

***ELECTRON SPECTROSCOPY IN BERKELEY:  
FROM THE FIELD FREE LAB TO FREE  
ELECTRON LASERS***



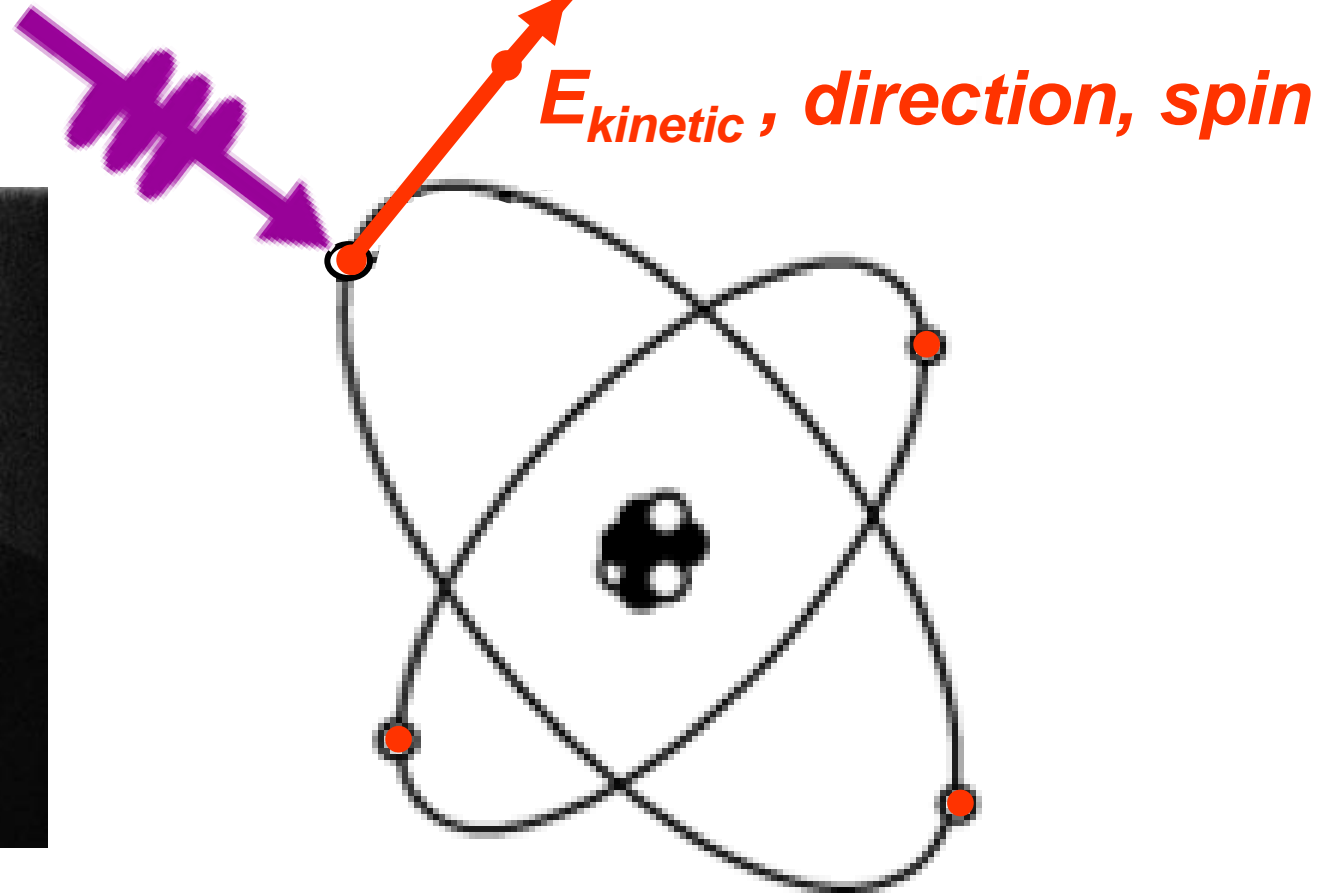
**Chuck Fadley  
Dept. of Physics, UC Davis  
and  
Materials Sciences Division  
Lawrence Berkeley National Laboratory**

