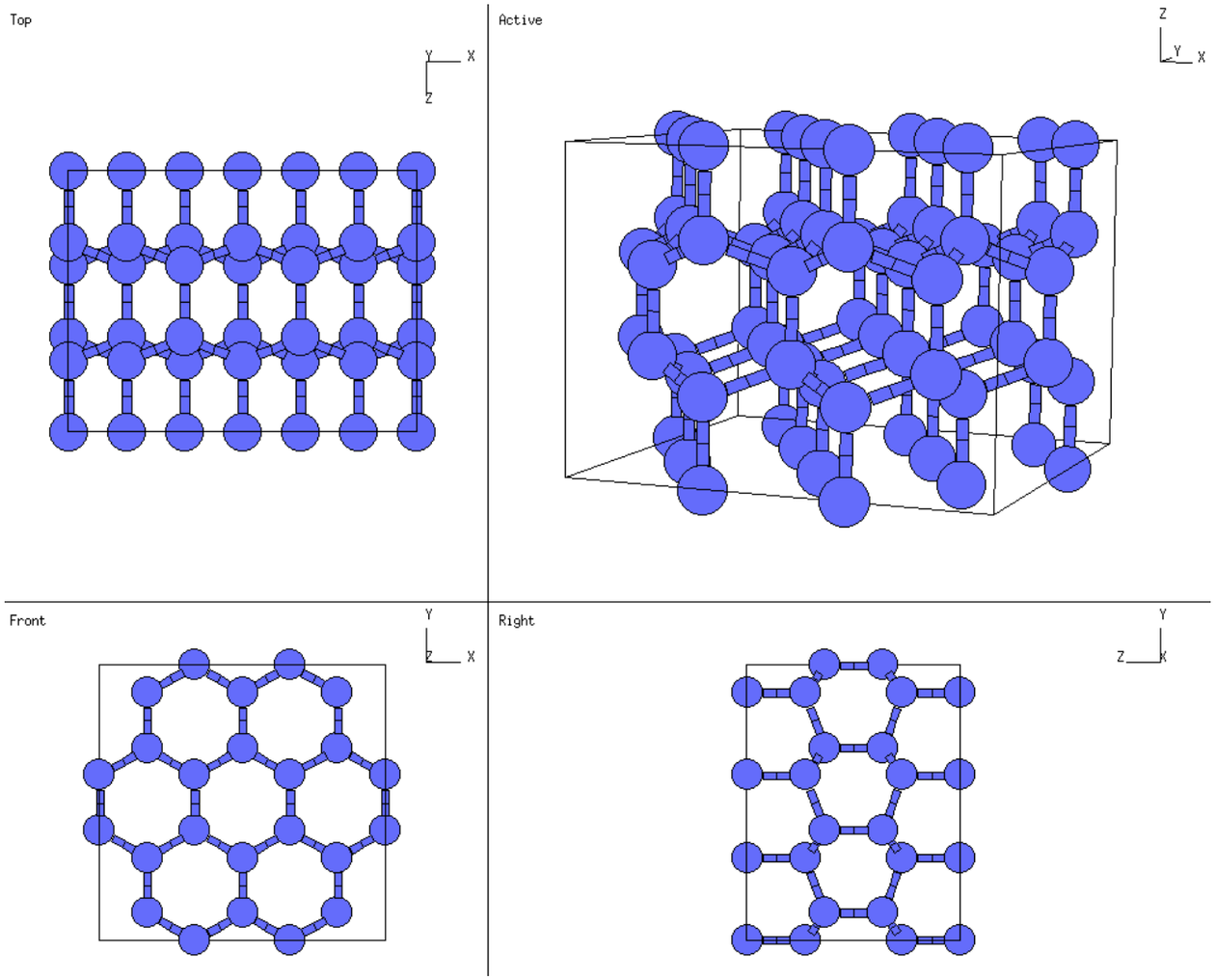
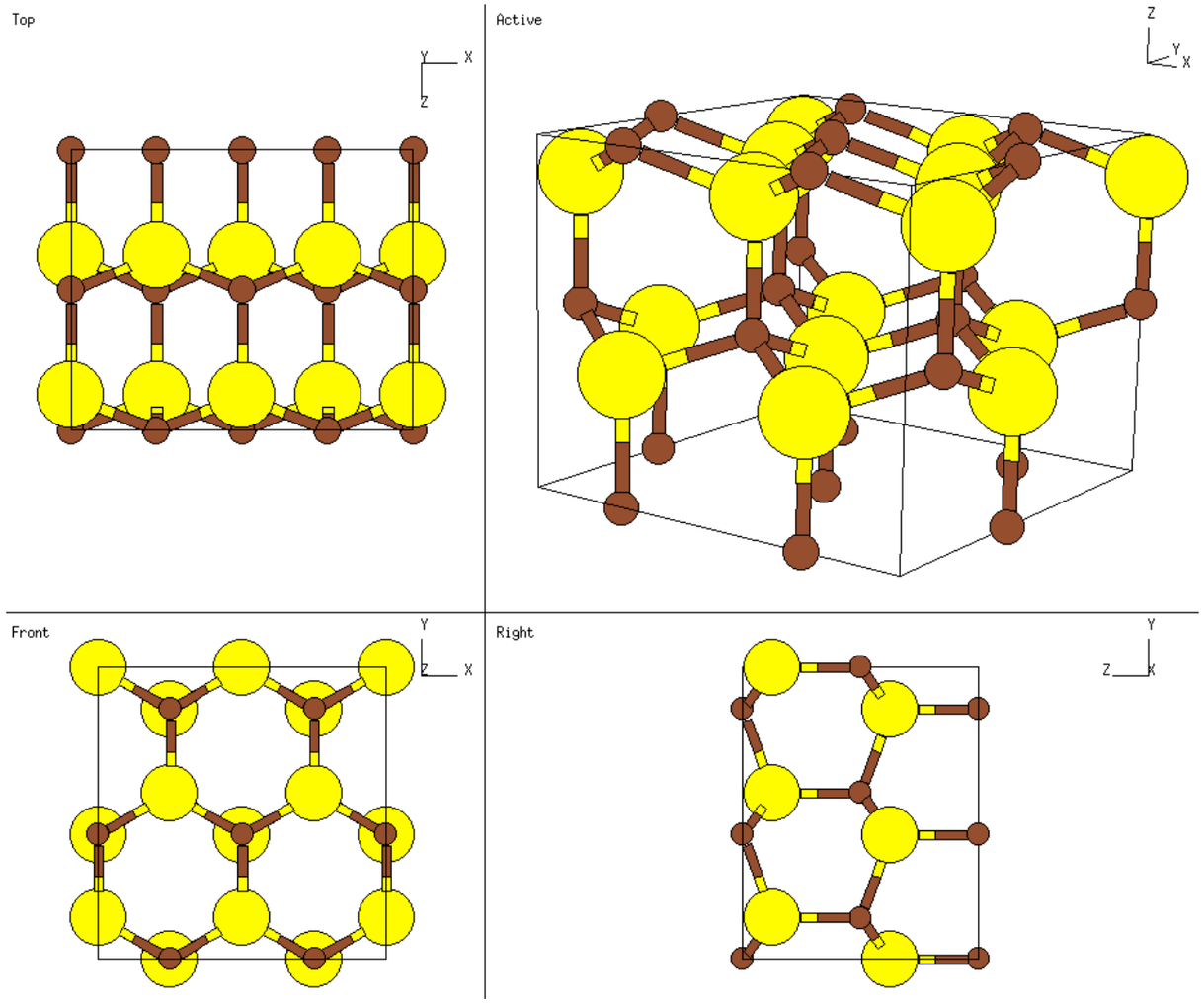




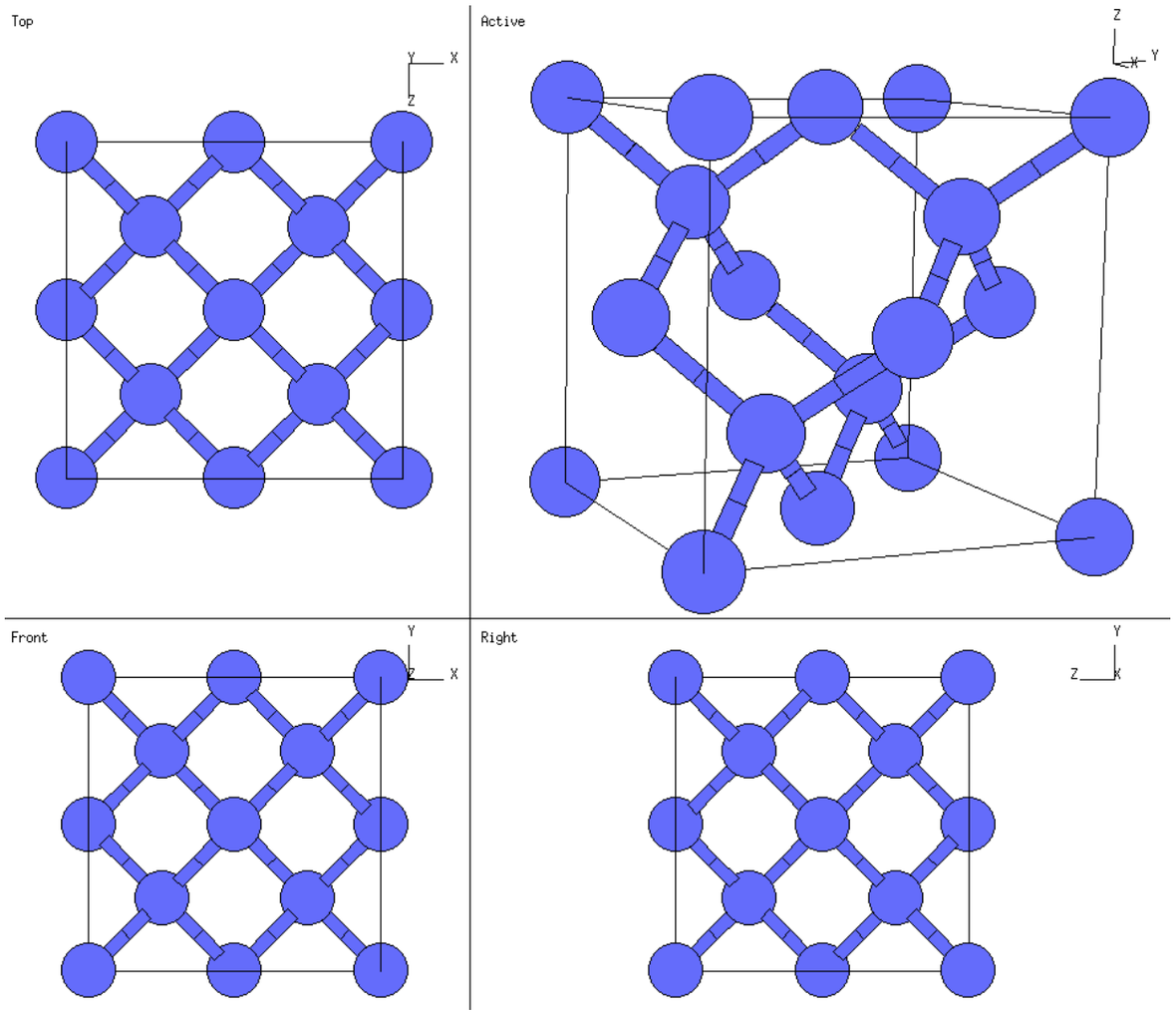
Londsdaleit

Wurtzit (ZnS)

