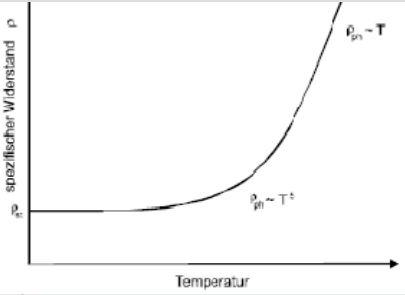


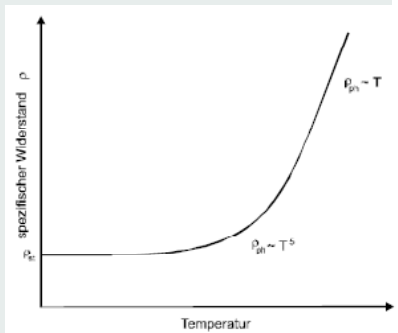
Metals, Semiconductors, Insulators



	ionisch	kovalent	metallisch
Bandstruktur			
totale DOS			
partielle DOS			

Metals, Semiconductors, Insulators

	ionisch	kovalent	metallisch
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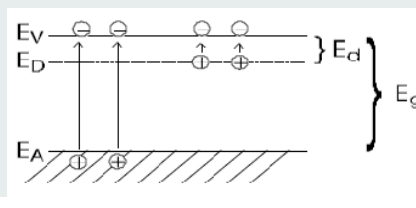


$T \ll \Theta_D : \rho_{ph} \propto T^5$ (Kleinwinkelstreuung)

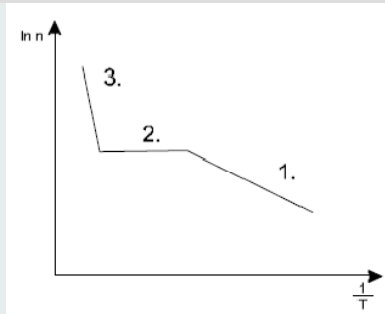
und

$T \gg \Theta_D : \rho_{ph} \propto T$

wobei Θ_D die Debye-Frequenz des Festkörpers ist.



$$\sigma = ne\mu_n + pe\mu_p$$



1. **Impurity reserve** ($E_d \gg kT$):

Thermal energy is too low to promote electrons from donatorniveaus into conduction band

$$n \propto e^{-\frac{E_d}{2kT}}$$

2. **Impurity depletion** ($E_d \ll kT \ll E_g$):

All donator centers are ionised, but thermal energy still to promote electrons via the intrinsic band gap.

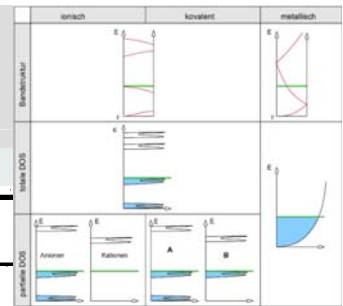
$$n = \text{const.}$$

3. **Intrinsic conductivity** ($E_g \ll kT$):

Thermal energy is large enough, to promote intrinsic charge carriers over the band gap. Now the donor carriers become the minority carriers and conductivity raises strongly

$$n \propto e^{-\frac{E_g}{2kT}}$$

Metals, Semiconductors, Insulators



R. NESPER, ETH ZÜRICH & COLLEGIUM HELVETICUM

I-VII compounds		II-VI compounds		III-V compounds	
LiF	11	ZnO	3.4	AlP	3.0
LiCl	9.5	ZnS	3.8	AlAs	2.3
NaF	11.5	ZnSe	2.8	AlSb	1.5
NaCl	8.5	ZnTe	2.4	GaP	2.3
NaBr	7.5	CdO	2.3	GaAs	1.4
KF	11	CdS	2.45	GaSb	0.7
KCl	8.5	CdSe	1.8	InP	1.3
KBr	7.5	CdTe	1.45	InAs	0.3
KI	5.8	PbS	0.37	InSb	0.2
		PbSe	0.27	β -SiC	2.2
		PbTe	0.33	α -SiC	3.1

Some of these values, especially for the alkali halides, are only approximate.

Nitrides, Carbides ??

Nanochemistry UIO

Color in Semiconductors II Bandgap-Tuning by Quanten-Size-Effect

R. NESPER, ETH ZÜRICH & COLLEGIUM HELVETICUM

CdTe



Growing particle diameter from 2 auf 5 nm results in color change from green to red \rightarrow bandgap becomes smaller

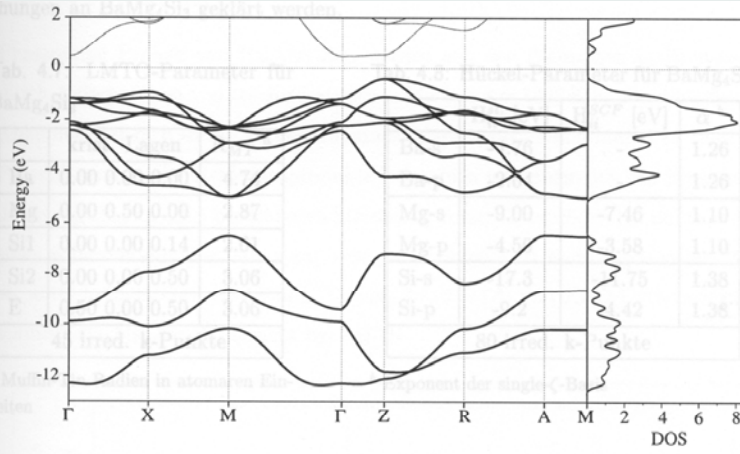
Nanochemistry UIO



Photoelectron spectra (ESCA)

