Photoemission

Semiconductors

Band structure in 1-D

Consider an electron moving in a periodic potential $V(x)$. The period of the potential is a, $V(x+a) = V(x)$. The Schrödinger equation for this case is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

Quantum mechanically, the electron moves as a wave through the potential. Due to the diffraction of these waves, there are bands of energies where the electron is allowed to propagate through the potential and bands of energies where no propagating solutions are possible. The Bloch theorem states that the propagating states have the form,

$$\psi = e^{ikx}u_k(x).$$

where k is the wavenumber and $u_k(x)$ is a periodic function with periodicity a.

The solutions to the Schrödinger equation for a 1-D periodic potential can be calculated numerically. The following form can be used to calculate the dispersion relation between E and k for any one dimensional potential. Input the periodic potential $V(x)$ in the interval between 0 and a.

The density of states is,

$$D(E) = \frac{2}{\pi}\frac{dk}{dE},$$

and the group velocity is,

$$v_g = \frac{1}{\hbar}\frac{dE}{dk}.$$

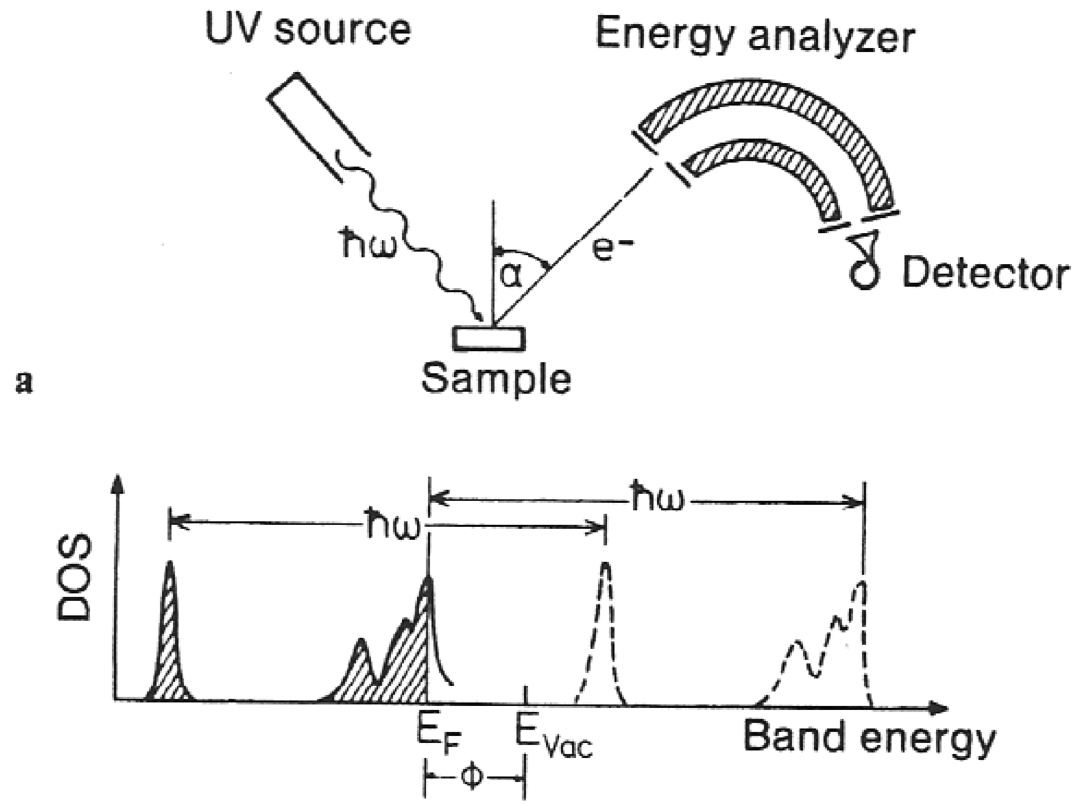
http://lampx.tugraz.at/~hadley/ss1/bloch/bloch.php

Photoemission spectroscopy

UPS - Ultraviolet photoemission spectroscopy

XPS - X-ray photoemission spectroscopy

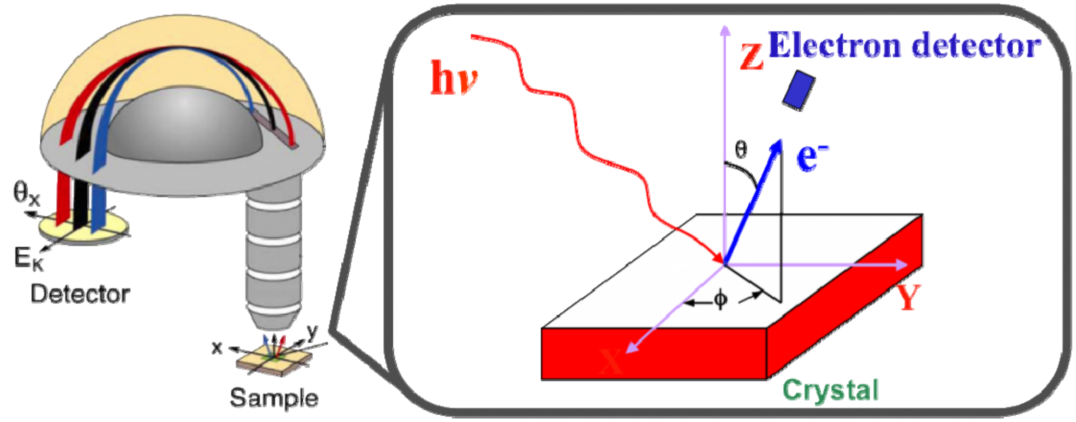
Measure the density of states with photoemission spectroscopy