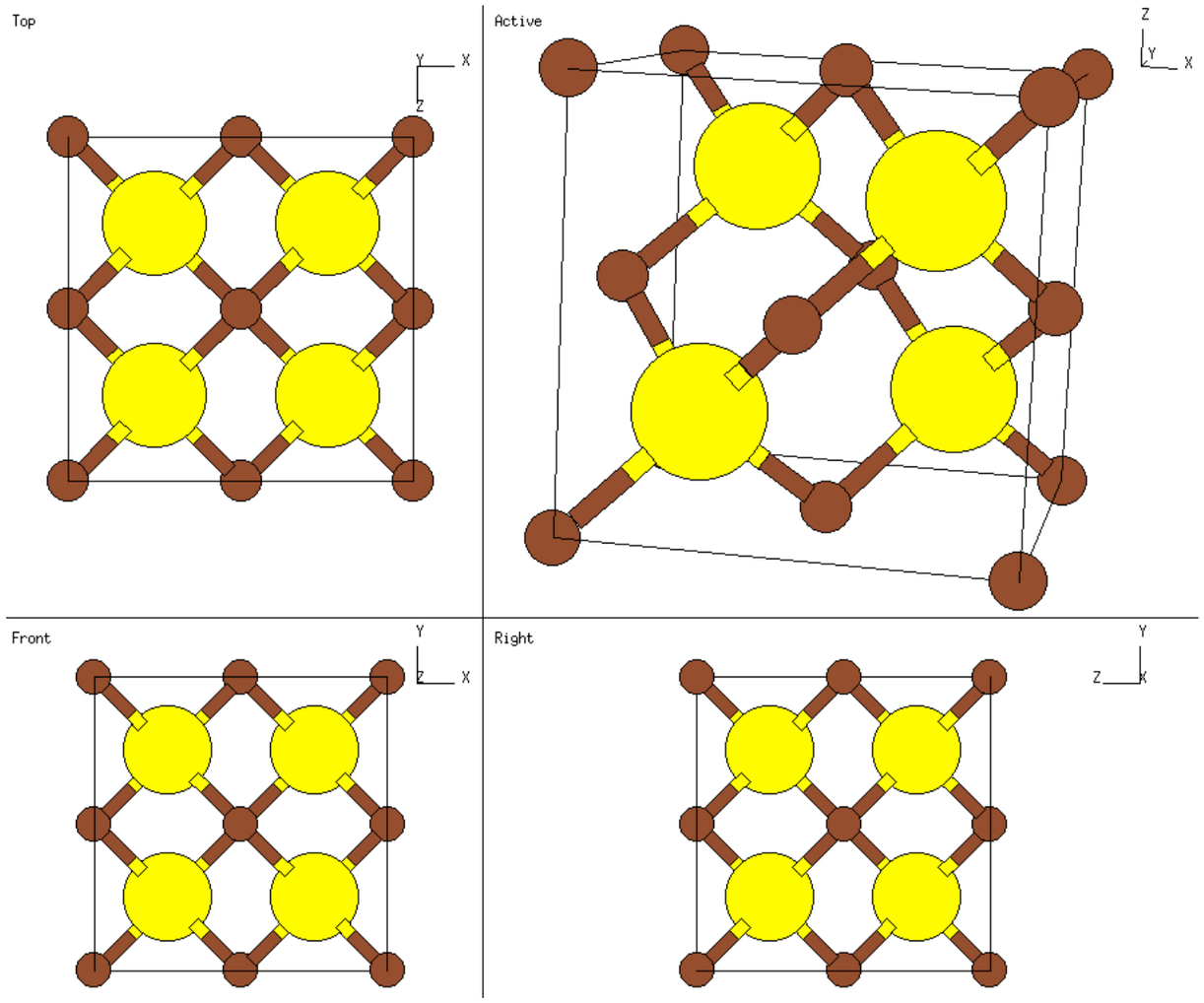
Tetraeder-Stapelung: ABABAB (hcp)

http://cst-www.nrl.navy.mil/lattice/

kovalente Kristalle: sp^3



Diamant

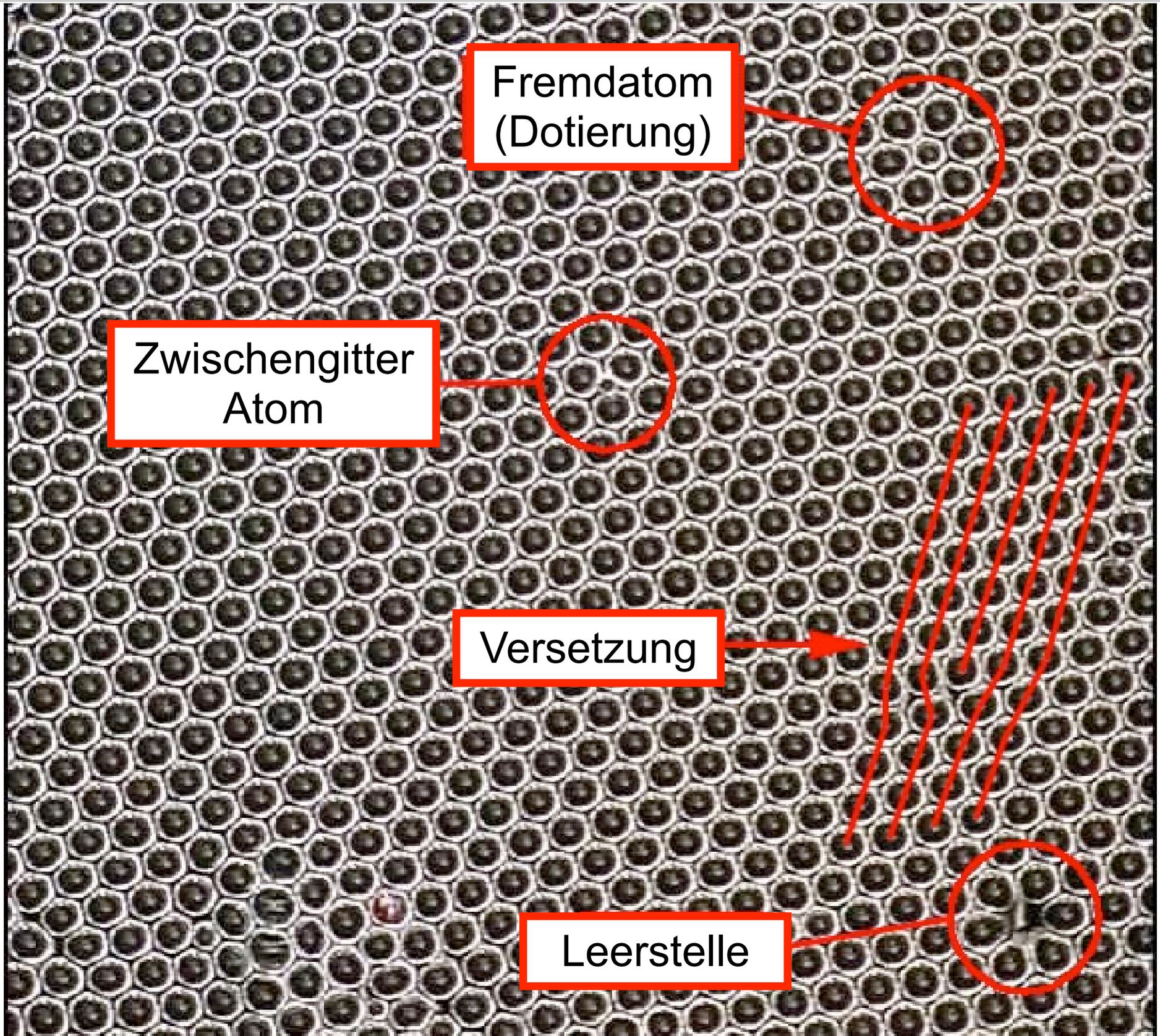


Zinkblende (ZnS)

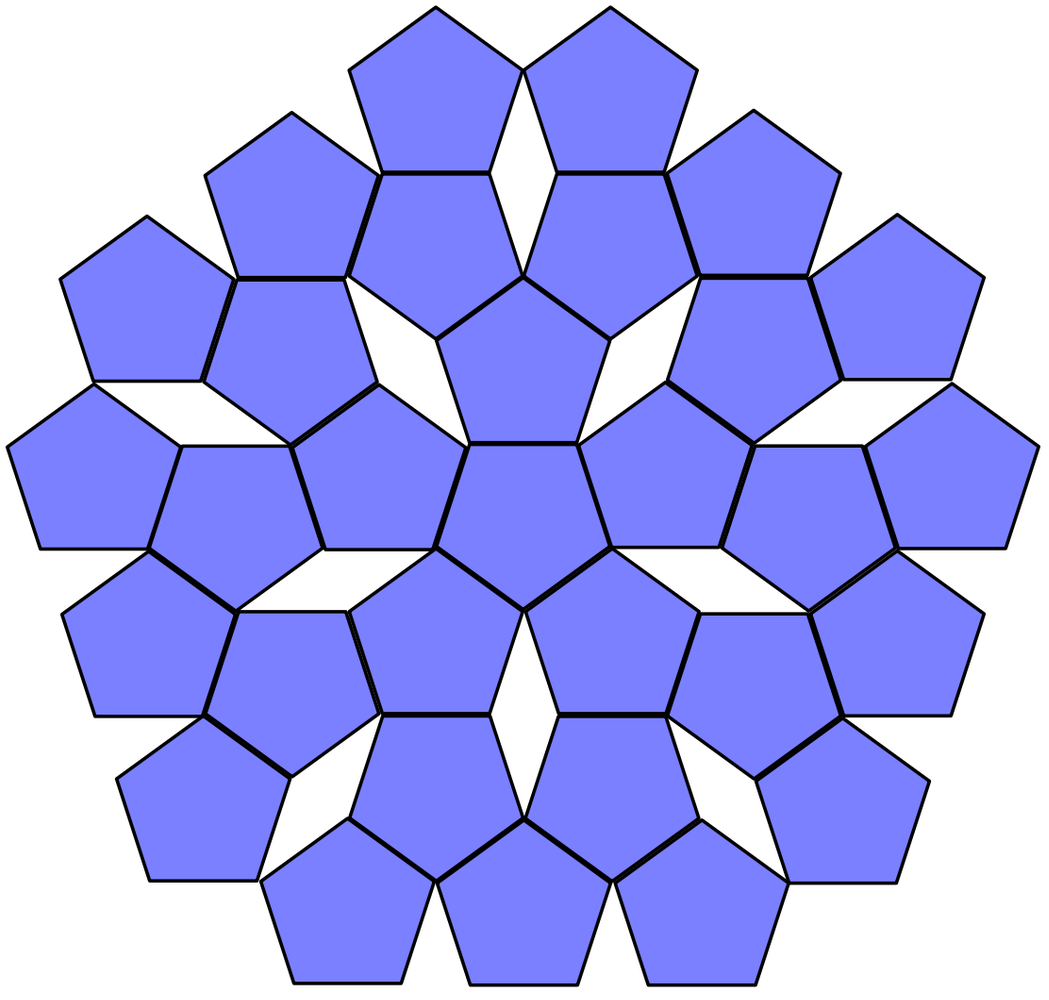
Tetraeder-Stapelung: ABC (fcc)

