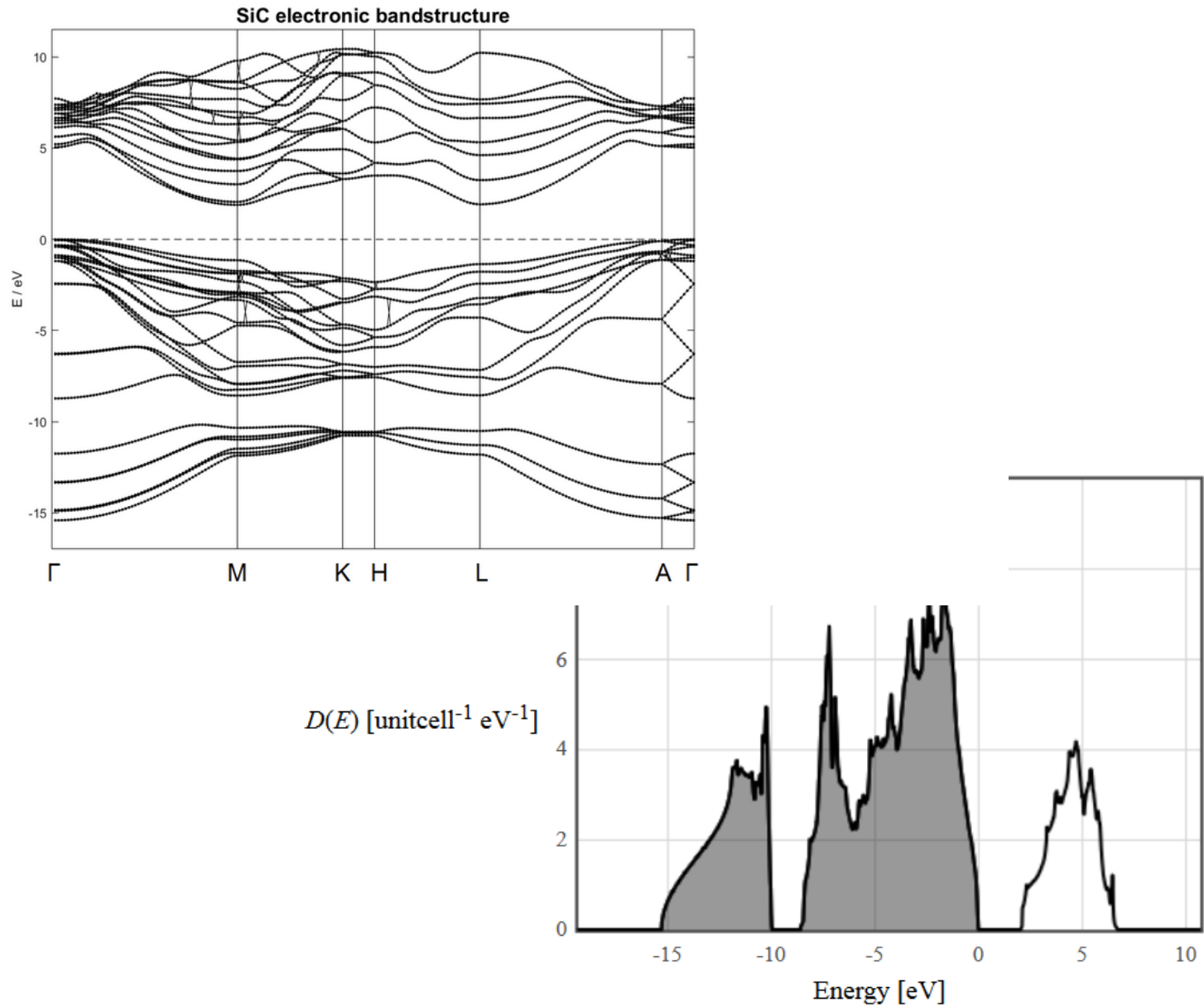


6. Photoemission

Oct 18, 2018

Bandstructure of hexagonal silicon carbide (SiC)

The bandstructure calculation for silicon carbide was calculated using the program [Quantum Espresso](#) (version 5.3.0) and the pseudopotentials for [Si](#) and [C](#).