**(PhD, 1970)**



# The Photoelectric Effect, Einstein, 1905

## Light can behave like a Particle!



$$h\nu = E_{initial} - E_{final} = E_{binding} + E_{kinetic}$$

From 1960s → Photoelectron Spectroscopy = Photoemission

# The first spectrometer in the U.S.—Made in Sweden

NUCLEAR INSTRUMENTS AND METHODS 27 (1964) 173-189; © NORTH-HOLLAND PUBLISHING CO.

## A 50-CM DOUBLE FOCUSING BETA SPECTROMETER OF THE CURRENT SHEET TYPE

K. SIEGBAHN, C. NORDLING, S.-E. KARLSSON, S. HAGSTRÖM, A. FAHLMAN and I. ANDERSSON

*Institute of Physics, University of Uppsala, Sweden*

Received 26 March 1964

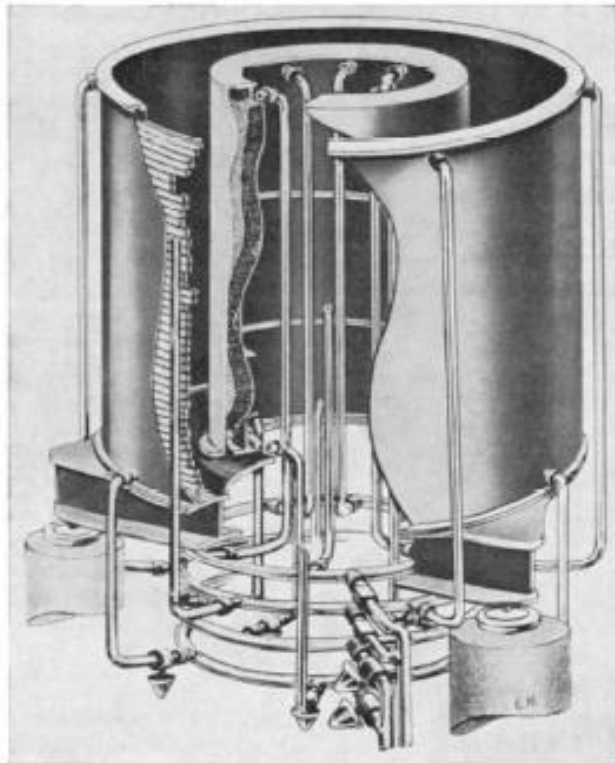


Fig. 1. Cut-away view of the spectrometer coils and cooling manifold. This is an artist's view and was made before the manufacturing of the coils.