http://cst-www.nrl.navy.mil/lattice/

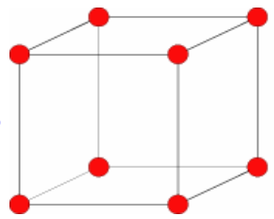
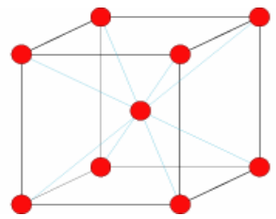
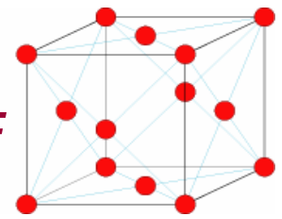
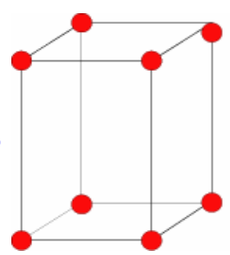
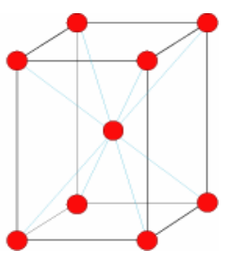
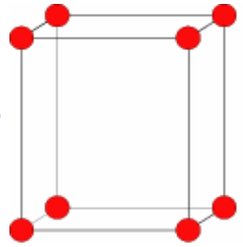
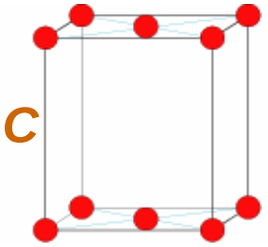
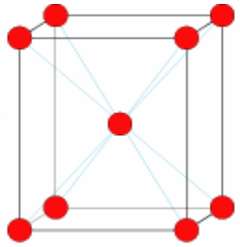
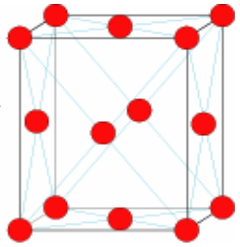
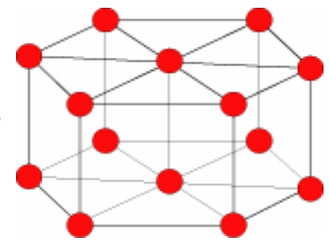
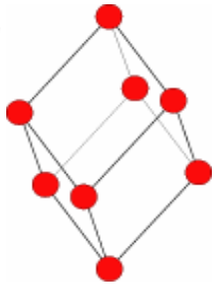
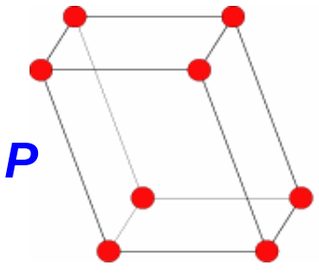
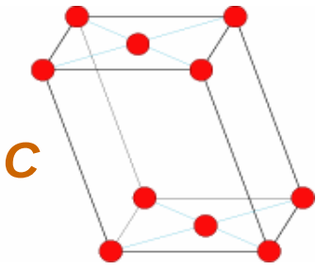
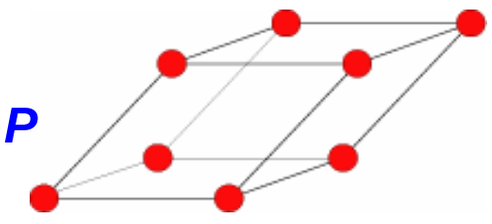
Kristalldefekte

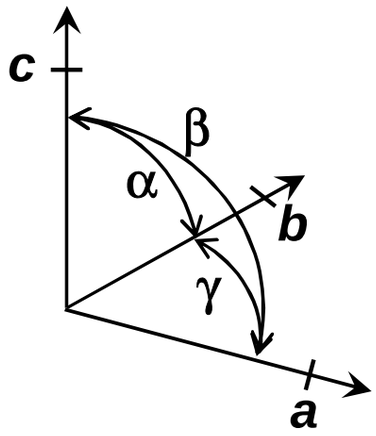


Quasi-Kristall



14 Bravais Gitter

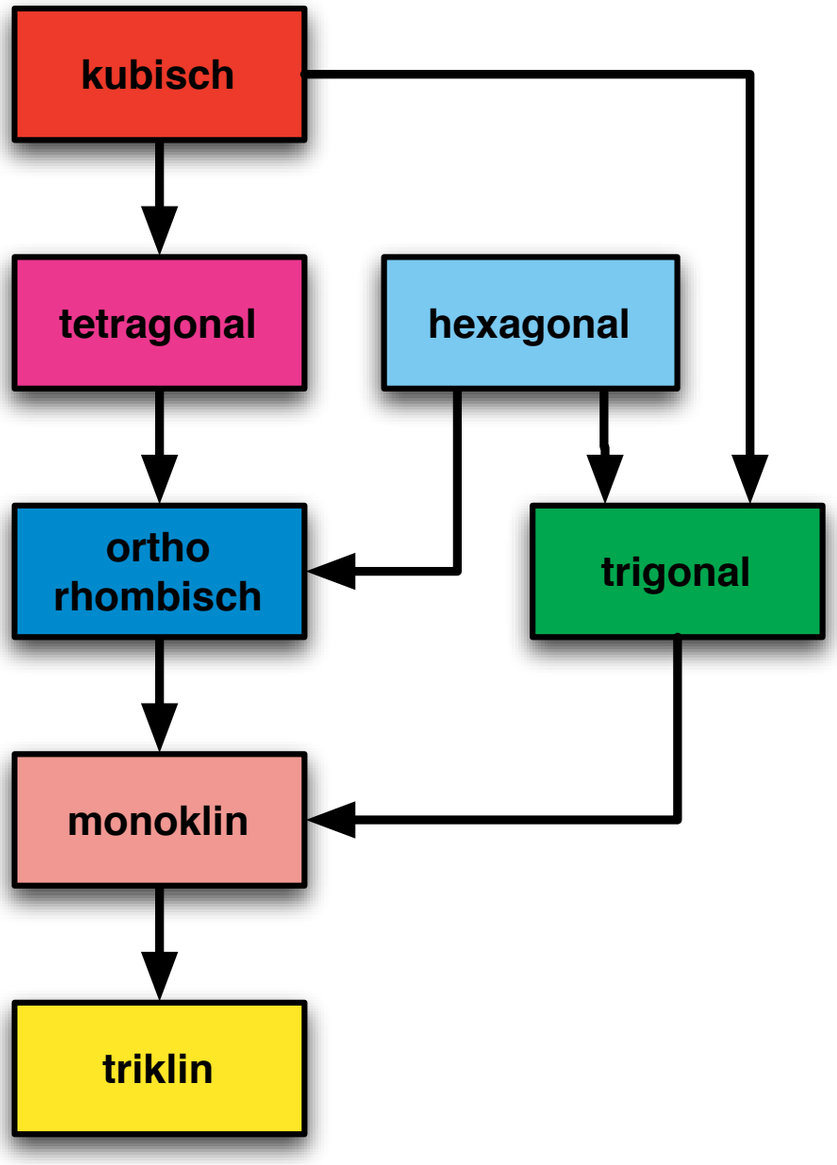
Kristallsystem	*zugehörige Bravais-Gitter*
1 *kubisch*	*P*  *I*  *F* 
2 *tetragonal*	*P*  *I* 
3 *rhombisch*	*P*  *C*  *I*  *F* 
4 *hexagonal*	*P* 
5 *trigonal*	*P* 
6 *monoklin*	*P*  *C* 
7 *triklin*	*P* 



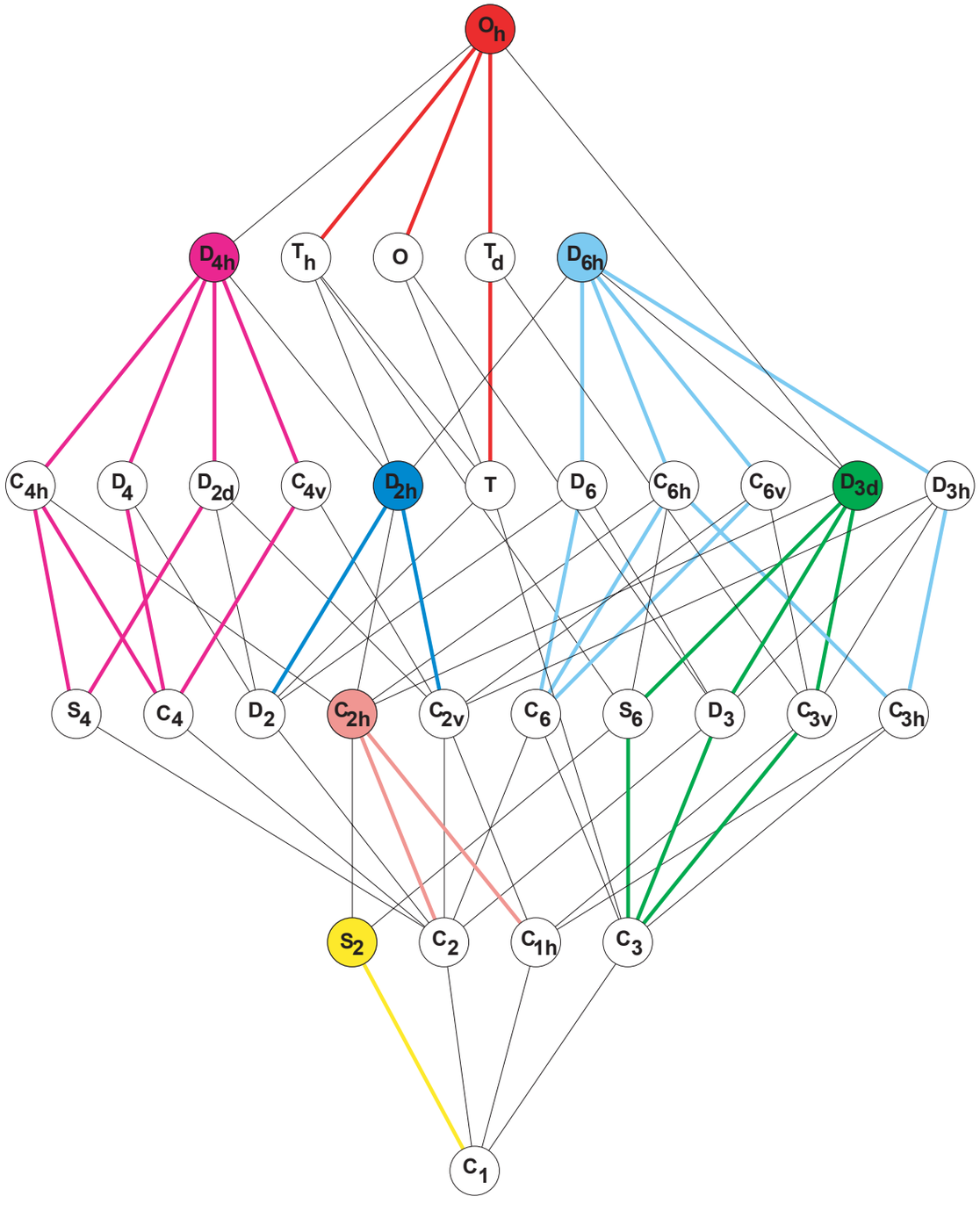
4 Arten von Einheitszellen:

P = *primitiv*
I = *raumzentriert*
F = *flächenzentriert*
C = *basiszentriert*

7 Kristallsysteme ➞ 32 Kristallklassen

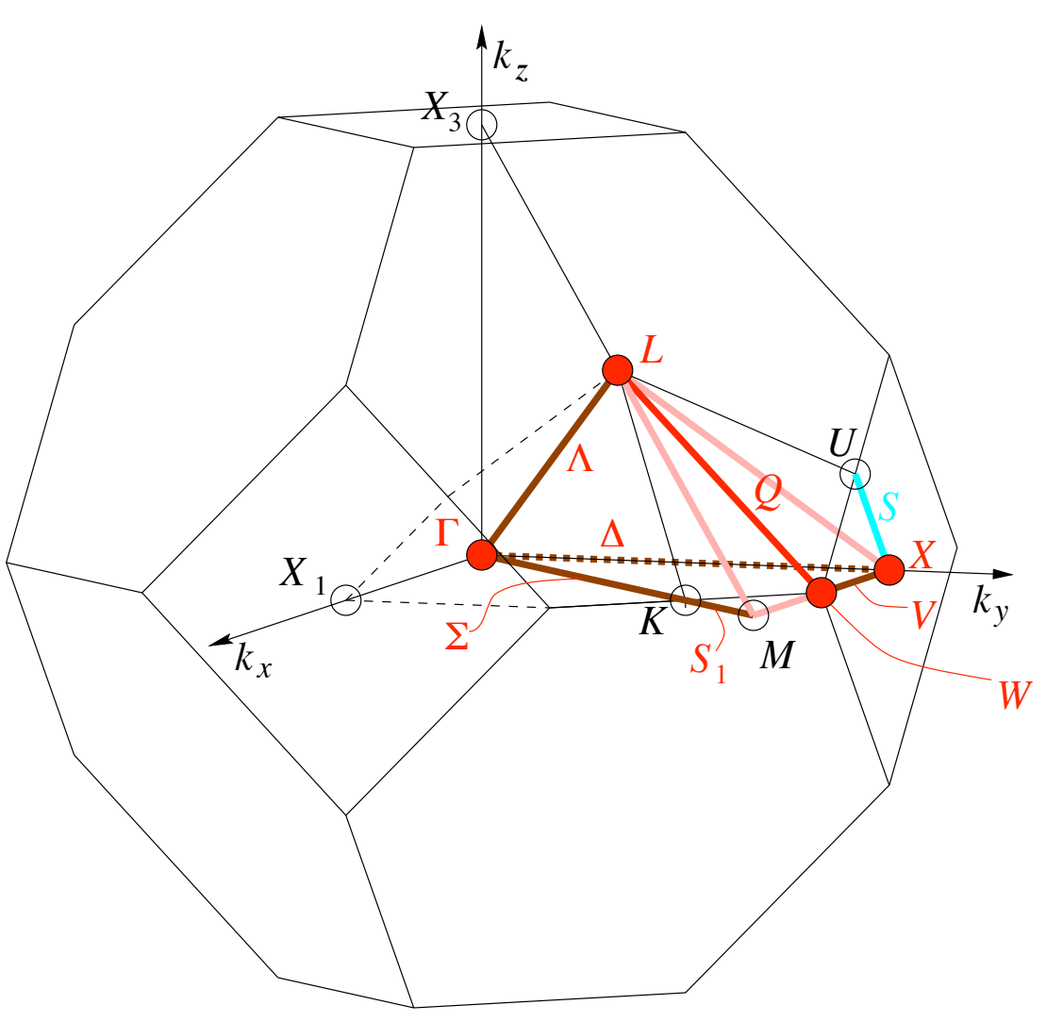


Untergruppenrelationen

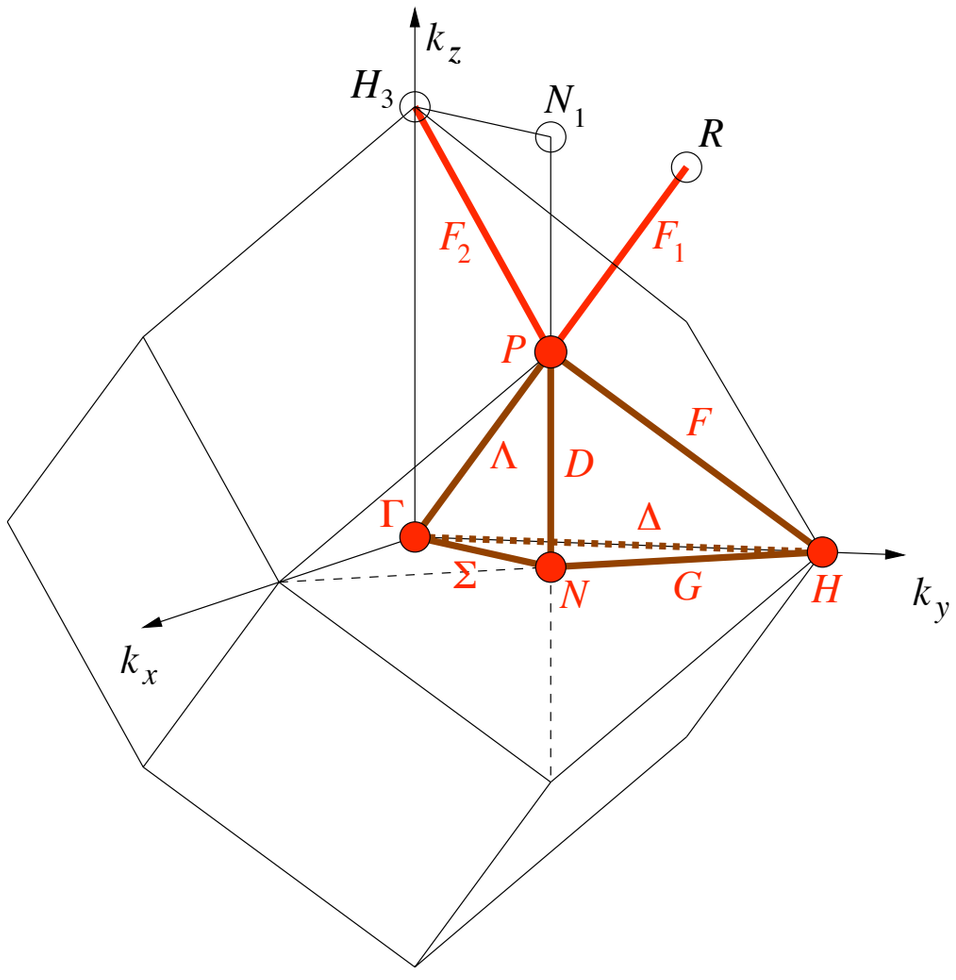


Brillouin Zone

fcc



bcc



Bilbao Crystallographic server: http://www.cryst.ehu.es/

crystallographic information file: cif

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primary 'Physikalische Zeitschrift' 1916 17 277 283 PHZTAO
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Debye, P.;Scherrer, P.
_cell_length_a                    3.70
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_cell_length_c                    3.70
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_cell_angle_beta                  39.75
_cell_angle_gamma                 39.75
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Veröffentlichung