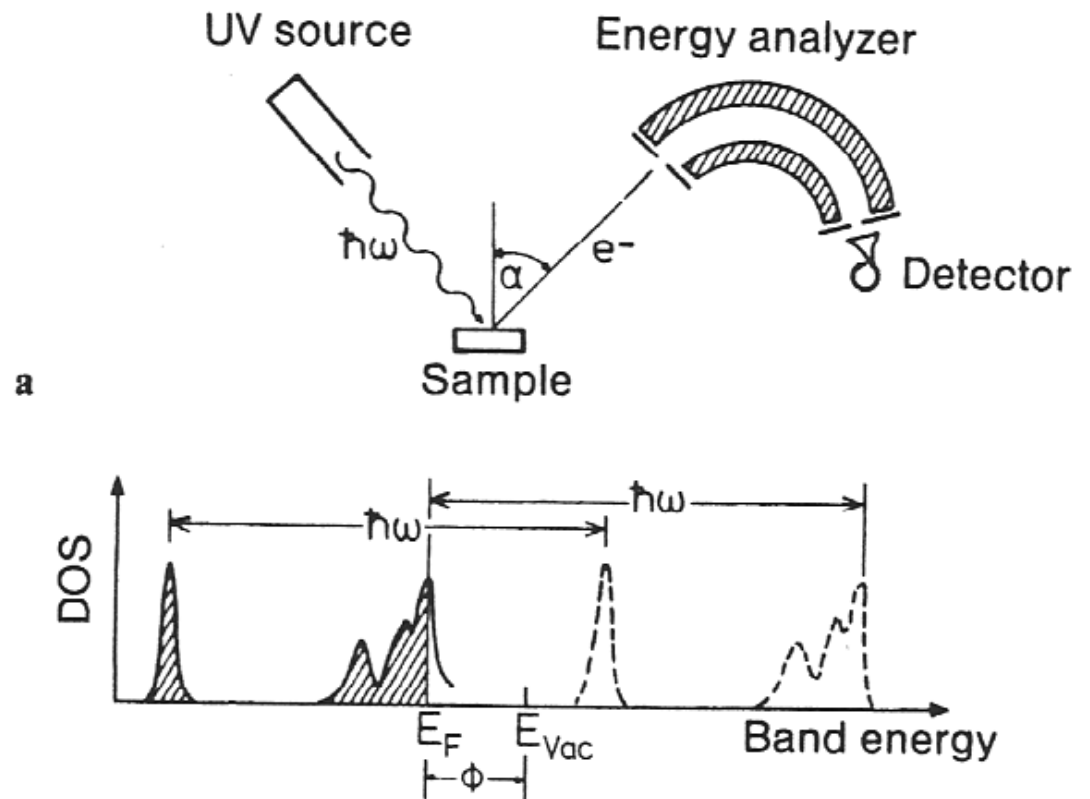


Photoemission spectroscopy

UPS - Ultraviolet photoemission spectroscopy

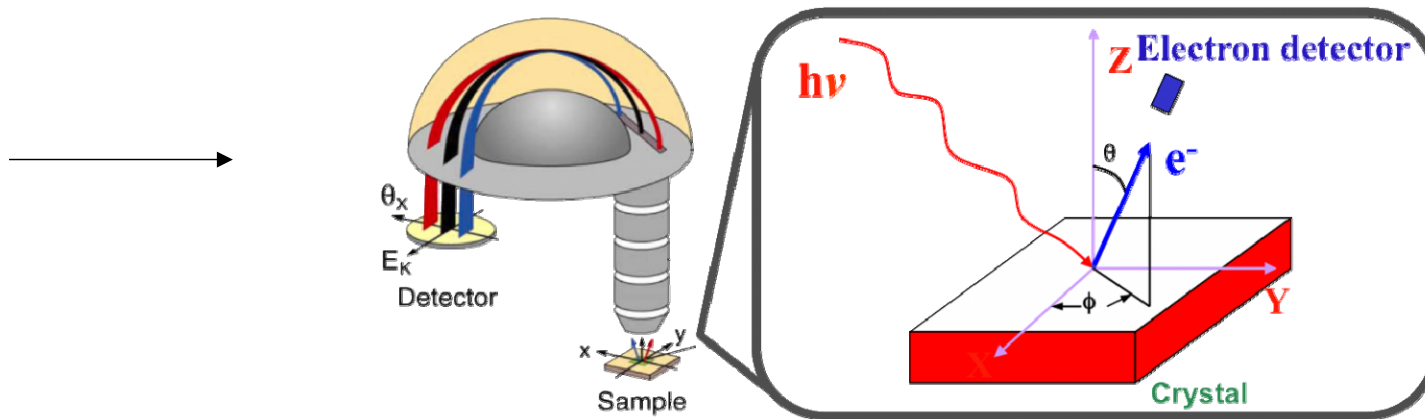
XPS - X-ray photoemission spectroscopy

Measure the density of states with photoemission spectroscopy

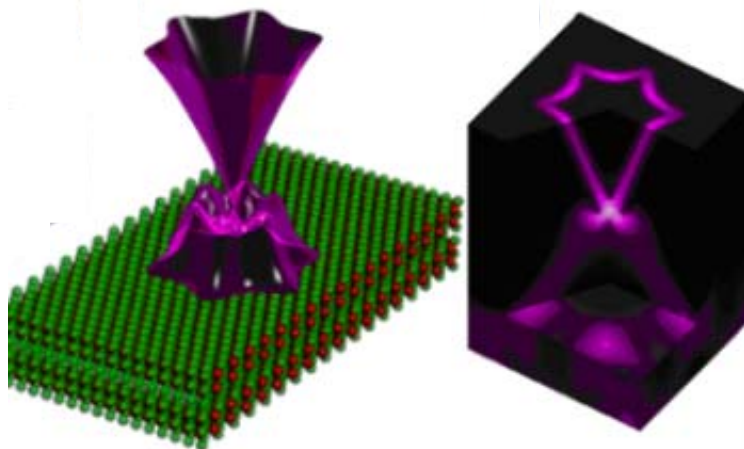


From: Ibach & Lueth

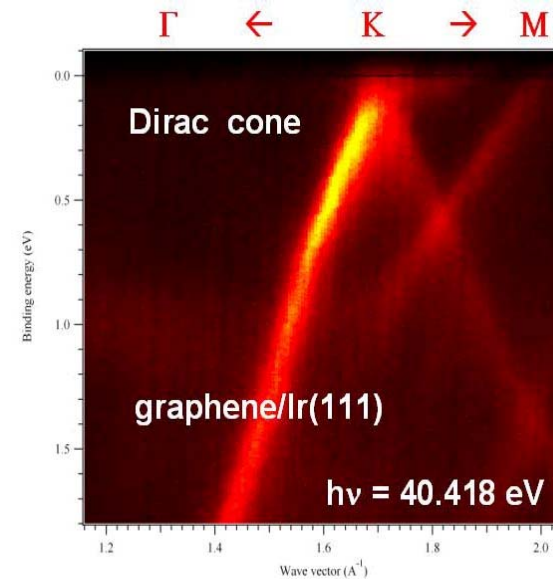
Angle resolved photoemission spectroscopy (ARPES)