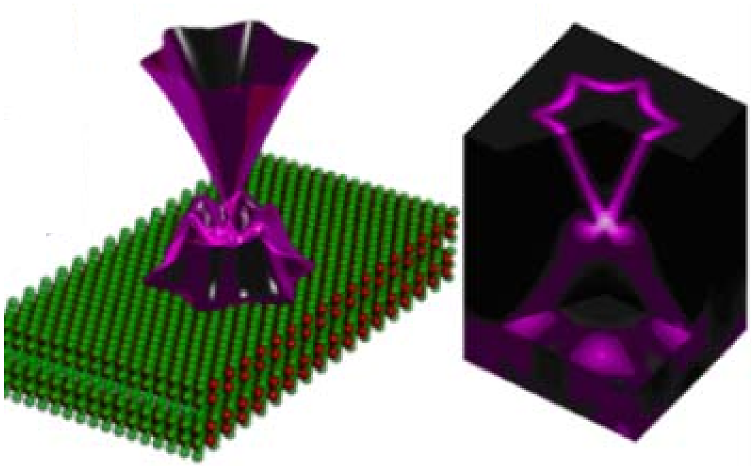
From: Ibach & Lueth

Angle resolved photoemission spectroscopy (ARPES)

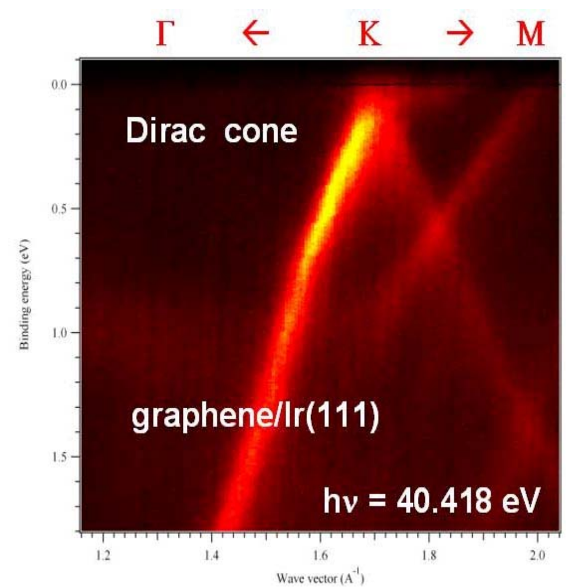
https://arpes.stanford.edu/research/tool-development/angle-resolved-photoemission-spectroscopy