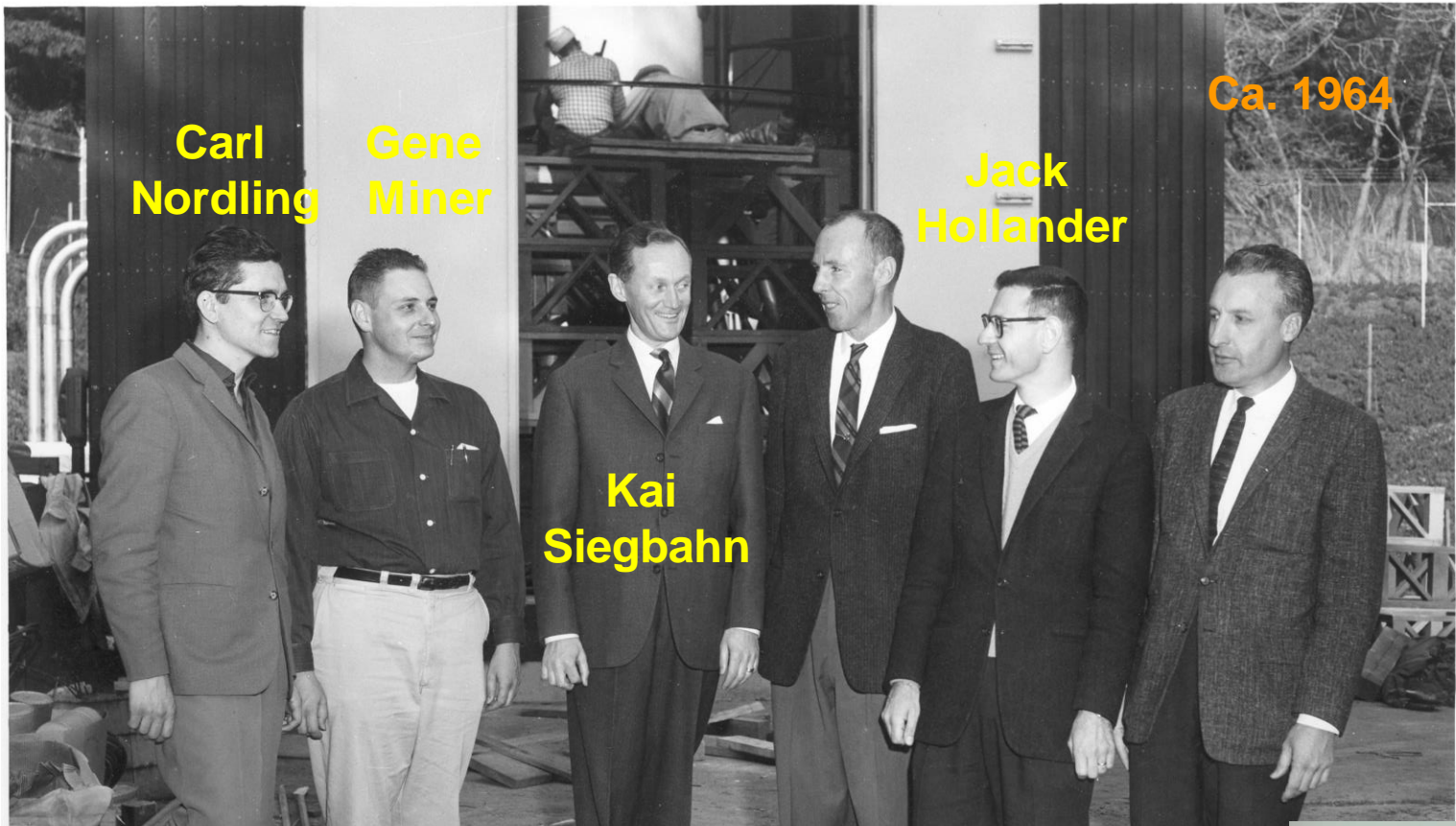
Jack Hollander

Carl Nordling

Kai Siegbahn

Ca. 1964





**Carl Nordling**

**Gene Miner**

**Kai Siegbahn**

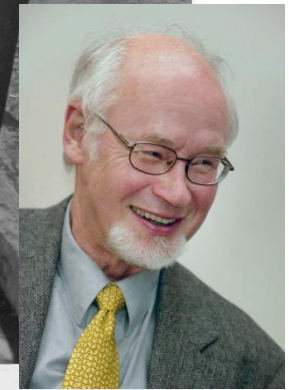
**Jack Hollander**

**Ca. 1964**



**Dave Shirley**

**Ca. 1966- Chuck, how would you like to