Bi_2Te_3

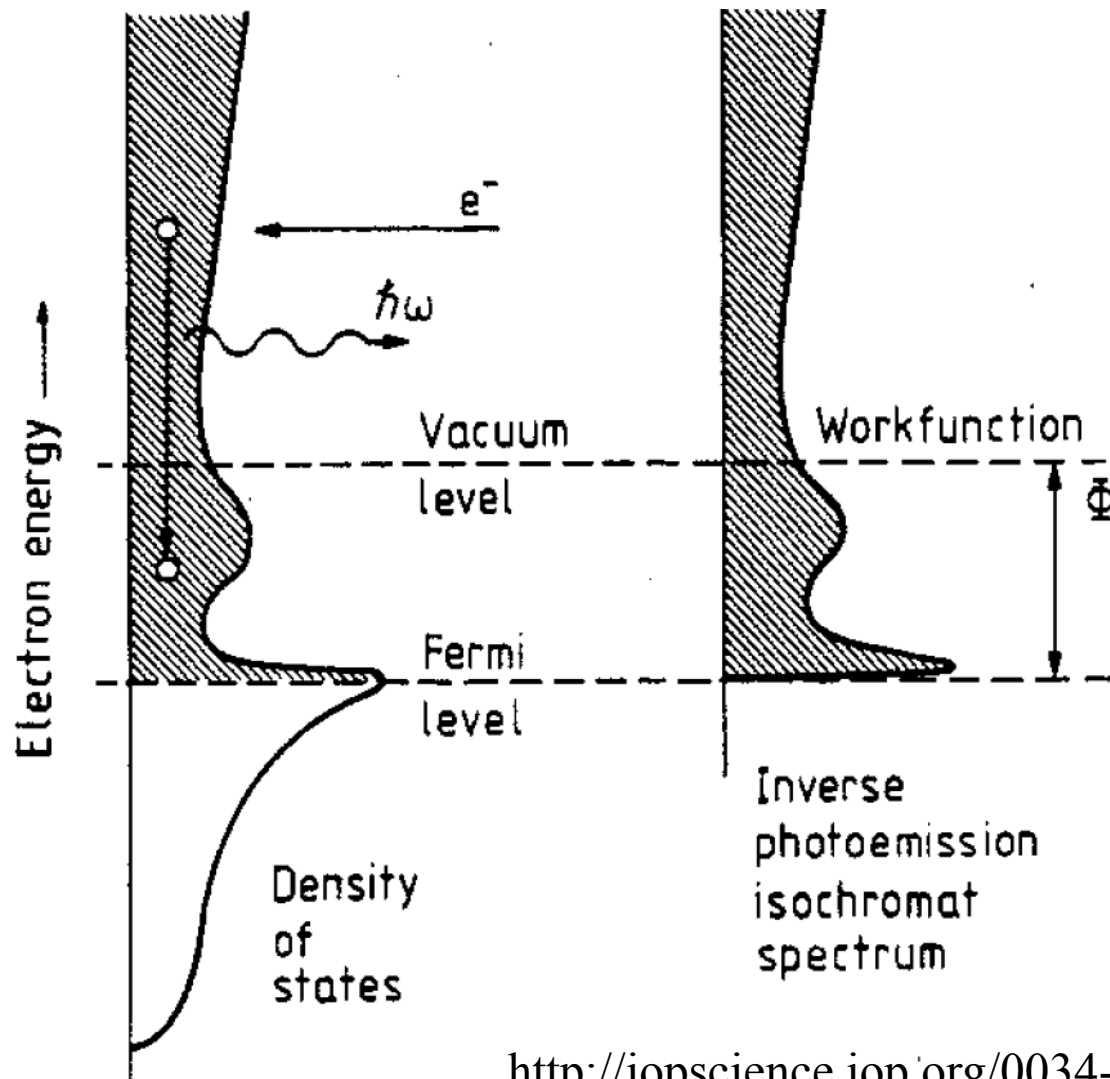


Topological insulator



Measure the dispersion relation with angle resolved photoemission

Inverse photoemission spectroscopy (IPES)



k -resolved Inverse Photoemission Spectroscopy (KRIPES)

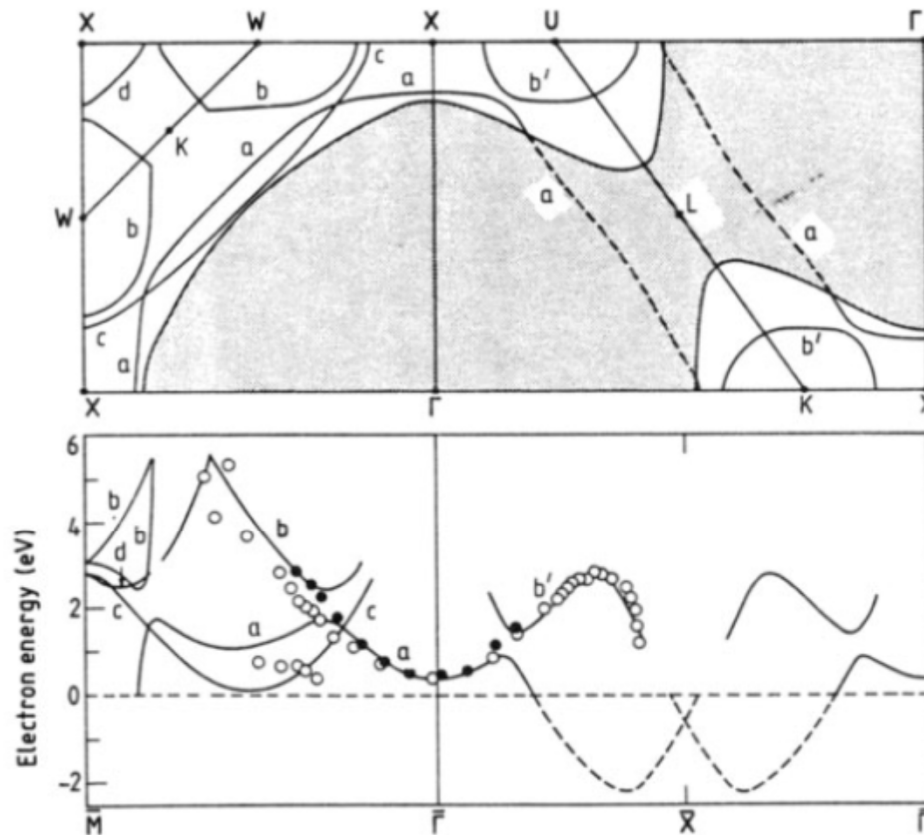
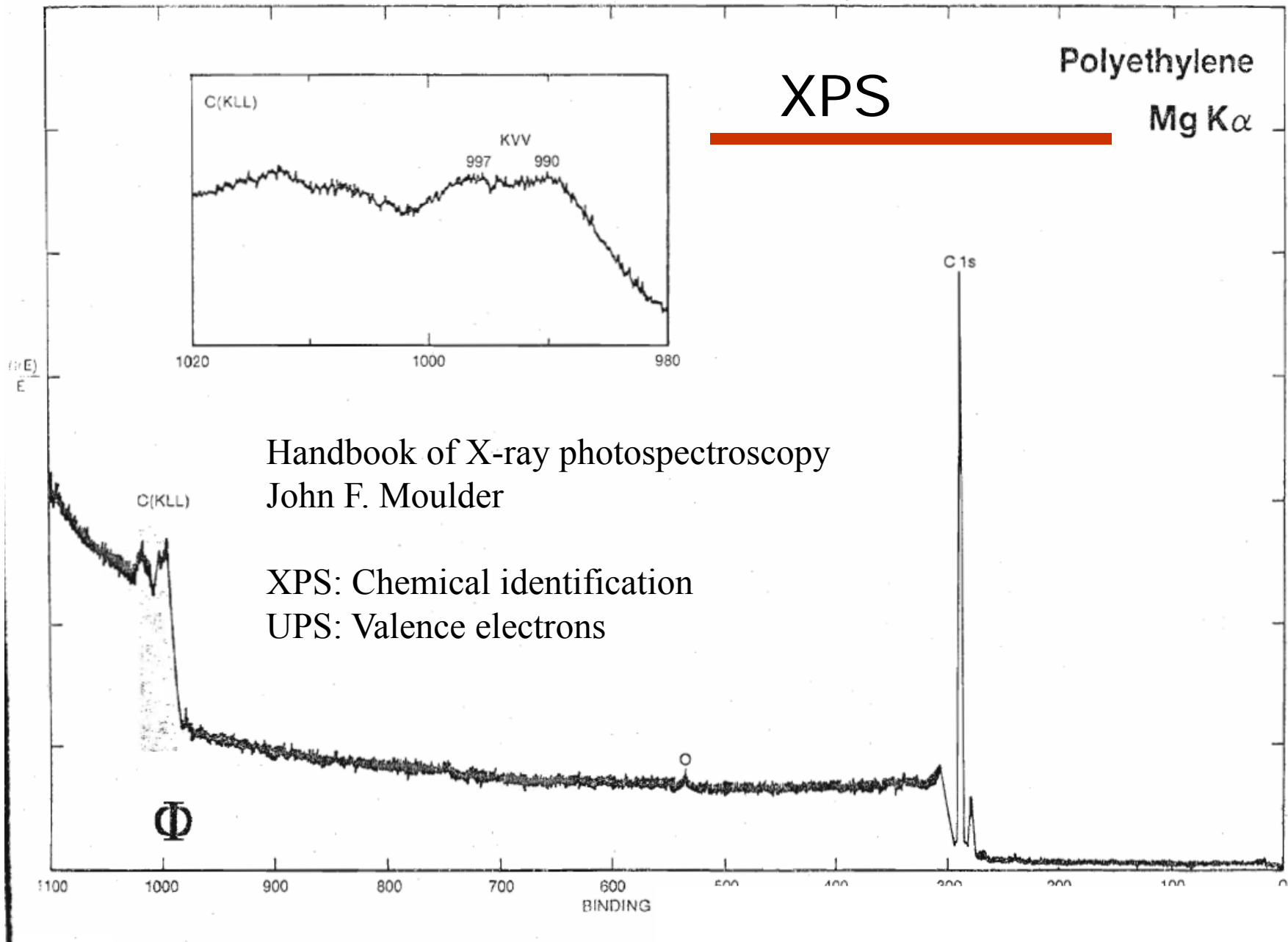