Bi_2Te_3



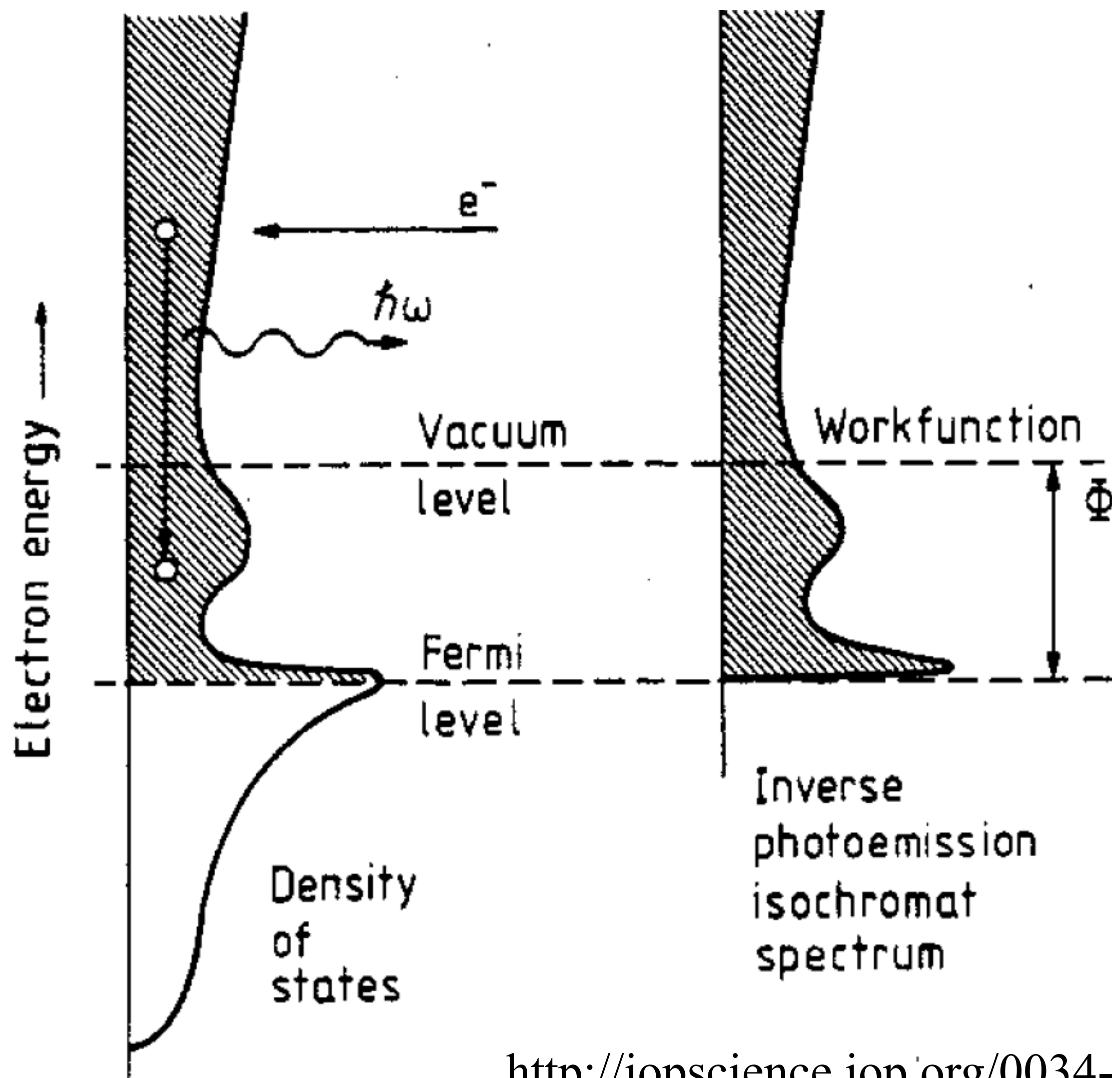
Topological insulator



http://server2.phys.uniroma1.it/gr/lotus/Instrumentation1_M.htm

Measure the dispersion relation with angle resolved photoemission

Inverse photoemission spectroscopy (IPES)



http://iopscience.iop.org/0034-4885/51/9/003

k-resolved Inverse Photoemission Spectroscopy (KRIPES)