work on a new kind of experiment with Stig Hagström, a guy from Sweden?**



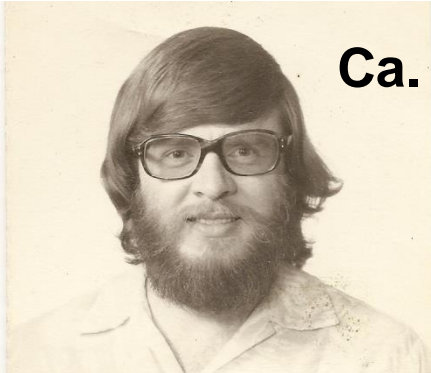
**Stig Hagström  
1932-2011**



Ca. 1966

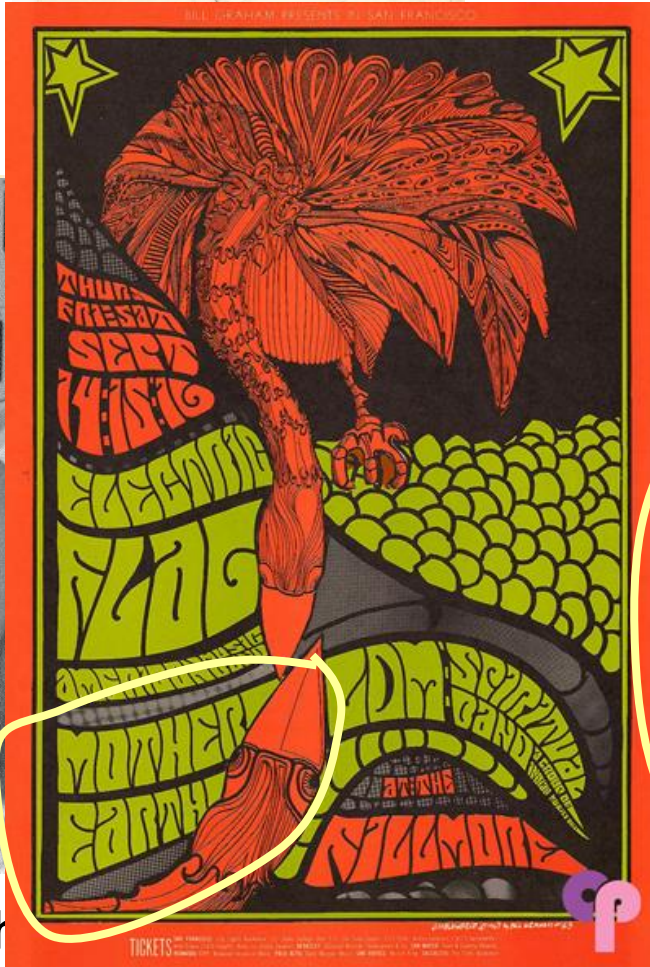
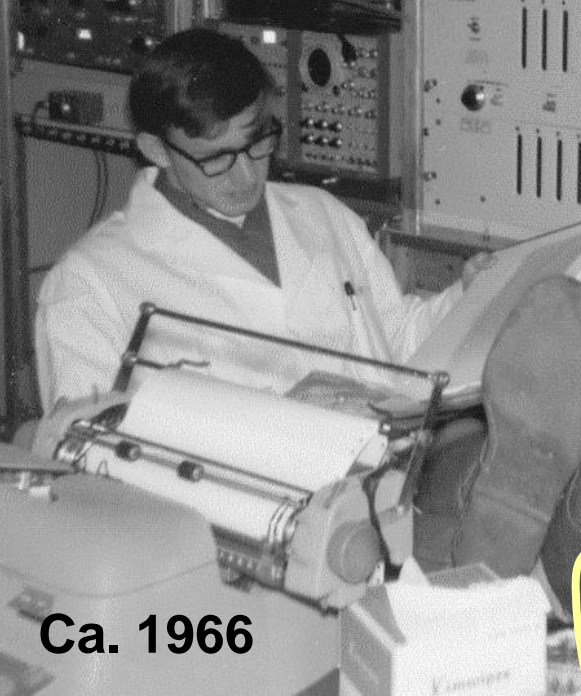


Ca. 1968



The "group bands" from my apt.