Figure 9. Band calculations and data for bulk direct transitions in the two principal azimuths $\Gamma\bar{M}$ and $\Gamma\bar{X}$ and Cu(001). Upper panel shows the Fermi surface and isochromat curves at $\hbar\omega = 9.7$ eV for transitions into band 6. Lower panel shows the corresponding $E_t(k_{||})$ projections. Computations and filled data circles are from Woodruff *et al* (1982); open circles are data from Jacob *et al* (1986).

Polyethylene

XPS

Mg K α



Handbook of X-ray photospectroscopy
John F. Moulder

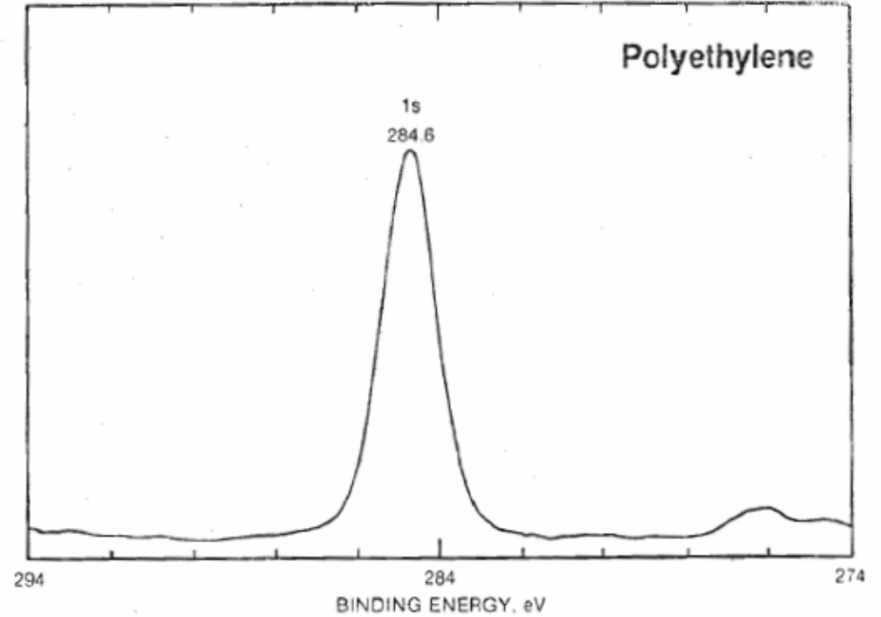
XPS: Chemical identification
UPS: Valence electrons