UPS: $E_{\text{rad}} = \text{UV radiation} \Rightarrow$

valence states (bonds, etc)



binding energy

Band structure

DOS

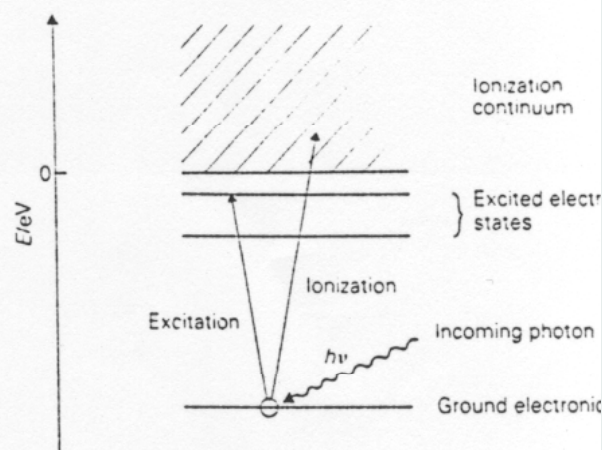
Nanochemistry UIO

Photoelectron spectra (ESCA)

$$E_{\text{kin}} (\text{electron}) = E_{\text{rad}} - E_{\text{bind}}$$

Surface method

2-3nm depth



Nanochemistry UIO

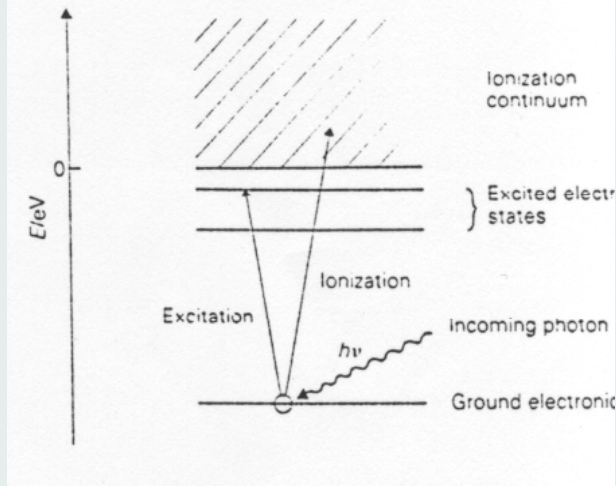
Photoelectron spectra (ESCA)

UPS: $E_{\text{rad}} = \text{UV radiation} \Rightarrow$

valence states (bonds, etc)

XPS: $E_{\text{rad}} = \text{X radiation} \Rightarrow$

core states (oxidation states)

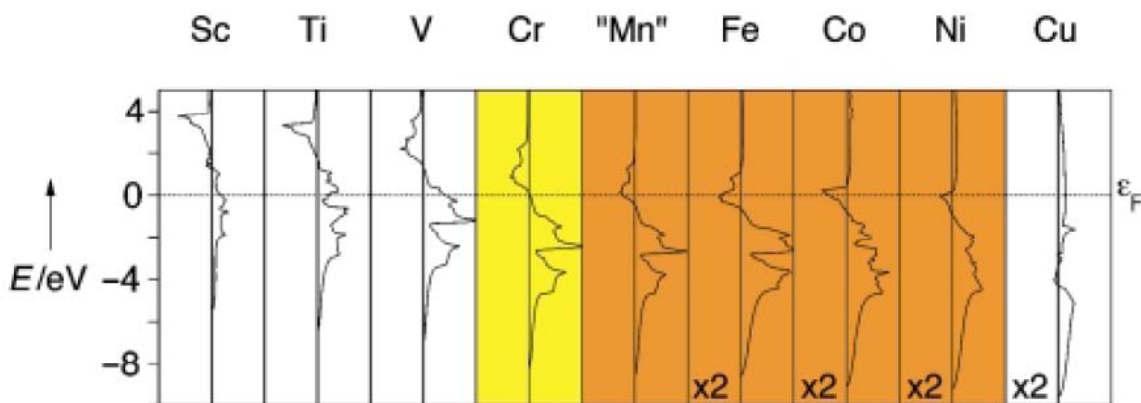


Nanochemistry UIO



Magnetism in Transition Metals

Angew. Chem. Int. Ed. **2000**, *39*, 1560–1585



Nanochemistry UIO



Magnetism - Spin Polarized Band Structures

Angew. Chem. Int. Ed. 2000, 39, 1560–1585

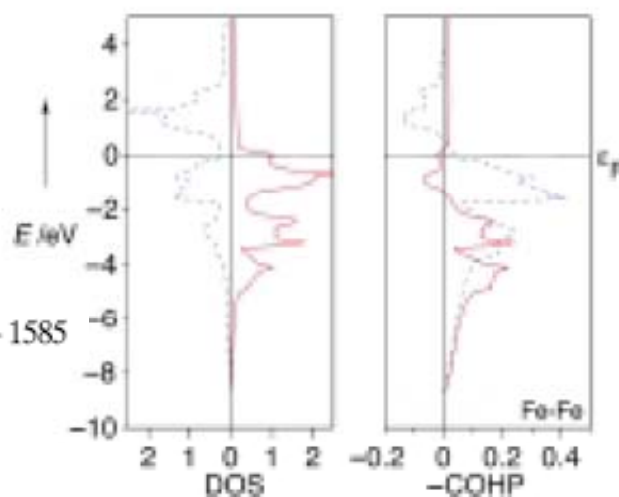


Figure 17. DOS and Fe-Fe COHP curves for ferromagnetic α -Fe. In each plot, the solid red/dashed blue line corresponds to the α/β spins. All curves have been shifted in energy so that ϵ_F , indicated with a horizontal dotted line, lies at 0.0 eV.