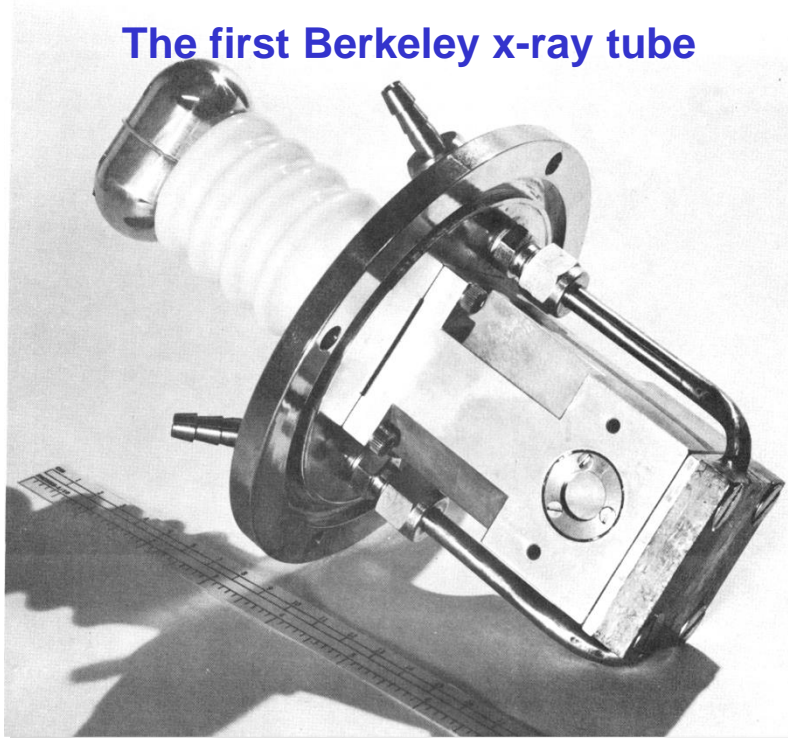
Ca. 1966



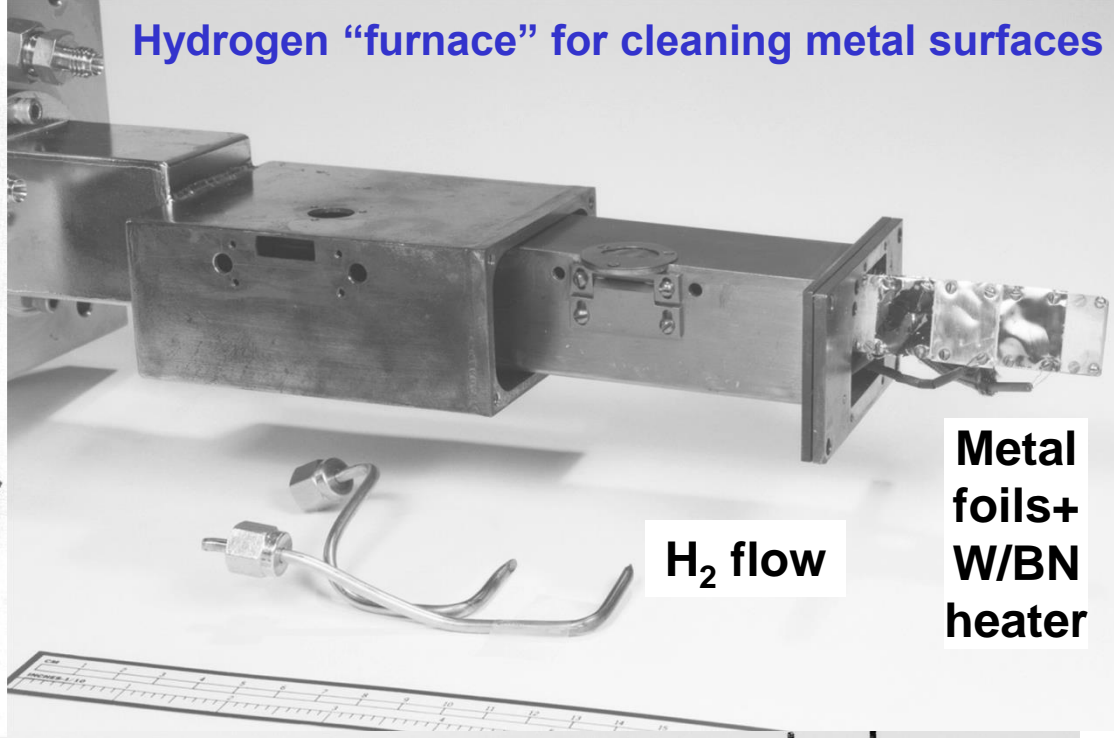
Typewriter for output, th