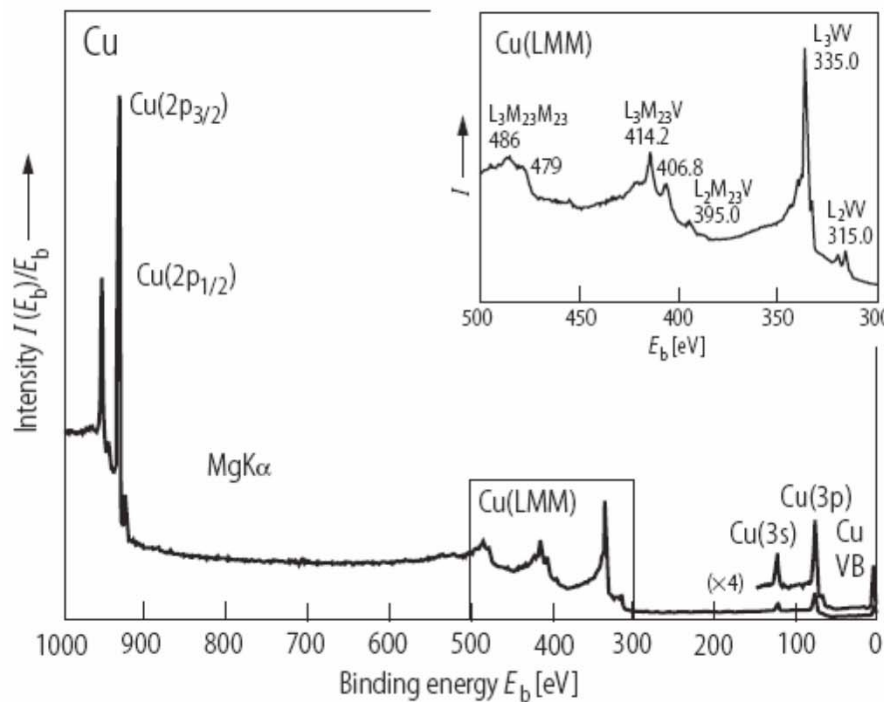
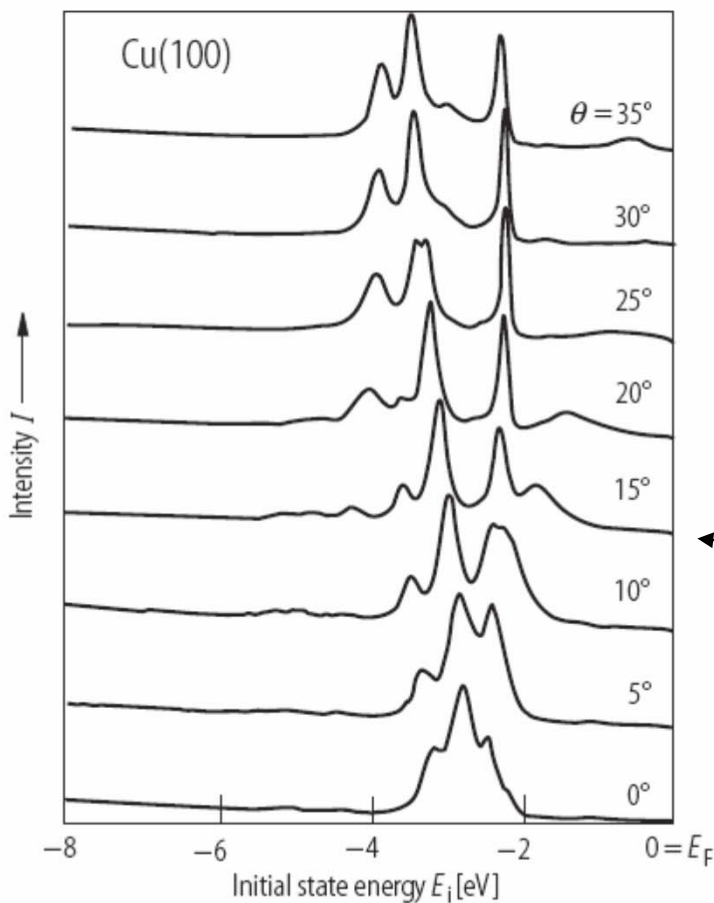
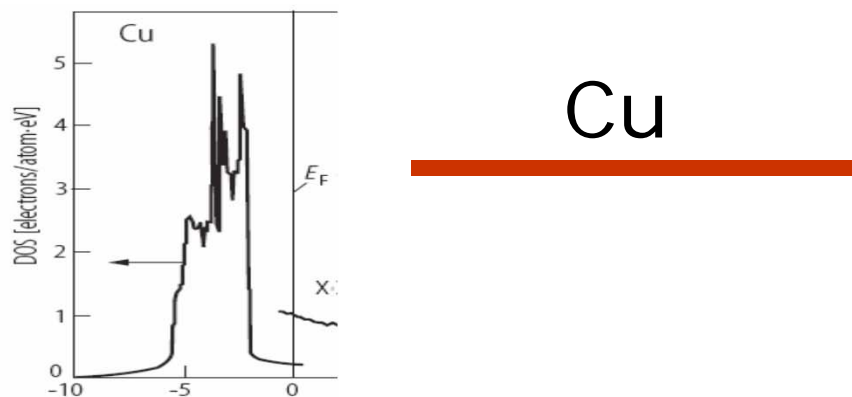
XPS

Carbon, C Atomic Number 6

HANDBOOK OF X-RAY PHOTOELECTRON SPECTROSCOPY

COMPOUND	1s BINDING ENERGY, eV					REF.
	280	284	288	292	296	
HfC						RH1
TiC						RH1
WC						RH1
C (graphite)						HJG
(CH ₂) _n						Φ
Mn(C ₅ H ₅) ₂						BCD
SnPh ₄						BAL
MeCH ₂ NH ₂						GHH
Cr(C ₆ H ₆) ₂						PFD
MeCH ₂ Cl						GHH
MeCH ₂ OH						GHH
MeCH ₂ OEt						GHH
MeCH ₂ OOCMe						GHH
CS ₂						GHH
Fe(CO) ₅						BC1
Me ₂ CO						GHH
(NH ₂) ₂ CO						GHH
C ₅ F ₆						GHH
MeCOONa						GHH
MeCOOEt						GHH
MeCOOH						GHH
Na ₂ CO ₃						GHH
NaHCO ₃						GHH
CO						BC1
CO ₂						GHH
(CHFCH ₂) _n						CFK
(CHFCHF) _n						CFK
(CHFCH ₂) _n						CFK
(CF ₂ CH ₂) _n						CFK
(CF ₂ CHF) _n						CFK
(CF ₂) _n						CFK
CF ₃ COONa						GHH
CCl ₄						GHH
CF ₃ COMe						GHH
CF ₃ COOEt						GHH



