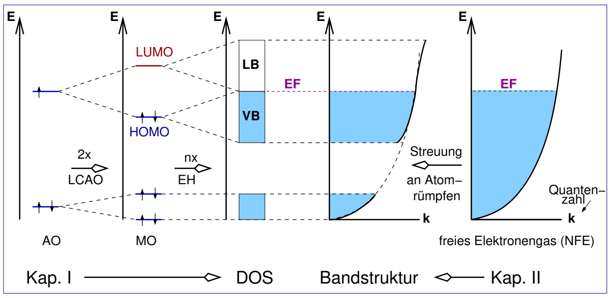
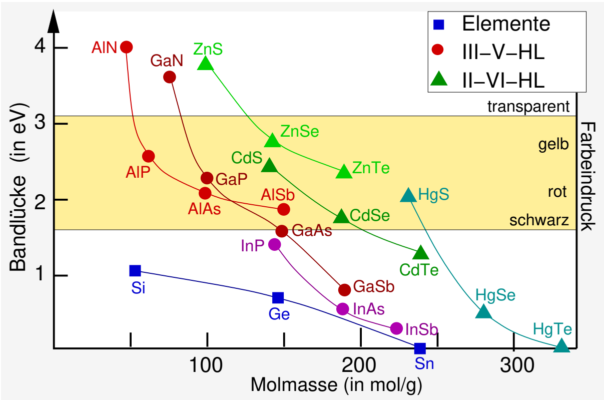
Einleitung



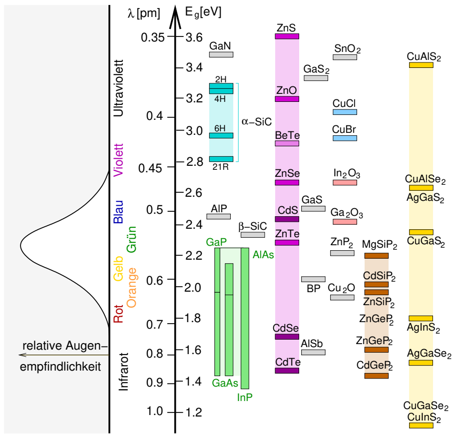
MO – NFE ↦ DOS/BS

Substanz	Typ	E_g [eV] (0 K)
C (Diamant)	i	5.4
Si	i	1.17
Ge	i	0.744
GaAs	d	1.52
Sn (α)	-	0
As		klein
Sb, Bi, Graphit	-	0
Se		2.2
Te	d	0.33

Übersicht Bandlücken

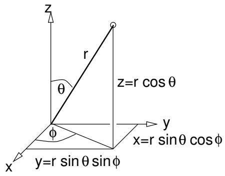


Bandlücken bei Verbindungshalbleitern



I. LCAO-Ansatz: Der Festkörper als 'Riesenmolekül' (EH-Methode)

Atomorbitale (Wdh.) (Lsg. d. Schrödinger-Gleichung für H-Atom)



Kugelkoordinaten

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$

☐ Eigenenergien: E_n

☐ Eigenfunktionen: $\psi_{n,l,m_l} = NR_{n,l}(r)\chi_{l,m_l}(\theta,\phi)$

Z=1, $a_0 = 52.917$pm (Bohr'scher Radius)

Quanten-zahlen n l	m_l	Orbital	Eigenwert E_n	norm. Radialfunktion $R_{n,l}(r)$	norm. Winkelfunktion sphär. Koord. $\chi_{l,m_l}(\theta,\phi)$	kart. Koord. $\chi_{l,m_l}(\frac{x}{r},\frac{y}{r},\frac{z}{r})$
1 0	0	1s	E_1	$\frac{2}{\sqrt{a_0^3}}e^{-\frac{r}{a_0}}$	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}}$
2 0	0	2s	$E_2 = \frac{E_1}{4}$	$\frac{1}{2\sqrt{2a_0^3}}(2-\frac{r}{a_0})e^{-\frac{r}{2a_0}}$	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}}$
2 1	0	$2p_z$	$E_2 = \frac{E_1}{4}$	$\frac{1}{2\sqrt{6a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}$	$\frac{\sqrt{3}}{2\sqrt{\pi}}\cos\theta$	$\frac{\sqrt{3}}{2\sqrt{\pi}}\frac{z}{r}$
2 1	1	$2p_x$	$E_2 = \frac{E_1}{4}$	$\frac{1}{2\sqrt{6a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}$	$\frac{\sqrt{3}}{2\sqrt{\pi}}\sin\theta\cos\phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}}\frac{x}{r}$
2 1	-1	$2p_y$	$E_2 = \frac{E_1}{4}$	$\frac{1}{2\sqrt{6a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}$	$\frac{\sqrt{3}}{2\sqrt{\pi}}\sin\theta\sin\phi$	$\frac{\sqrt{3}}{2\sqrt{\pi}}\frac{y}{r}$
3 0	0	3s	$E_3 = \frac{E_1}{9}$		$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{2\sqrt{\pi}}$
3 1	0	$3p_z$	$E_3 = \frac{E_1}{9}$			
3 1	1	$3p_x$	$E_3 = \frac{E_1}{9}$			
3 1	-1	$3p_y$	$E_3 = \frac{E_1}{9}$			
3 2	-1	$3d_{xy}$	$E_3 = \frac{E_1}{9}$		$\sqrt{\frac{15}{4\pi}}\sin^2\theta\sin\phi\cos\phi$	$\sqrt{\frac{15}{4\pi}\frac{xy}{r^2}}$
3 2	1	$3d_{xz}$	$E_3 = \frac{E_1}{9}$		$\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\phi$	$\sqrt{\frac{15}{4\pi}\frac{xz}{r^2}}$
3 2	0	$3d_{yz}$	$E_3 = \frac{E_1}{9}$		$\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\phi$	$\sqrt{\frac{15}{4\pi}\frac{yz}{r^2}}$
3 2	2	$3d_{z^2}$	$E_3 = \frac{E_1}{9}$		$\sqrt{\frac{15}{4\pi}}3\cos^2\theta - 1$	$\sqrt{\frac{15}{4\pi}\frac{3z^2-r^2}{r^2}}$
3 2	-2	$3d_{x^2-y^2}$	$E_3 = \frac{E_1}{9}$		$\sqrt{\frac{15}{4\pi}}\sin^2\theta\cos 2\phi$	$\sqrt{\frac{15}{4\pi}\frac{x^2-y^2}{r^2}}$