The first Berkeley x-ray tube

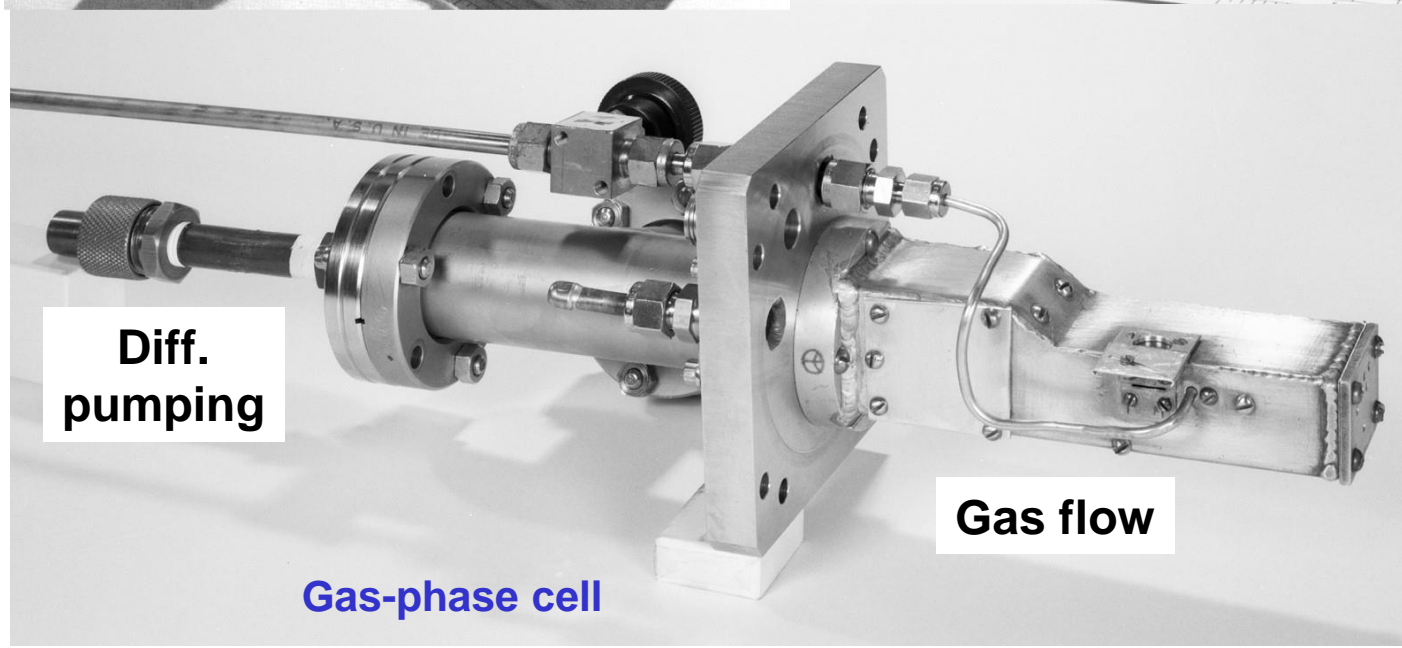


Hydrogen "furnace" for cleaning metal surfaces