Kristallachsen

Punktgruppe

crystallographic information file: cif

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_symmetry_equiv_pos_as_xyz
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   2   '-z, -x, -y'
   3   '-x, -z, -y'
   4   '-y, -z, -x'
   5   '-y, -x, -z'
   6   '-x, -y, -z'
   7   'z, y, x'
   8   'z, x, y'
   9   'x, z, y'
  10   'y, z, x'
  11   'y, x, z'
  12   'x, y, z'
```

Symmetrieoperationen
in Kristallachsen

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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_B_iso_or_equiv
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C1 C0+ 2 c 0.167 0.167 0.167 0.0 1.
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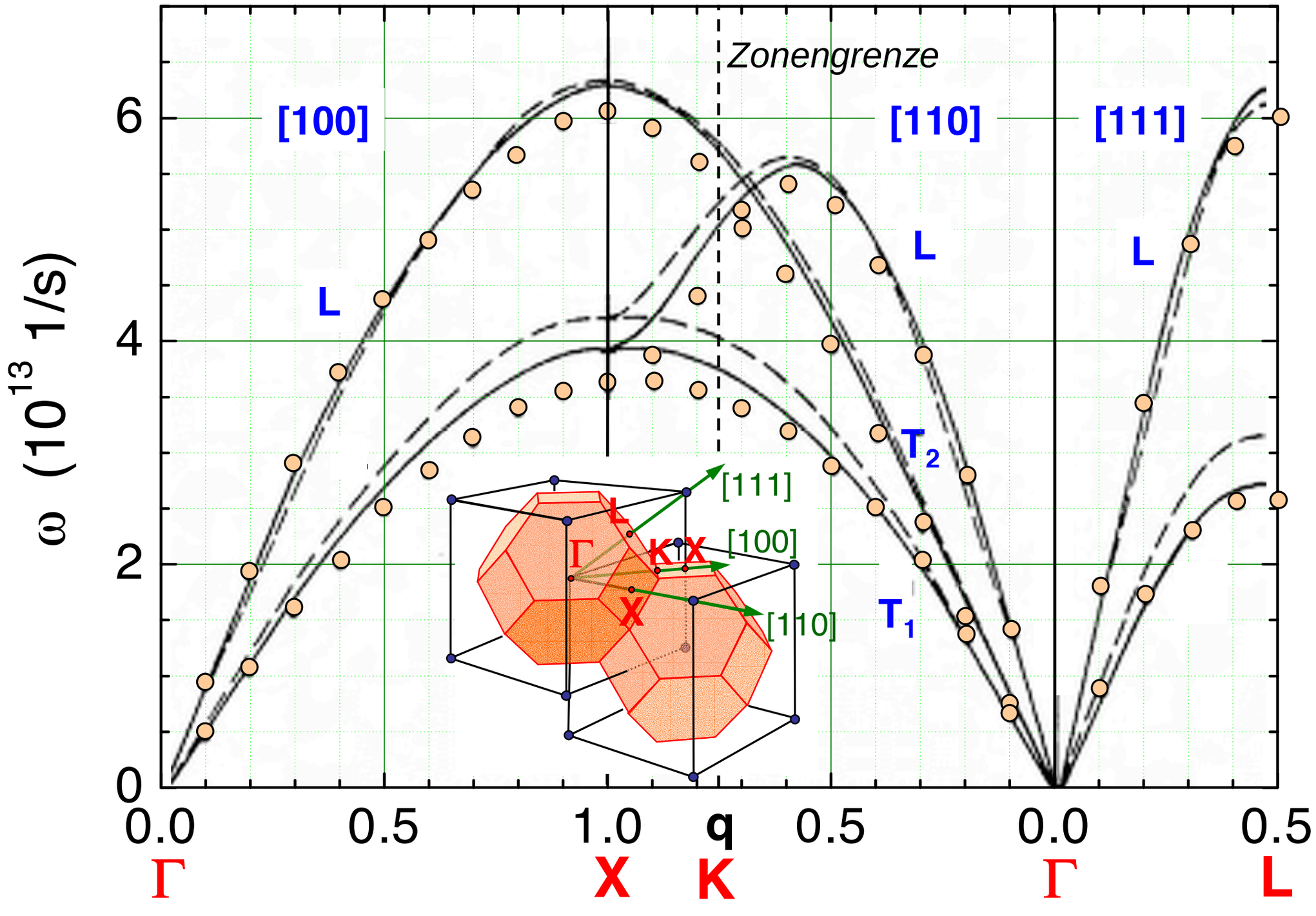
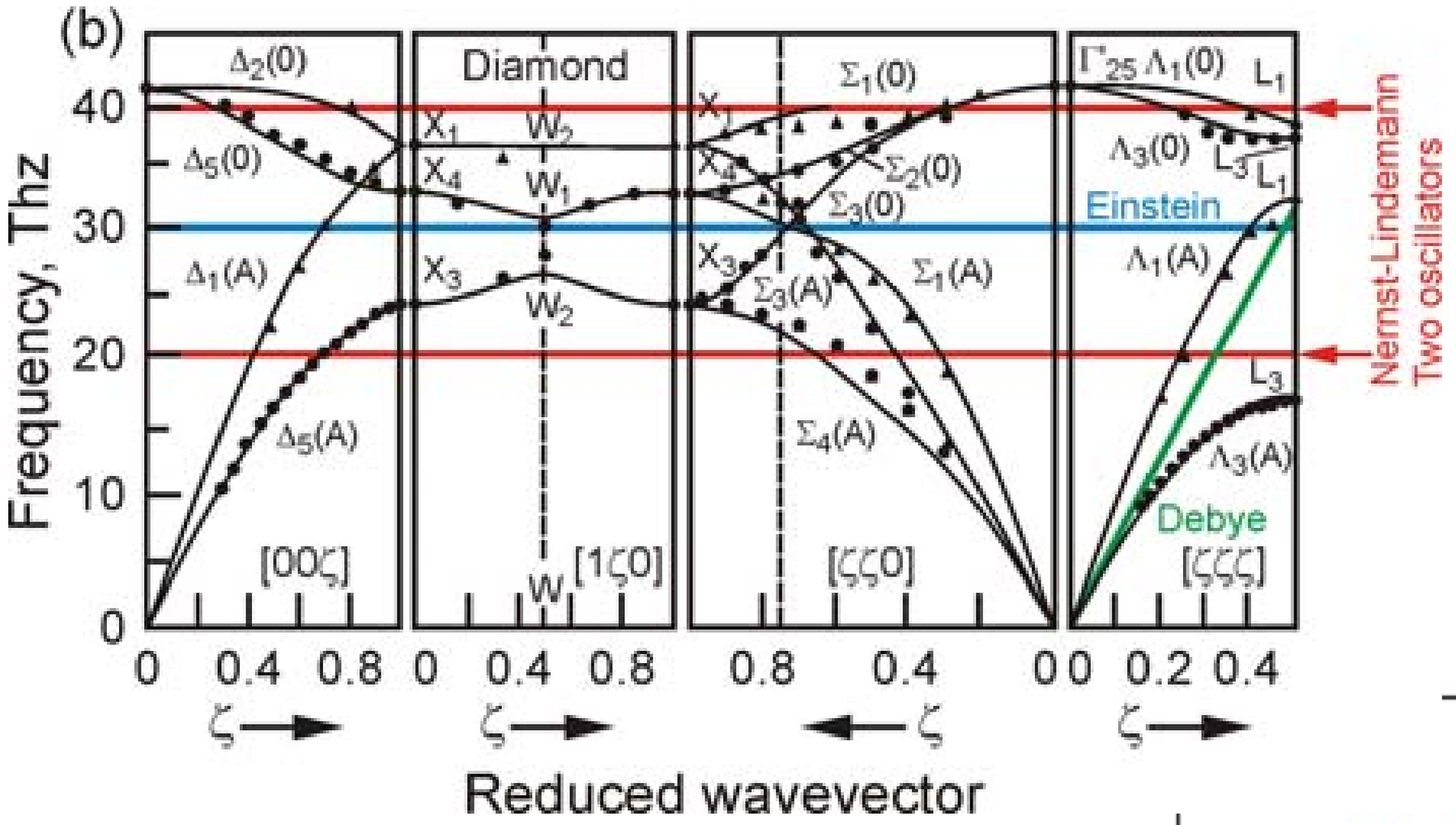
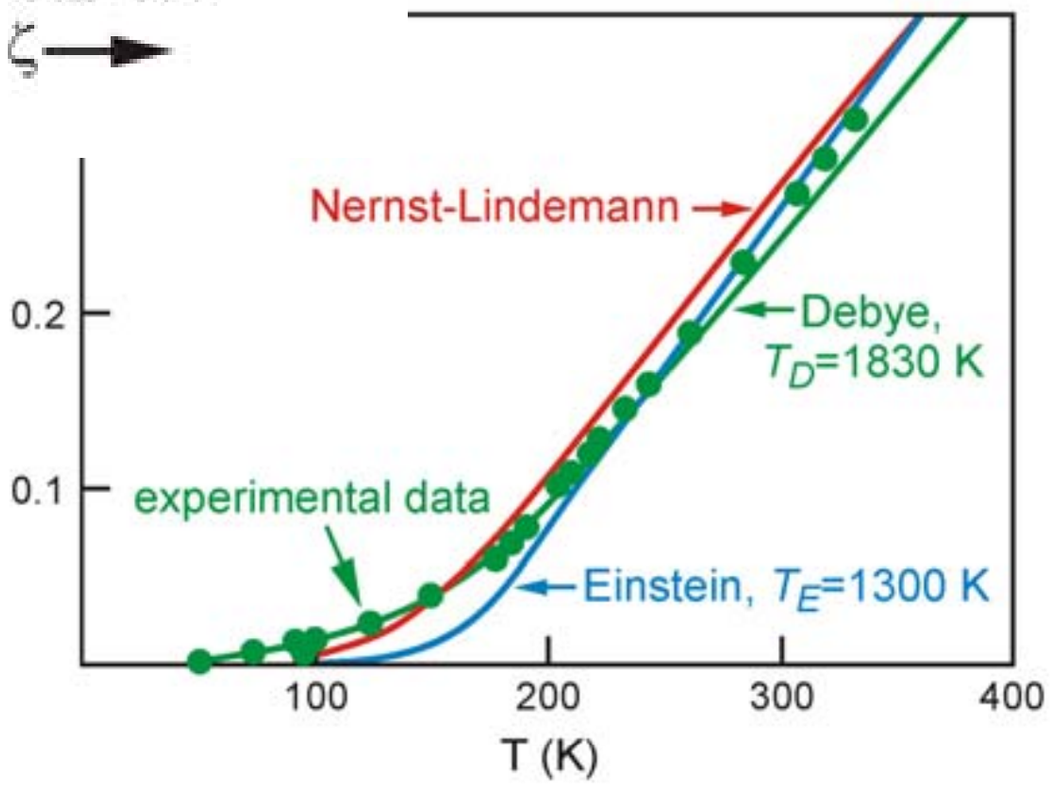
Atompositionen

Phononen Dispersion: Al (fcc)

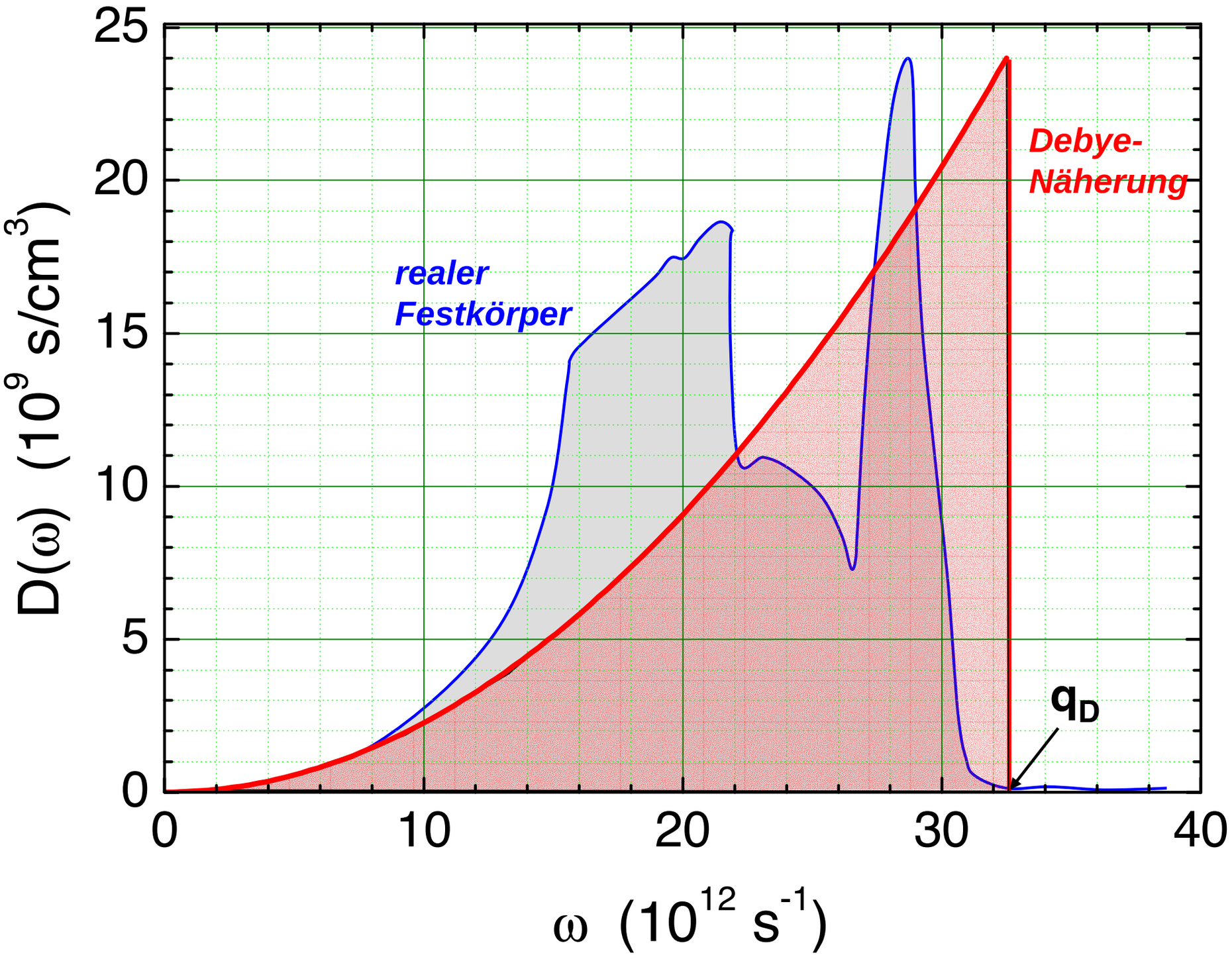


spezifische Wärme: Diamant





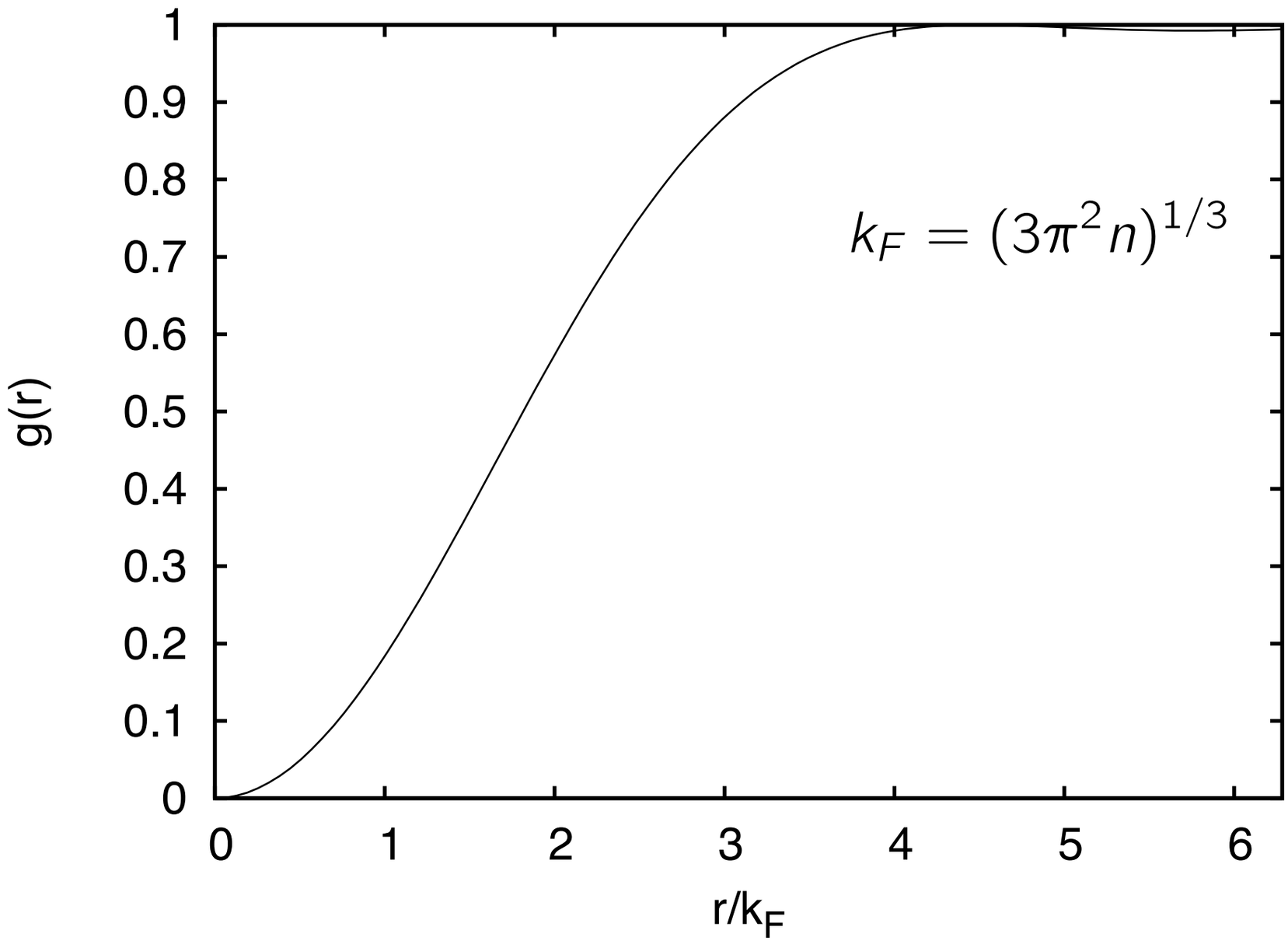
Zustandsdichte: Debye Näherung