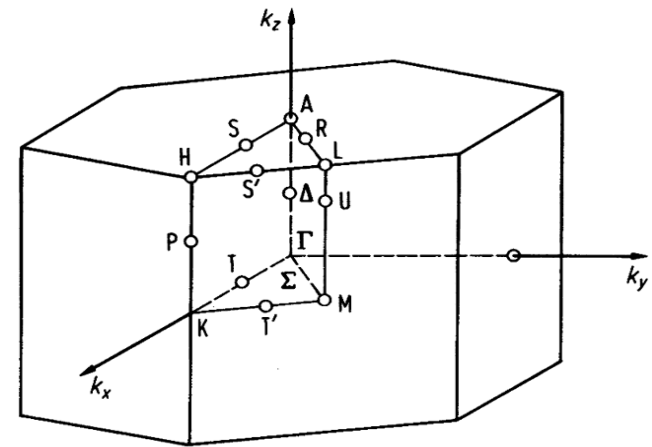
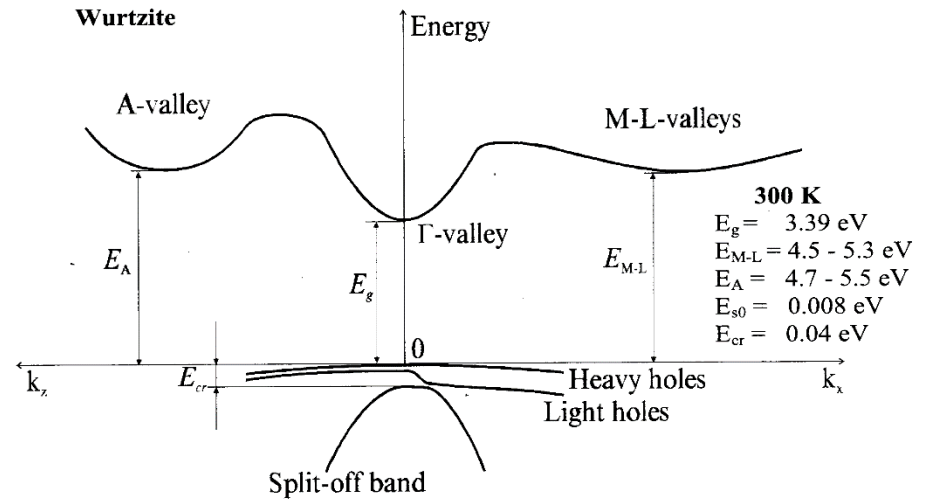
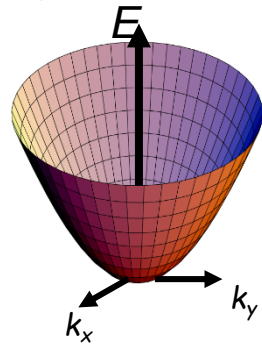
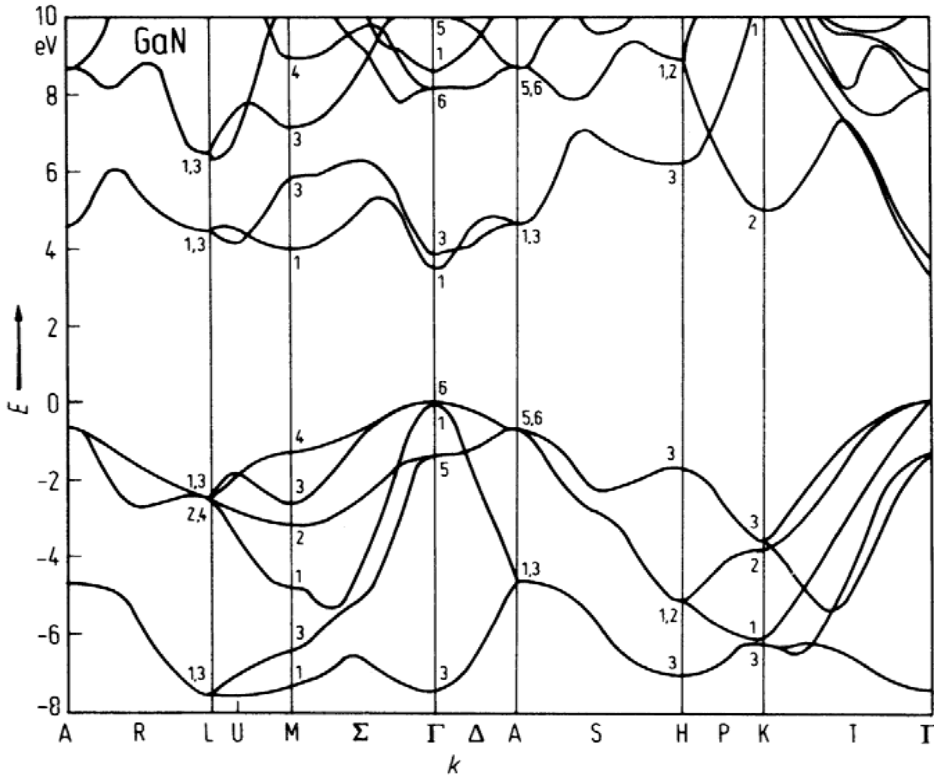


XPS

ARPES

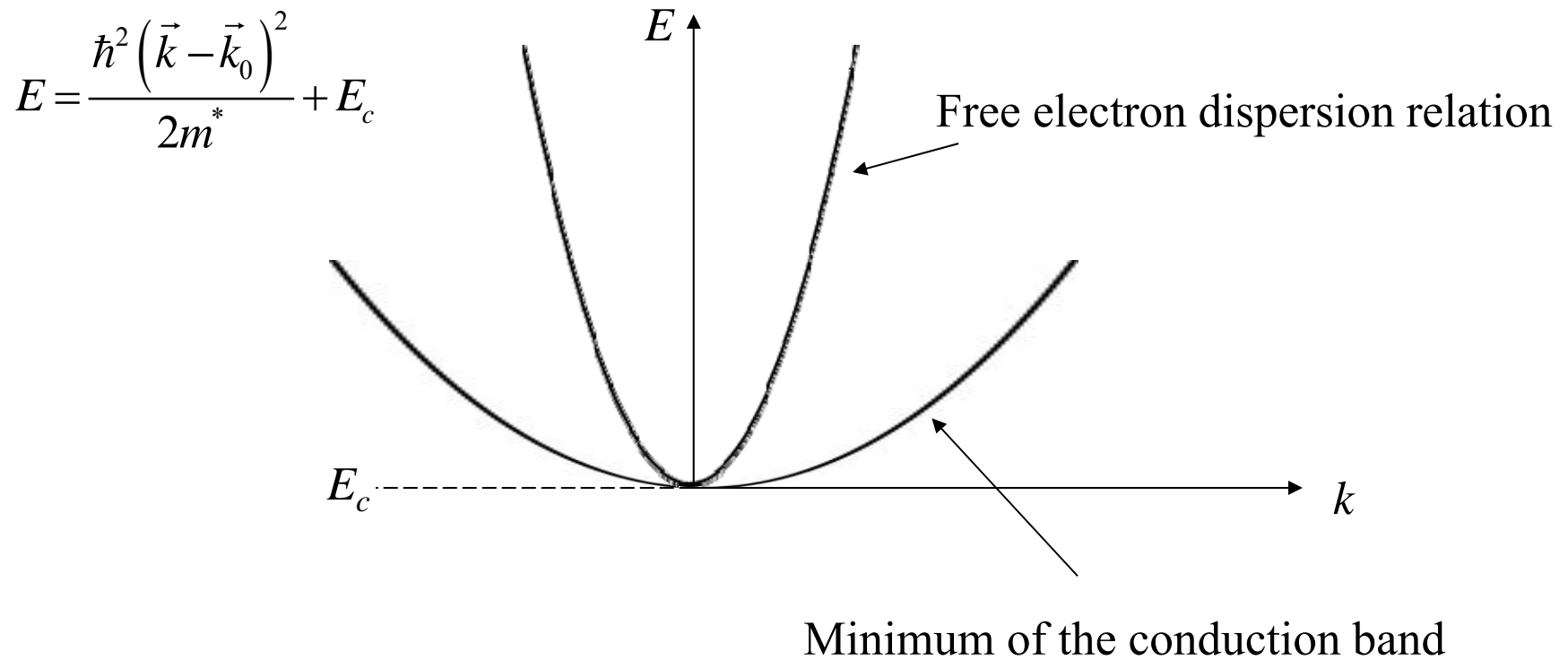
Fig. 28. Cu(100). Angle-resolved photoelectron spectra taken at different polar angles θ along the ΓXUL bulk mirror plane. Photon energy $h\nu = 21.2$ eV, sample temperature $T = 50$ K [93M1]. For further data taken at room temperature see [79H1]. For data taken with linear-polarized photons at $h\nu = 40^\circ$ see [83G].

GaN



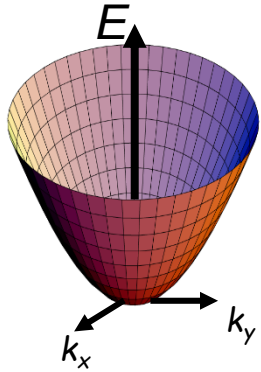
1st Brillouin zone of hcp

Conduction band minimum



Near the conduction band minimum, the bands are approximately parabolic.