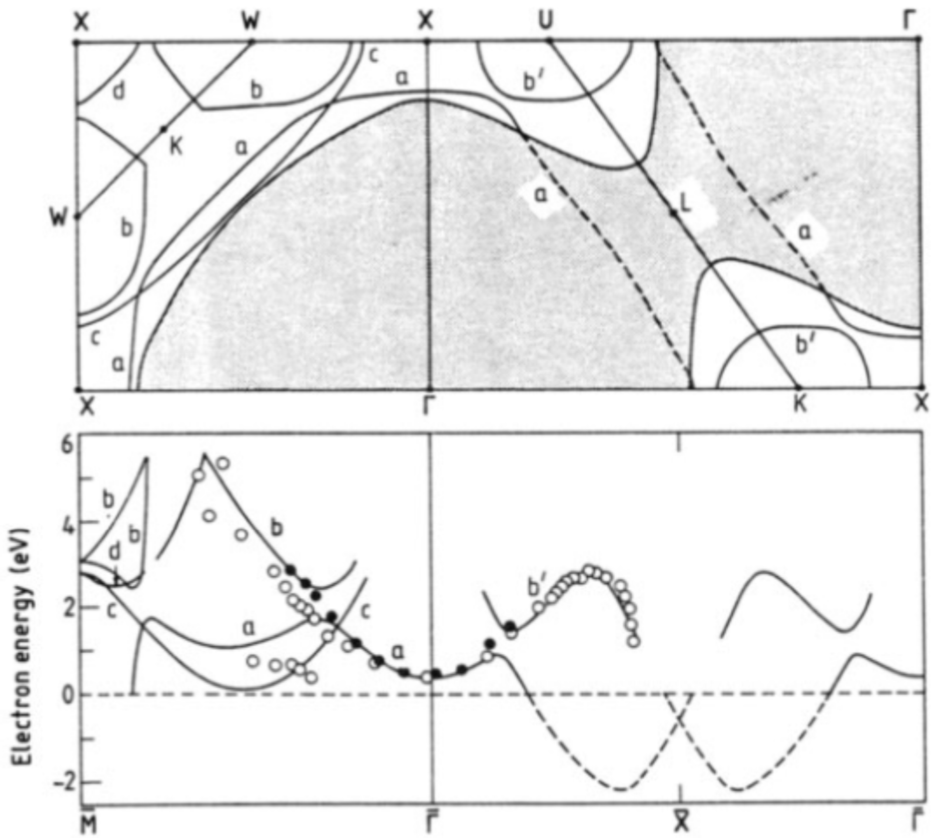
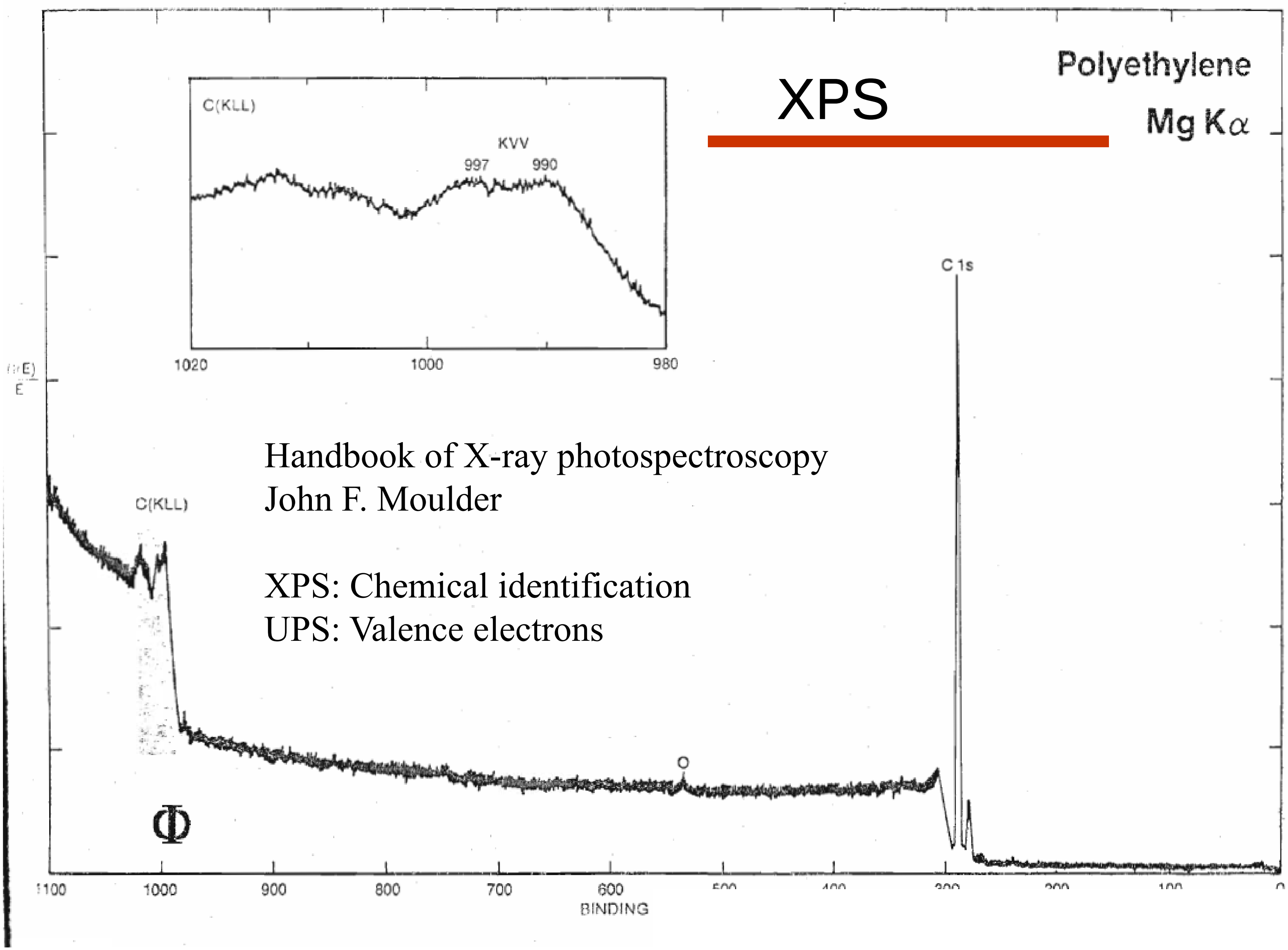


Figure 9. Band calculations and data for bulk direct transitions in the two principal azimuths $\bar{\Gamma}\bar{M}$ and $\bar{\Gamma}\bar{X}$ and Cu(001). Upper panel shows the Fermi surface and isochromat curves at $\hbar\omega = 9.7$ eV for transitions into band 6. Lower panel shows the corresponding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