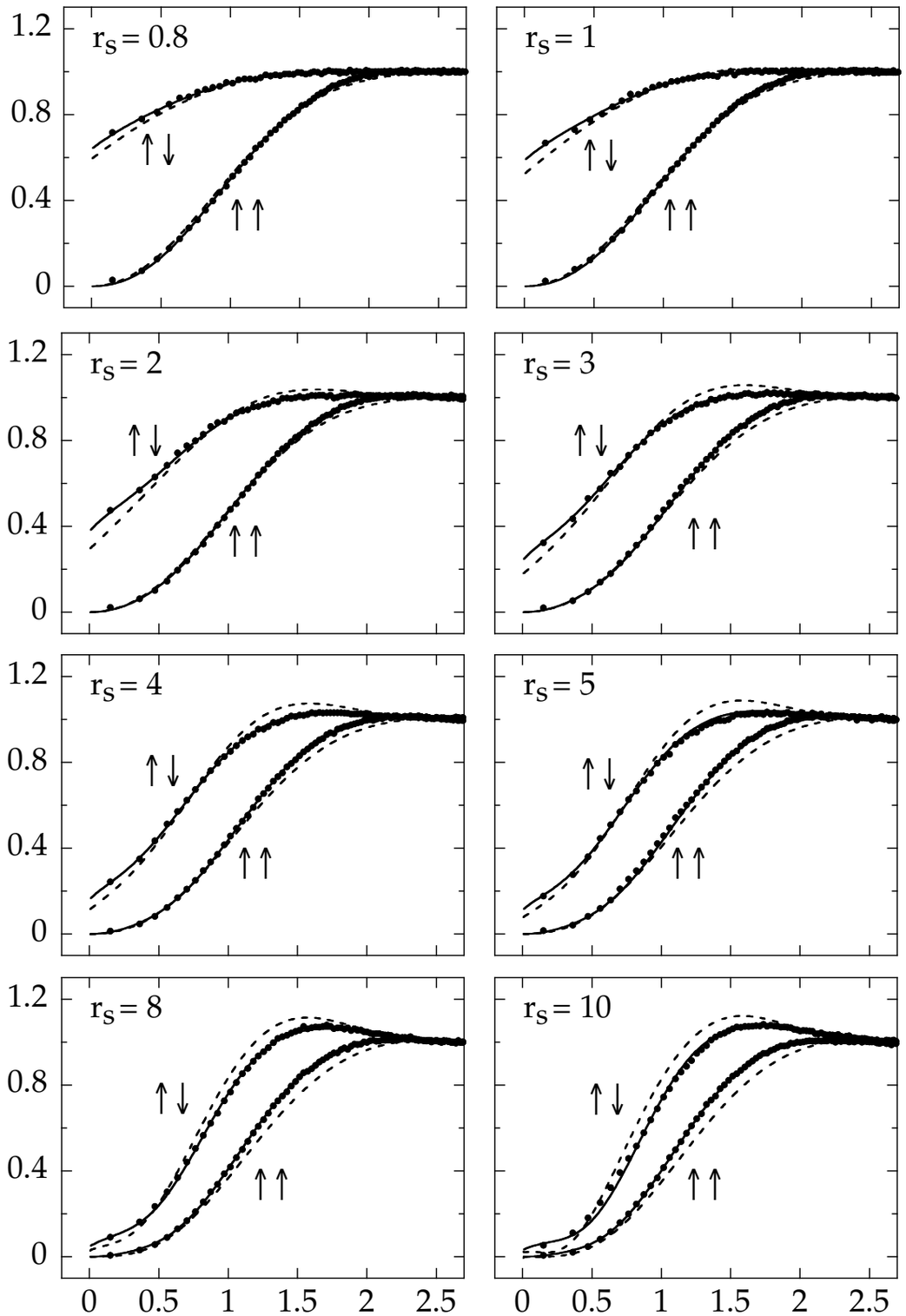
Austausch Loch

unpolarisiertes, homogenes Elektronengas

$$g_x(r) = 1 - \left[\frac{3}{(k_F r)^3} \Big(\sin(k_F r) - k_F r \cos(k_F r) \Big) \right]^2$$



Austausch-Korrelations Loch (QMC)



unpolarisiertes, homogenes Elektronengas

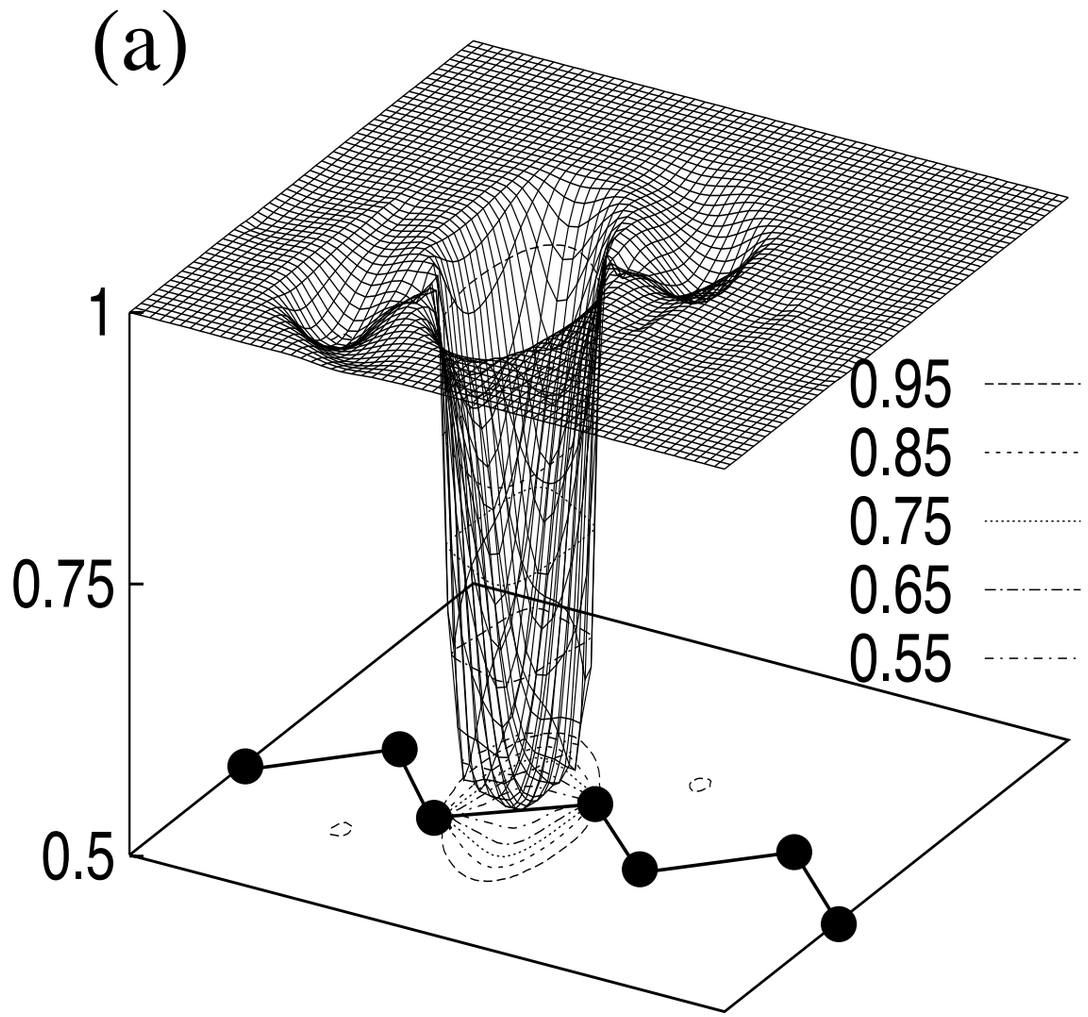
$$g_{xc}^{\sigma\sigma'}(r/r_s)$$

$$r_s = (3/4\pi n)^{1/3}$$

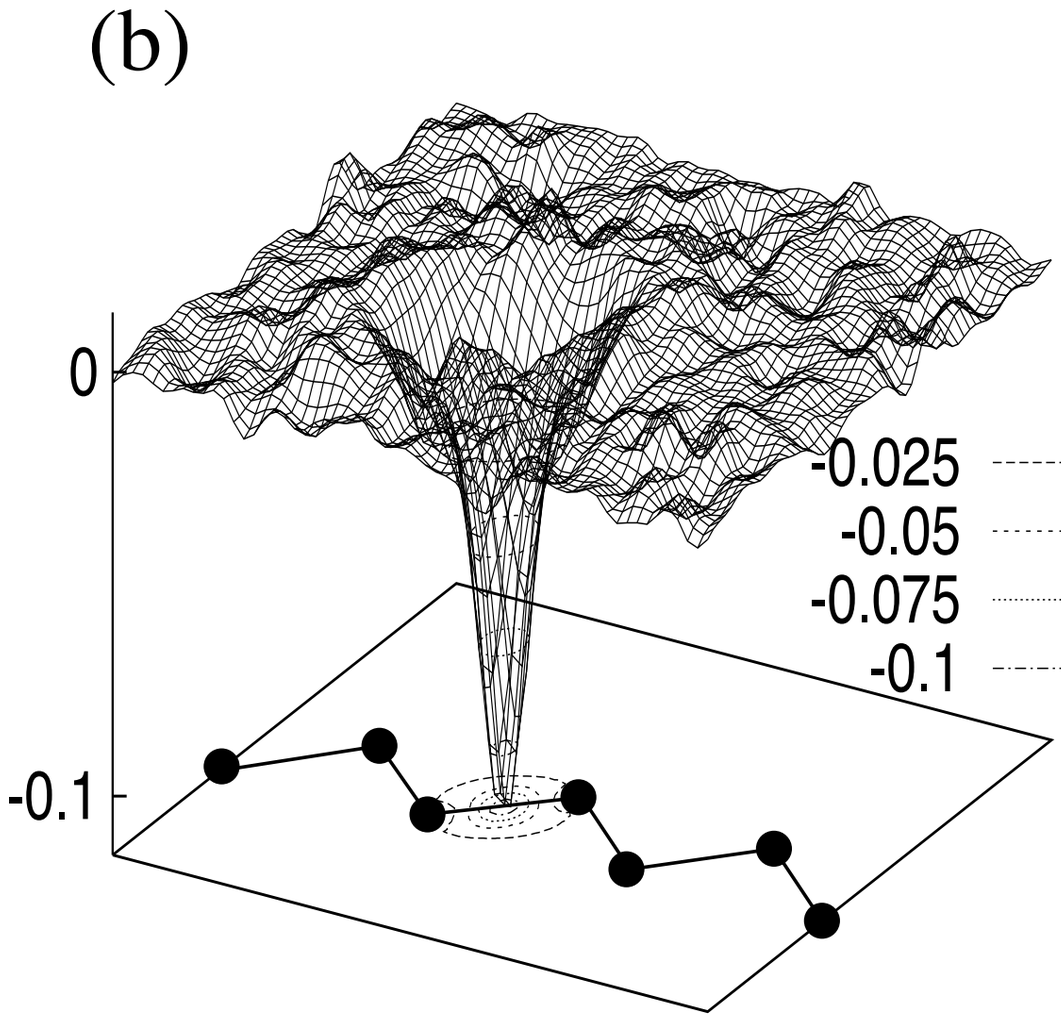
G. Ortiz, M. Harris, P. Ballone
Phys. Rev. Lett. **82**, 5317 (1999)
P. Gori-Giorgi, F. Sacchetti, G.B. Bachelet
Phys. Rev. B **61**, 7353 (200)

Austausch-Korrelations Loch

Elektron im Zentrum einer Si-Si Bindung



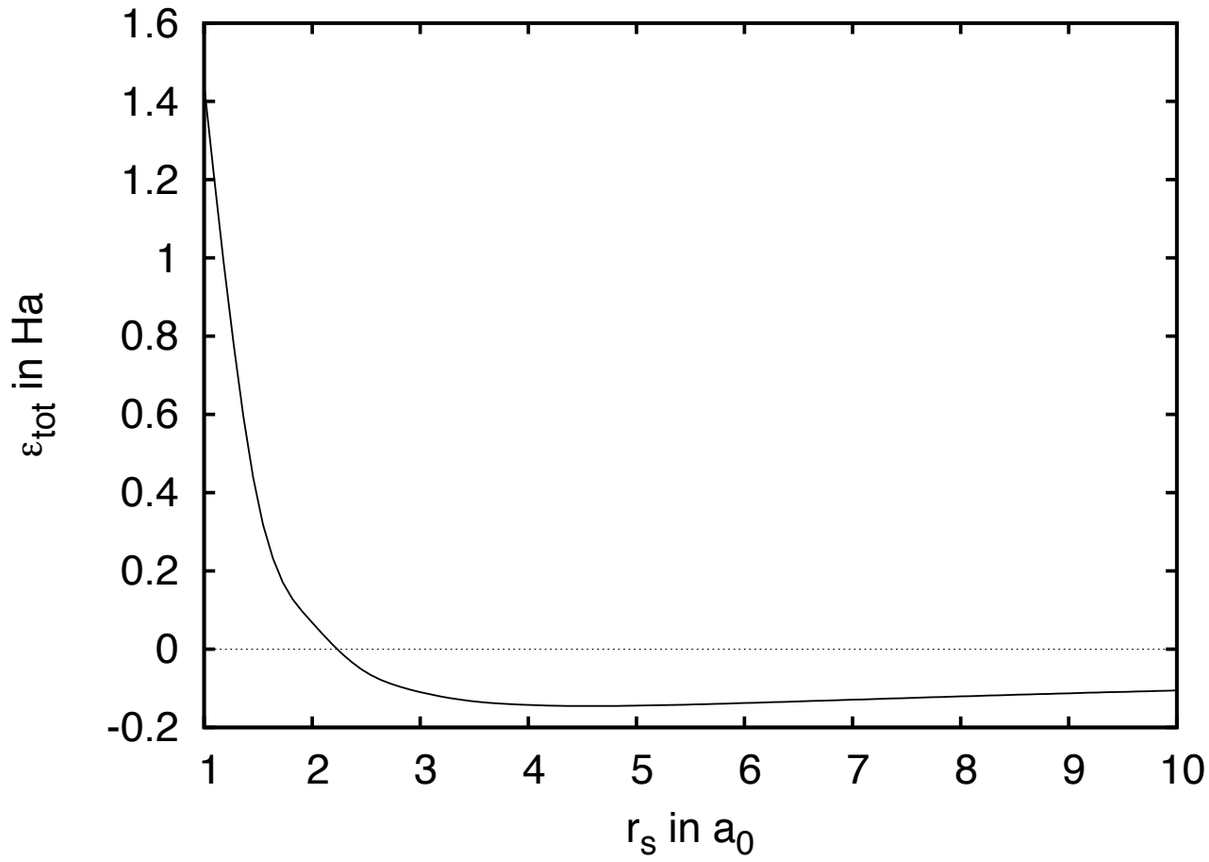
Austausch Loch

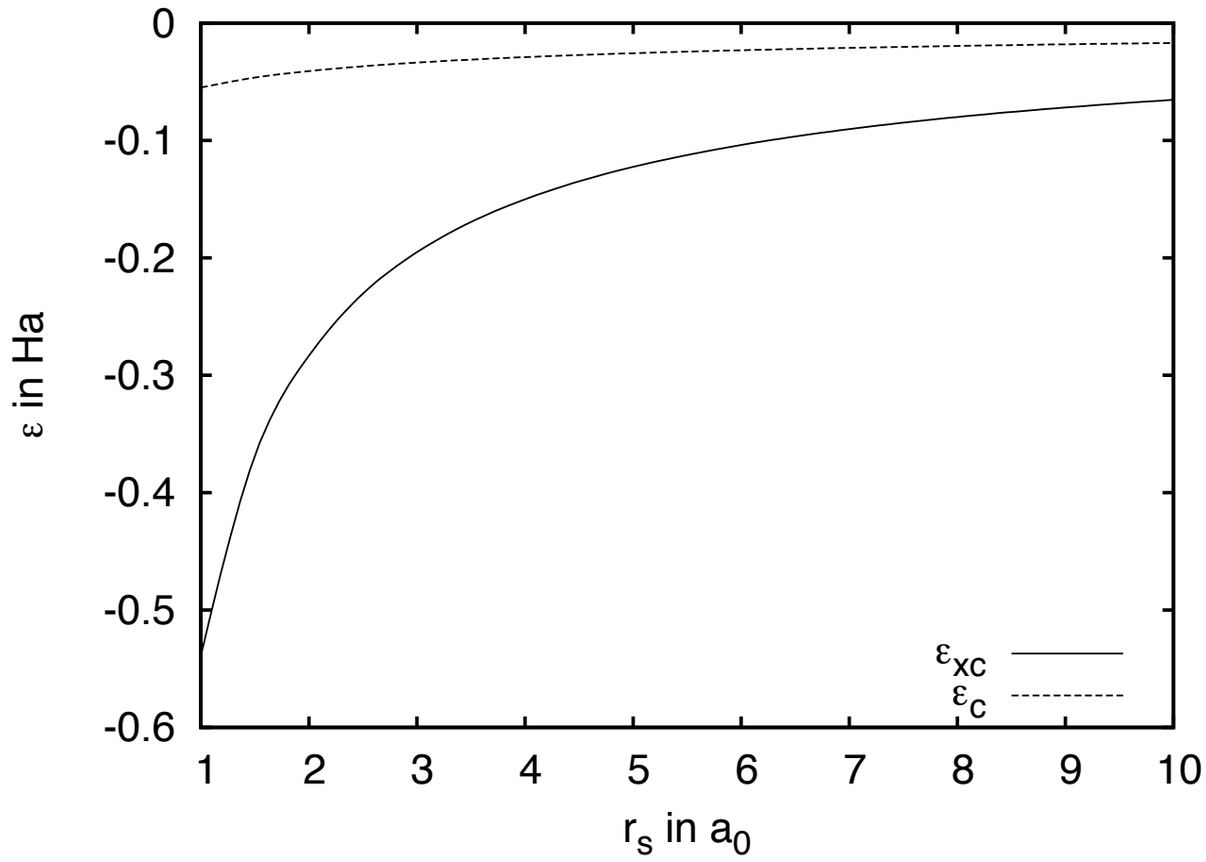


λ-integriertes Korrelations Loch

R.Q. Hood, M.Y. Chou, A.J. Williamson, G. Rajagopal, R.J. Needs, W.M.C. Foulkes
Phys. Rev. B **57**, 8972 (1998)

homogenes Elektronengas (QMC)





D.M. Ceperley, B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980)

Ladungsdichte in C_{60}