Effective mass



$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*} + E_c$$

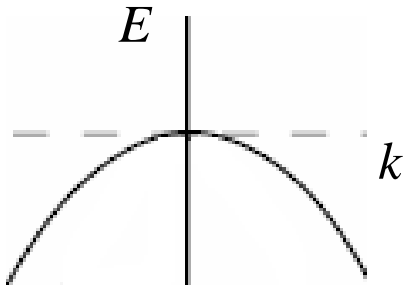
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

$$m^* = \frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

This effective mass is used to describe the response of electrons to external forces in the particle picture.

Top of the valence band

In the valence band, the effective mass is negative.



$$m^* = \frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}} < 0$$

Charge carriers in the valence band are positively charged holes.

m_h^* = effective mass of holes

$$m_h^* = \frac{-\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

Holes

A completely filled band does not contribute to the current.

$$\begin{aligned}\vec{j} &= \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} \\ &= \int_{\text{band}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} \\ &= \int_{\text{empty states}} e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}\end{aligned}$$

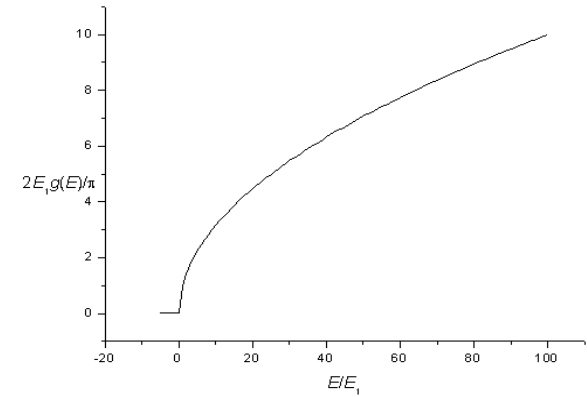
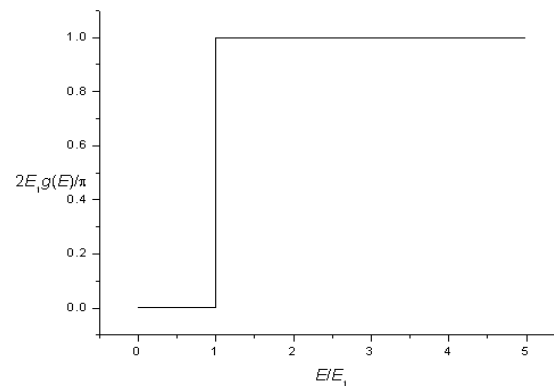
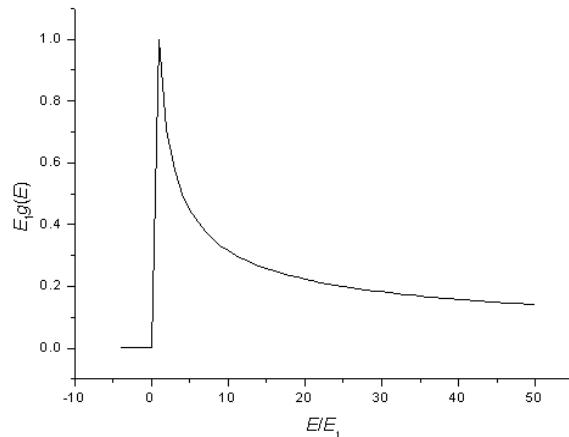
Holes have a positive charge and a positive mass.

Free electron Fermi gas

$$1 - d \quad D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1} \text{m}^{-1}$$

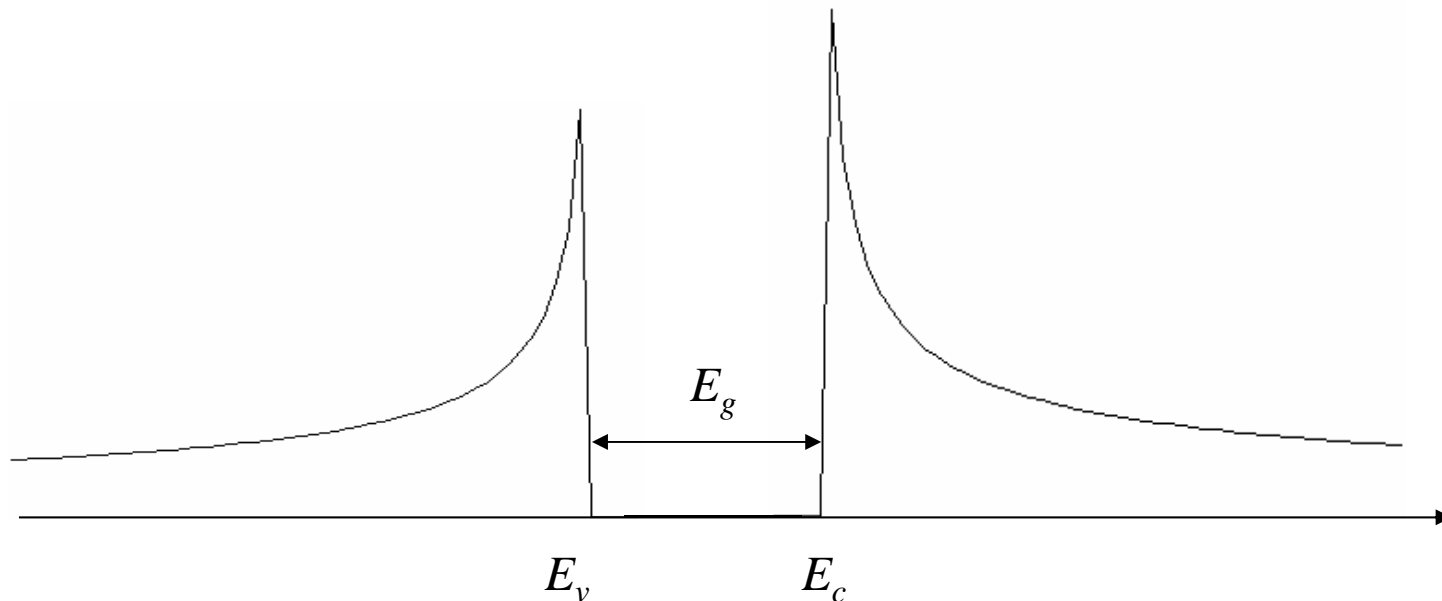
$$2 - d \quad D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1} \text{m}^{-2}$$

$$3 - d \quad D(E) = \frac{\pi}{2} \left(\frac{2m}{\hbar^2 \pi^2} \right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \quad \text{J}^{-1} \text{m}^{-3}$$