http://iopscience.iop.org/0034-4885/51/9/003

XPS



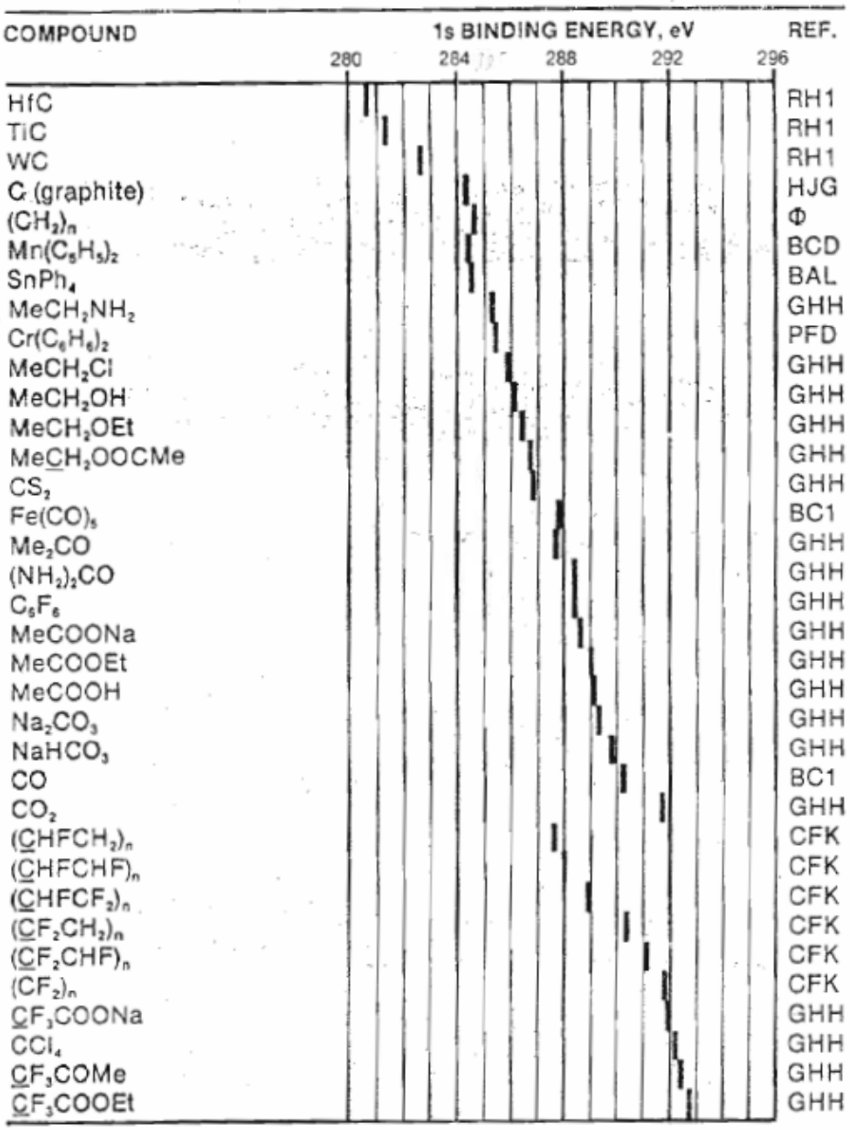
Handbook of X-ray photospectroscopy
John F. Moulder

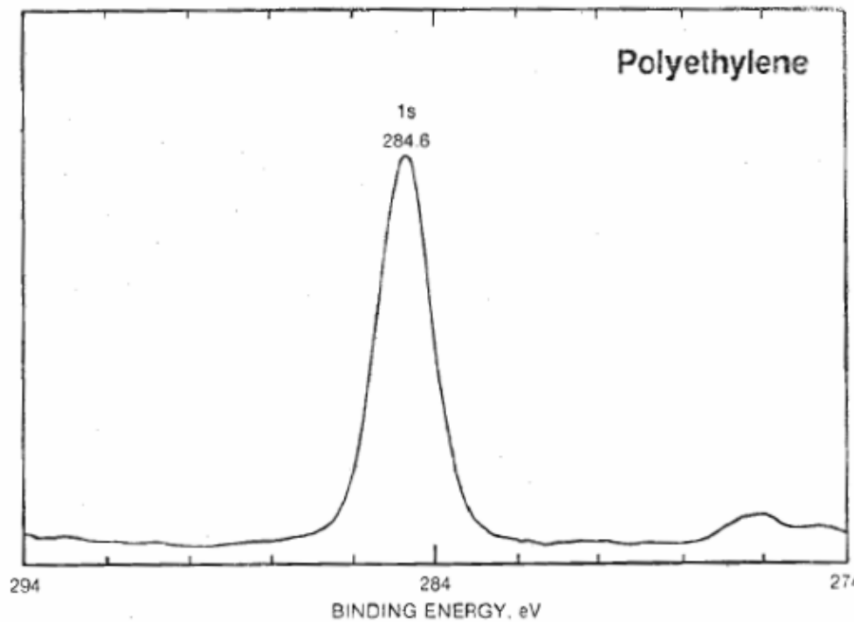
XPS: Chemical identification
UPS: Valence electrons