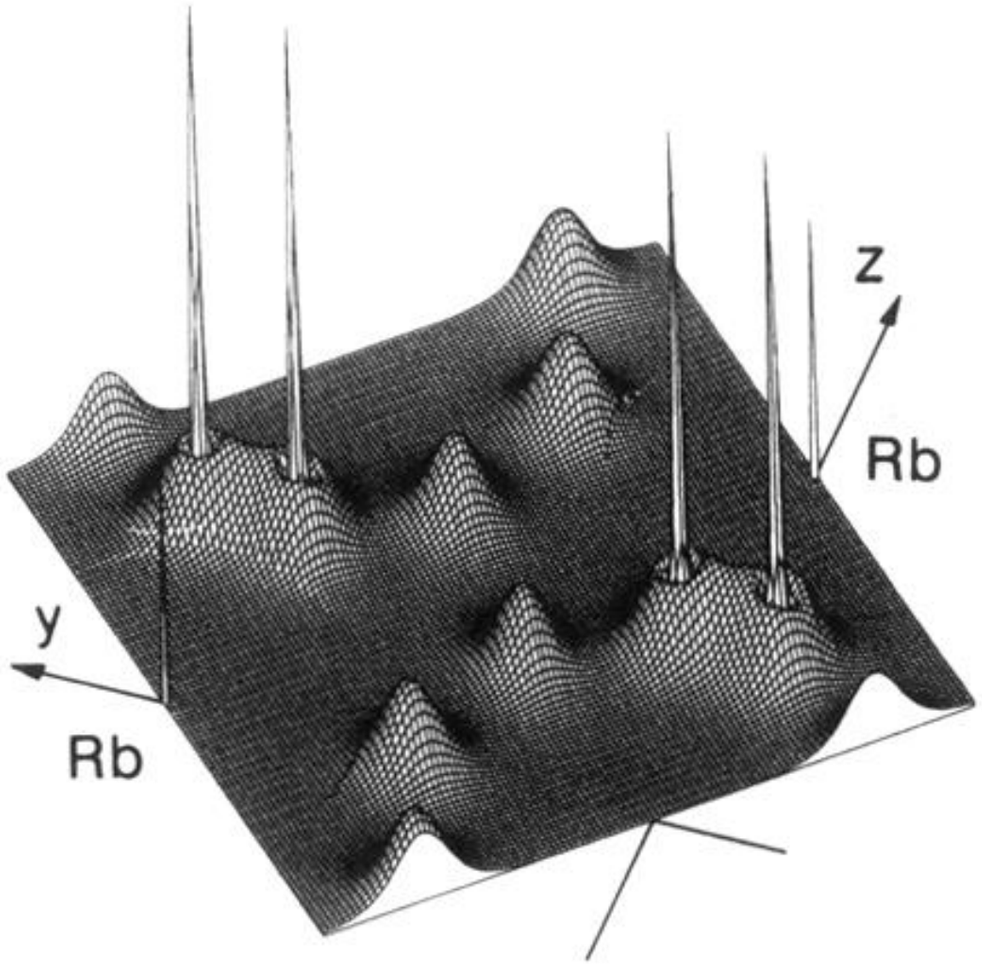


FIG. 12. Valence charge-density in the yz plane (see Fig. 2) for RbC_{60} in the fcc unidirectional structure. The plane passes through the Rb octahedral sites and, for each of two neighboring molecules, it contains a top hexagon edge and passes between two contact atoms plus the midpoint of another top hexagon edge. The Rb $5s$ electron is seen to be transferred to the C_{60} molecule.

Die Suche nach guten Dichtefunktionalen

PERSPECTIVES: DENSITY FUNCTIONAL THEORY

In Pursuit of the "Divine" Functional

Ann E. Mattsson

Paul Dirac reputedly said that the Schrödinger equation (SE) marked the end of chemistry: All answers could be calculated from the SE. The SE

lated exactly, just as the properties of small systems can be calculated from the SE.

The first step toward the divine functional was the local density approximation (LDA),

sively used in gas-phase catalysis, where the metallic character of the catalyst makes traditional SE methods inappropriate, and for determining phase diagrams (e.g., for steels).