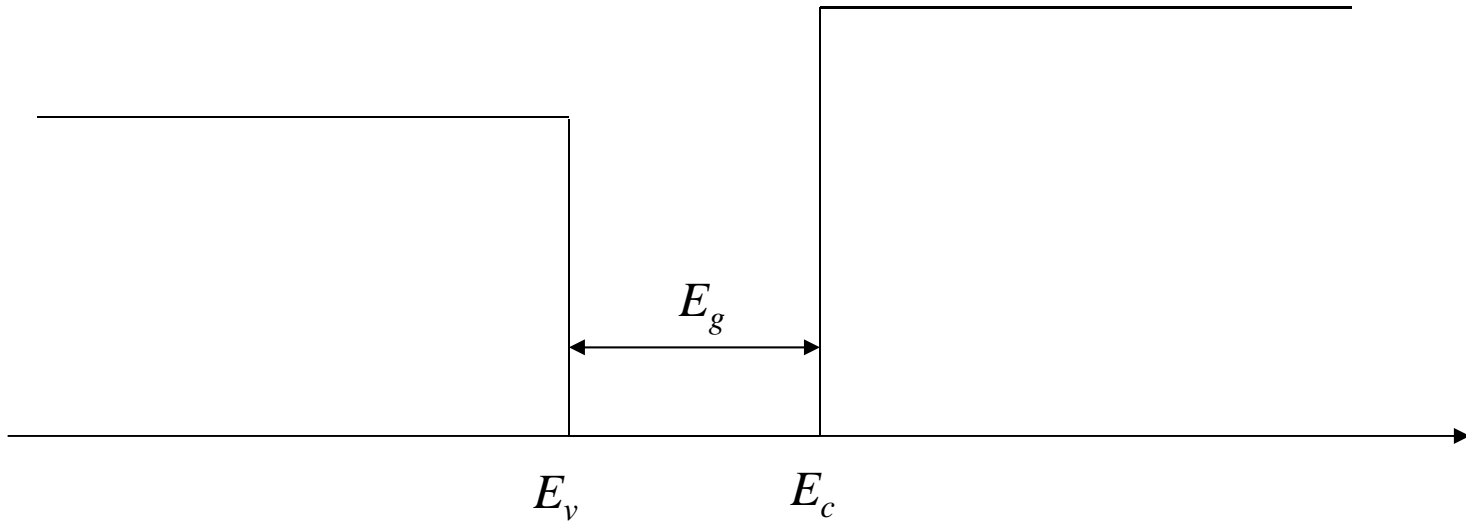
Semiconductors and insulators - 1d

$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$
$$D(E) = \begin{cases} \frac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



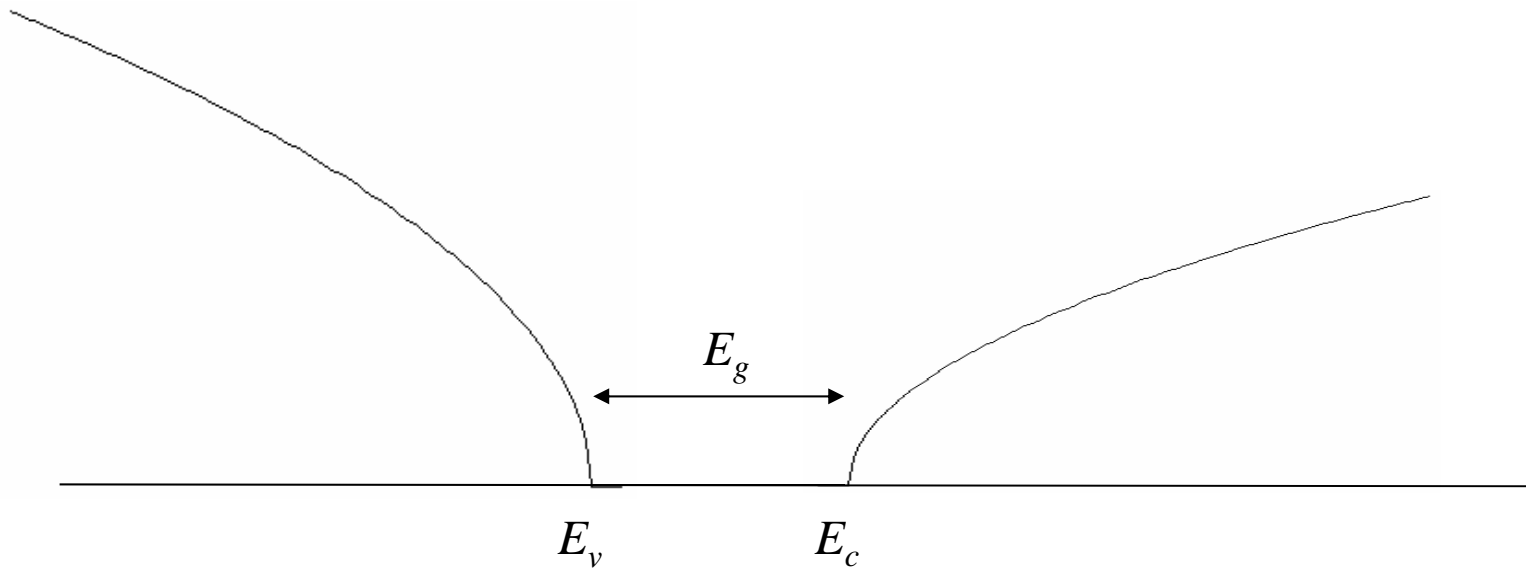
Semiconductors and insulators - 2d

$$D(E) = \begin{cases} D_c & E < E_v \\ 0 & E_v < E < E_c \\ D_v & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



Semiconductors and insulators - 3d

$$D(E) = \begin{cases} D_c \sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ D_v \sqrt{E - E_c} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



The electrical contribution to the thermodynamic properties of insulators depend on band edges

Boltzmann approximation

The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results were calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_B T$ from the band edge. The electronic contribution to the thermodynamic quantities are usually much smaller than the contribution of the phonons and thus the electronic components are often simply ignored.

	1-d	2-d
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi} \sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi} \sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$ $H(x) = 0 \text{ for } x < 0 \text{ and } H(x) = 1 \text{ for } x > 0$
Density of states N_v and N_c are the effective densities of states	$D(E) = \begin{cases} N_v(300) \sqrt{\frac{2}{300\pi k_B (E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ N_c(300) \sqrt{\frac{2}{300\pi k_B (E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{N_v(300)}{300k_B} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{N_c(300)}{300k_B} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$
Density of electrons in the conduction band $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-1}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2 \pi} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-2}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E) (1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-1}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2 \pi} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-2}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

Silicon density of states