XPS

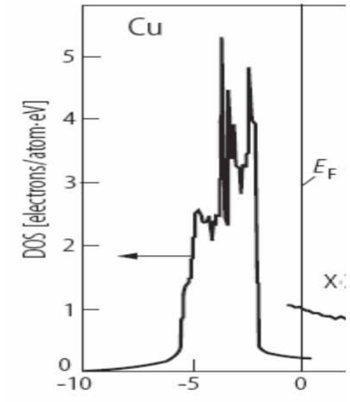
Carbon, C Atomic Number 6

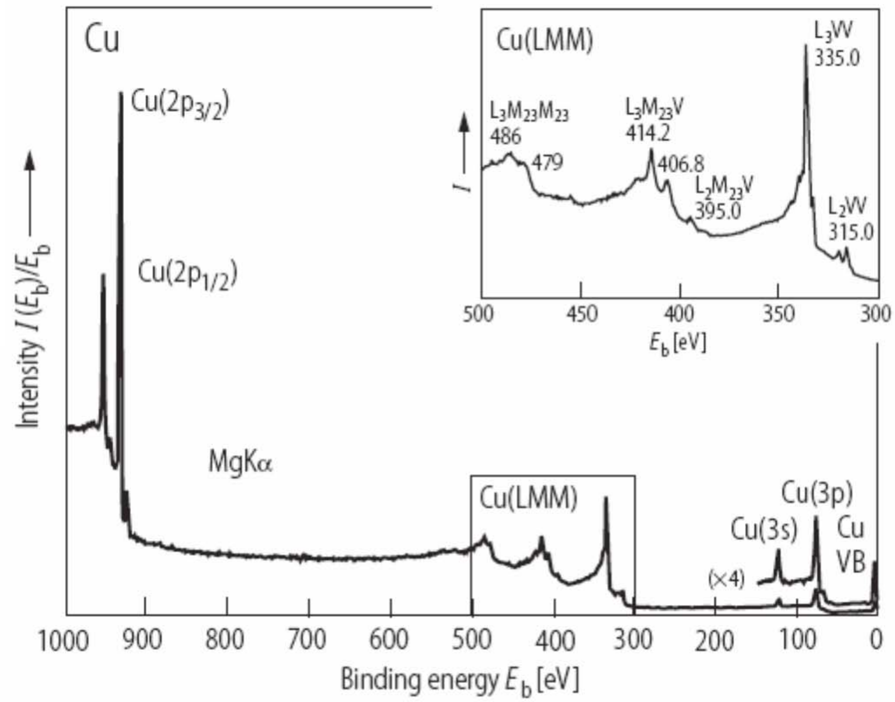
HANDBOOK OF X-RAY PHOTOELECTRON SPECTROSCOPY



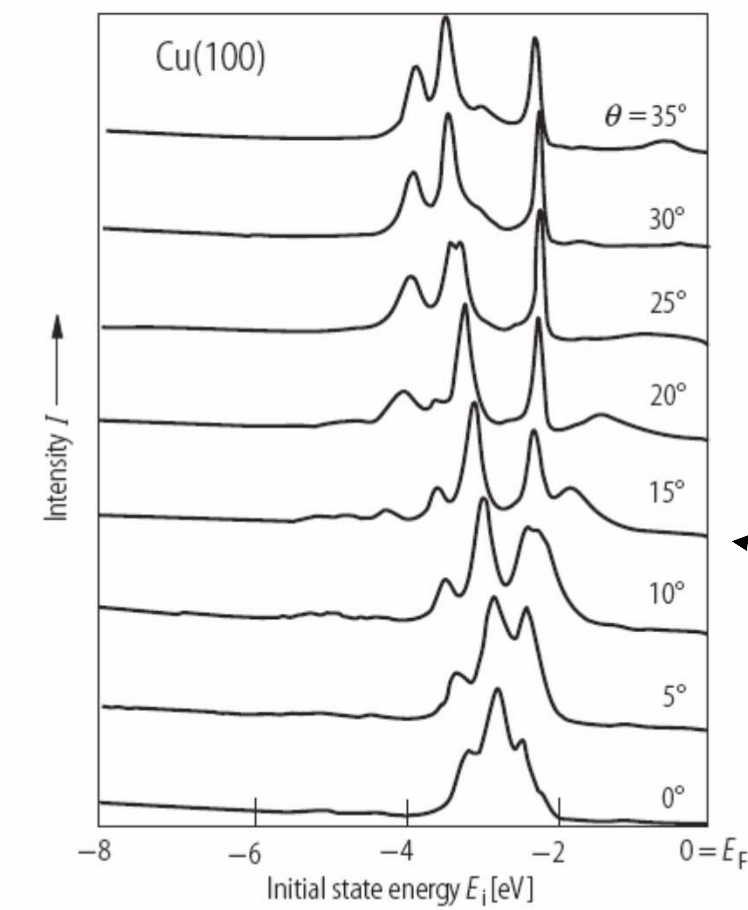


Cu





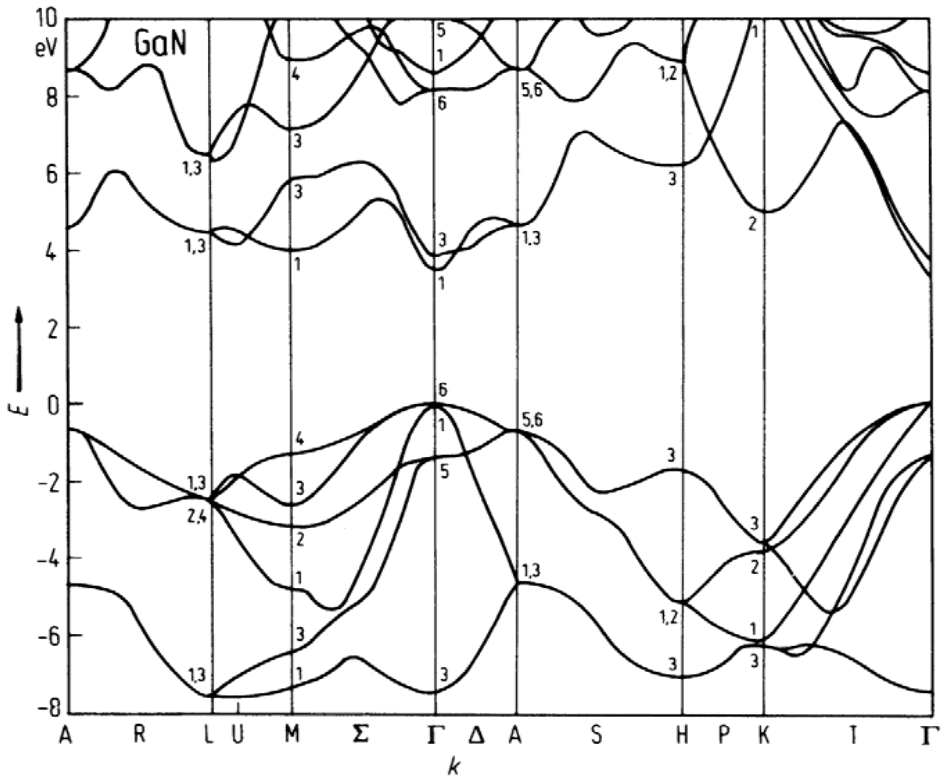
XPS

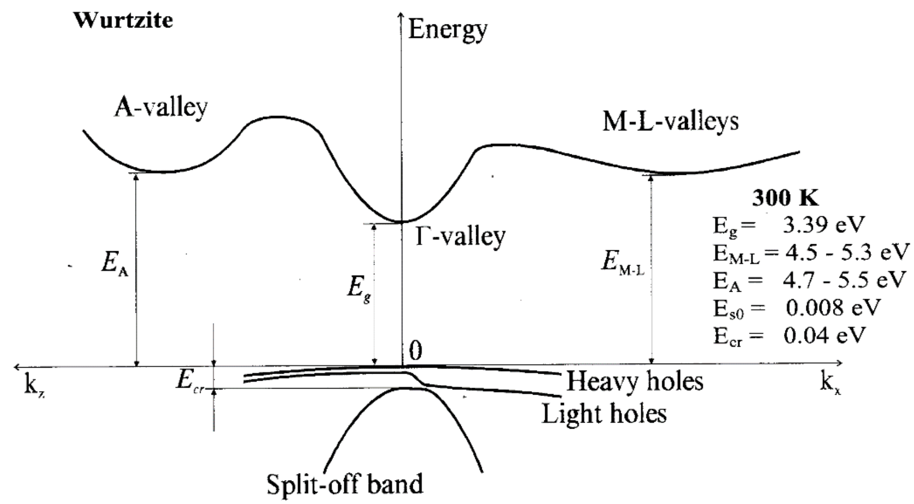


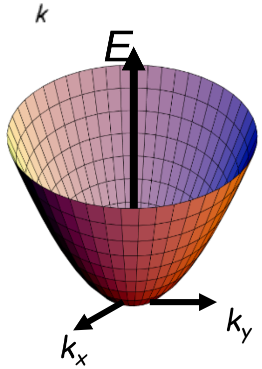
ARPES

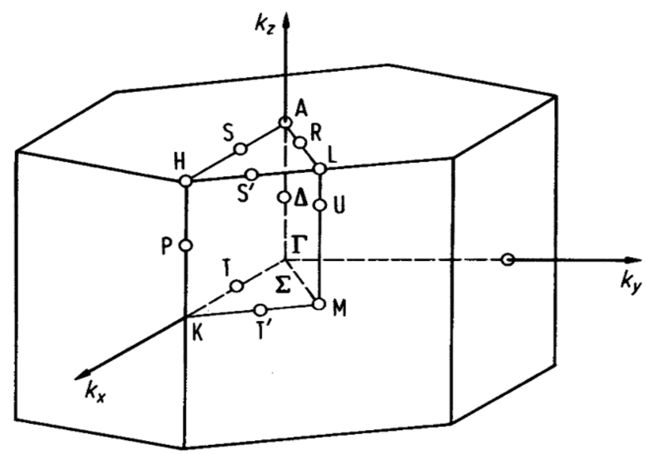
Fig. 28. Cu(100). Angle-resolved photoelectron spectra taken at different polar angles θ along the ΓXUL bulk mirror plane. Photon energy $h\nu$ = 21.2 eV, sample temperature T = 50 K [93M1]. For further data taken at room temperature see [79H1]. For data taken with linear-polarized photons at $h\nu$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