In recognition of the importance of DFT, Walter Kohn was awarded half of the 1998 Nobel Prize in Chemistry (the other half was awarded to John Pople) (*10*). Today numerous approximate functionals are in use (*11*)—a sign of the method's utility but also an indication that none is suitable for all systems. As the complexity of systems investigated by DFT grows (see the figure), the

Science **298**, 759 (2002)

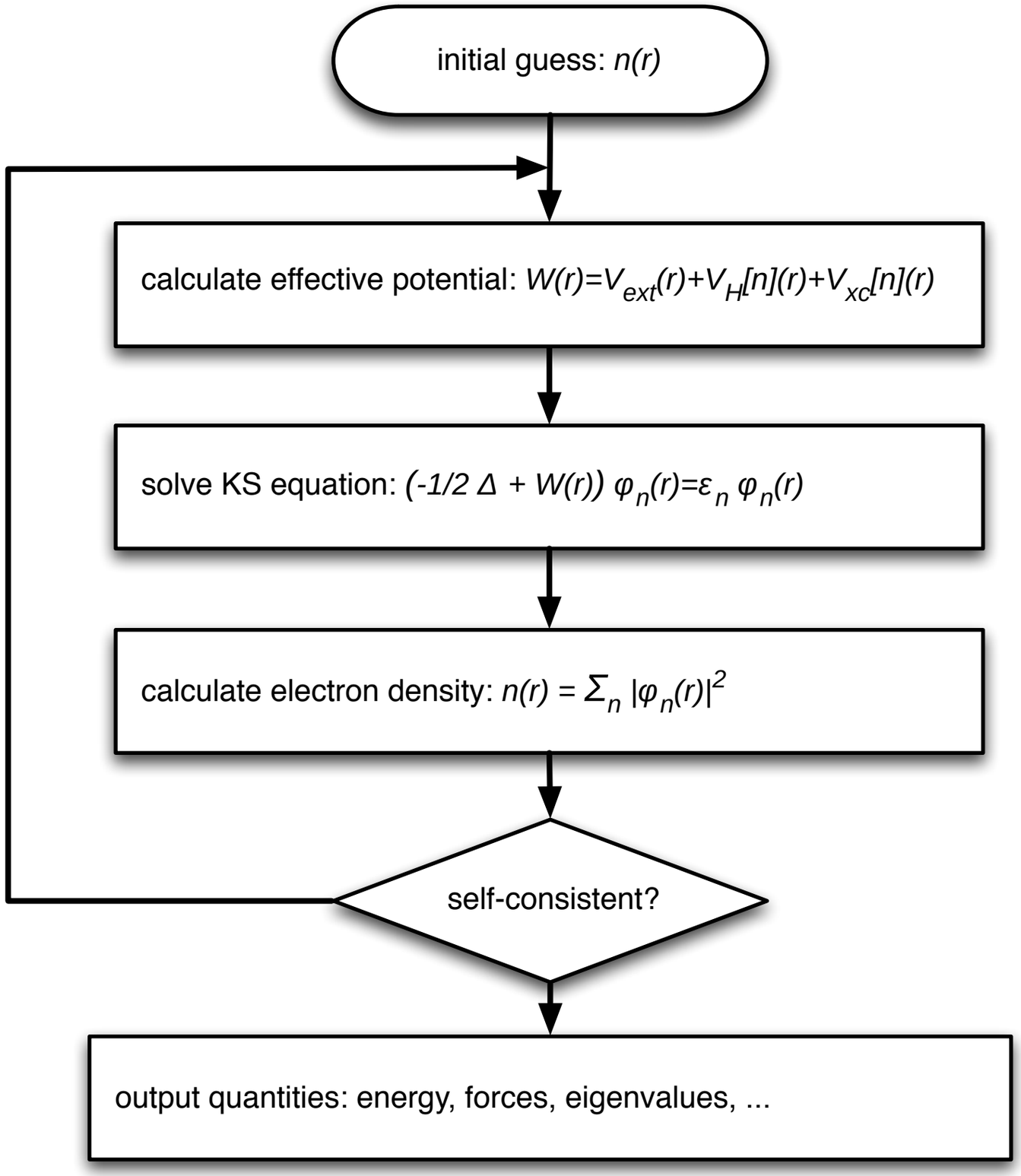
Comparison shopping for a gradient-corrected density functional

John P. Perdew and Kieron Burke
Int. J. Quant. Chem. **57**, 309 (1996)

Parametrised local spin density exchange-correlation energies and potentials for electronic structure calculations

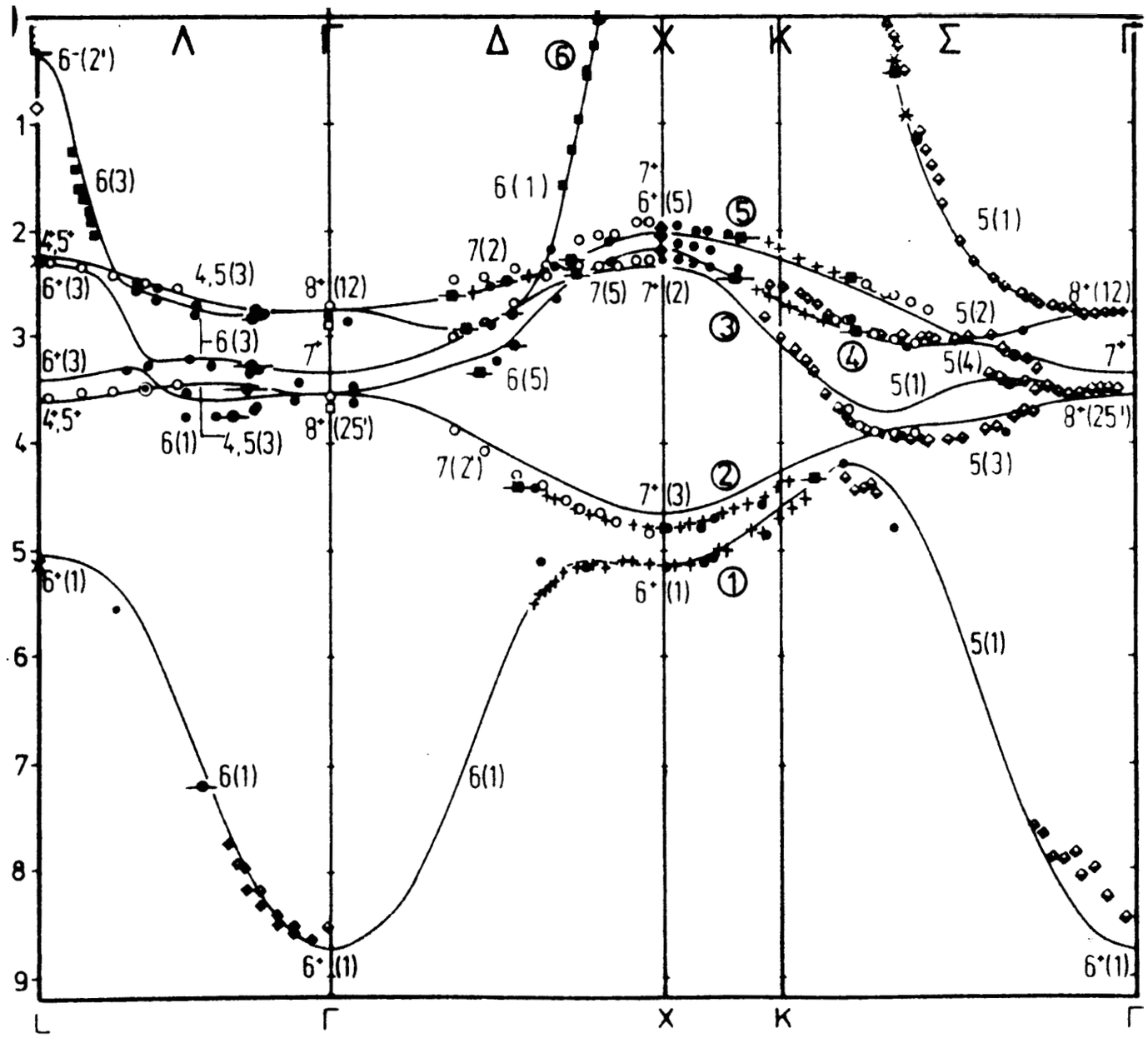
Computer Physics Communications **66**, 383 (1991)

Lösen der Kohn-Sham Gleichungen



Bandstruktur von Kupfer

winkelaufgelöste Photoemission (ARPES) vs. DFT Rechnung



P. Thiry *et al.*, Phys. Rev. Lett. **43**, 82 (1979)
G.A. Burdick, Phys. Rev. **129**, 138 (1963)