GaN





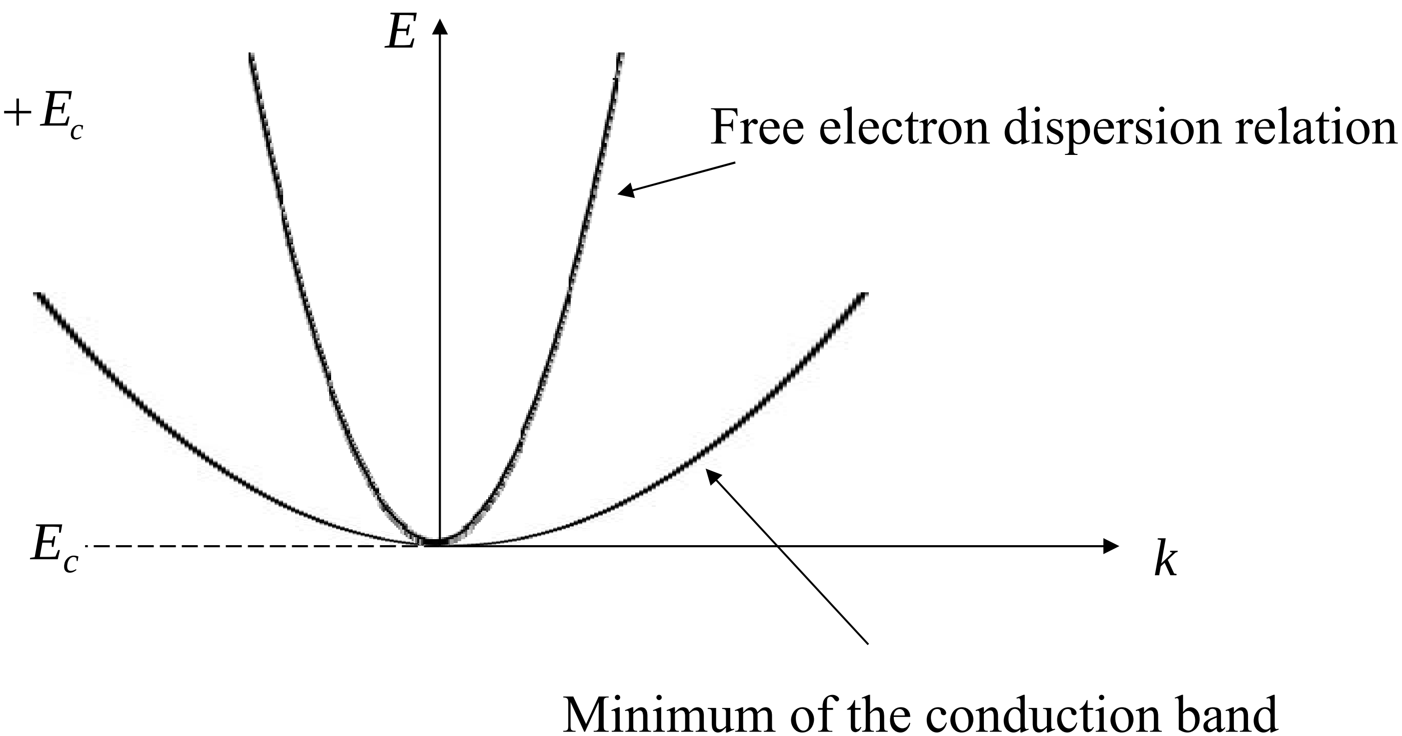




1st Brillioun zone of hcp

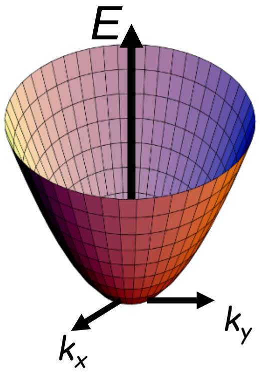
Conduction band minimum

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



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

Effective mass



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

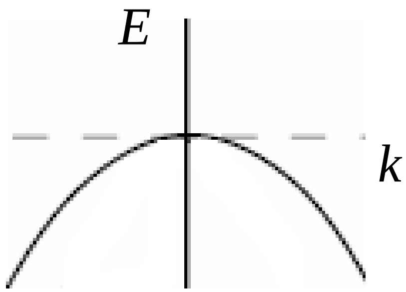
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

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

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.



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

Charge carriers in the valence band are positively charged holes.

m^*_h = effective mass of holes

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

Holes

A completely filled band does not contribute to the current.

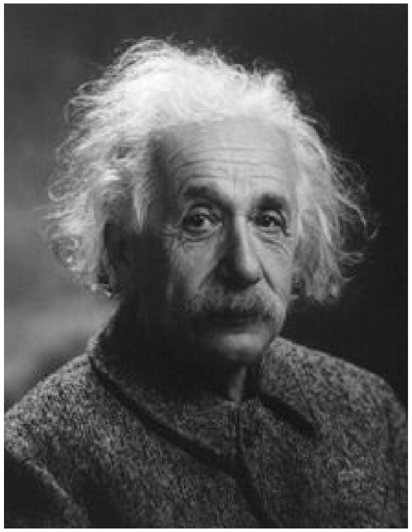
$$\vec{j} = \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

$$= \int_{\text{band}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

$$= \int_{\text{empty states}} e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

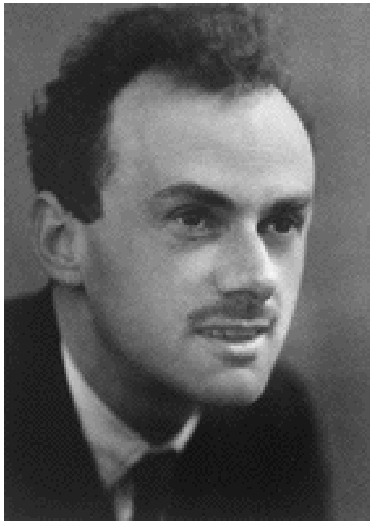
Holes have a positive charge and a positive mass.

Holes



Albert Einstein

Erwin Schrödinger



Paul Adrien Maurice Dirac