H<sub>2</sub> flow

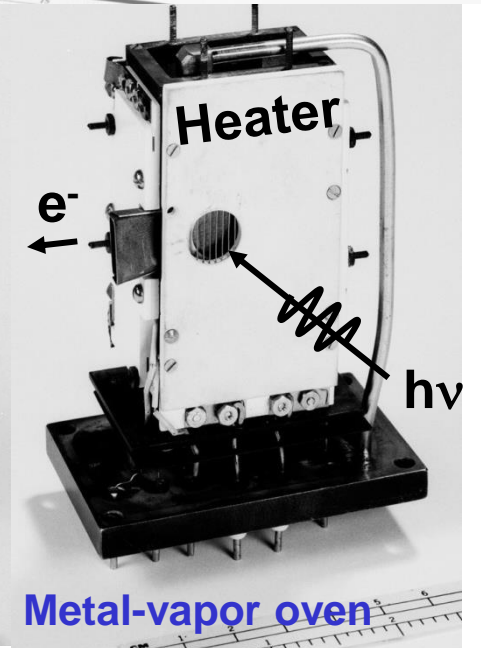
Metal foils+  
W/BN  
heater



Diff.  
pumping

Gas flow

Gas-phase cell



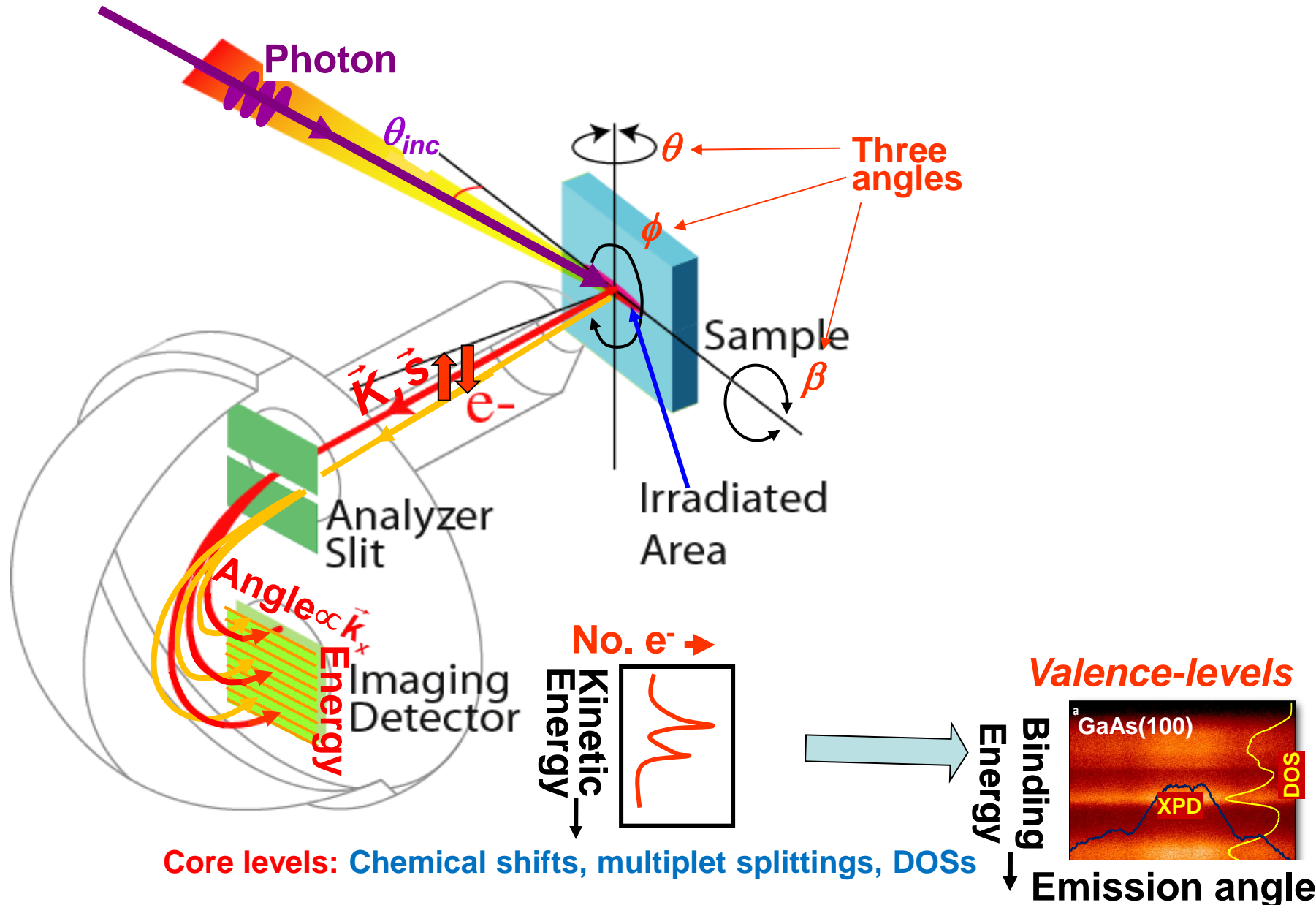
Heater

e<sup>-</sup>

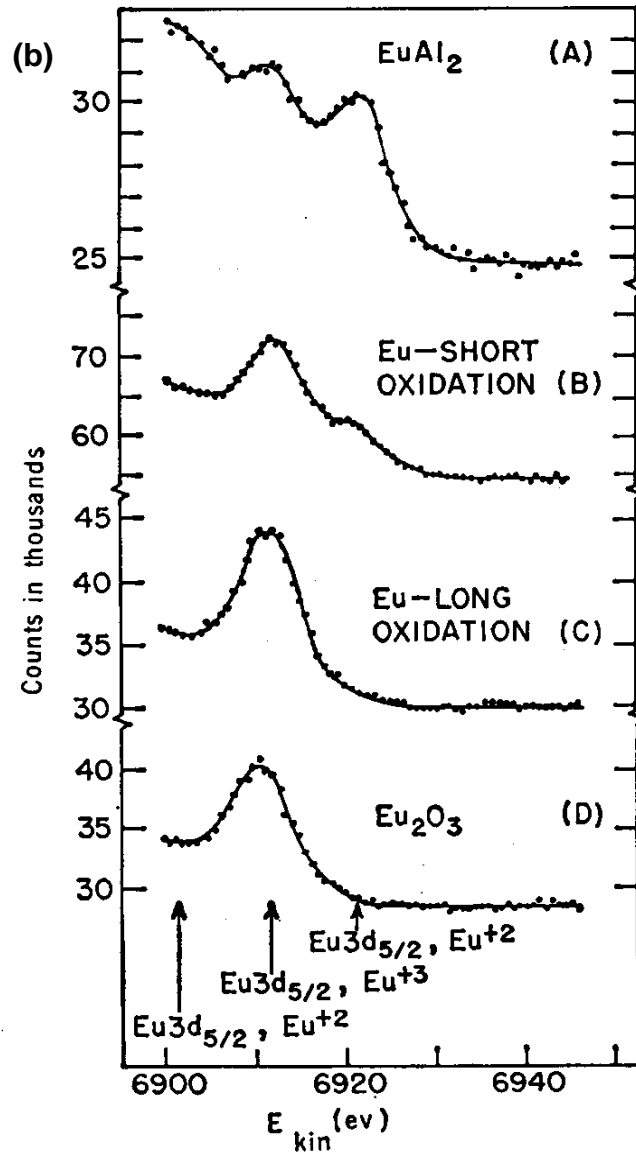
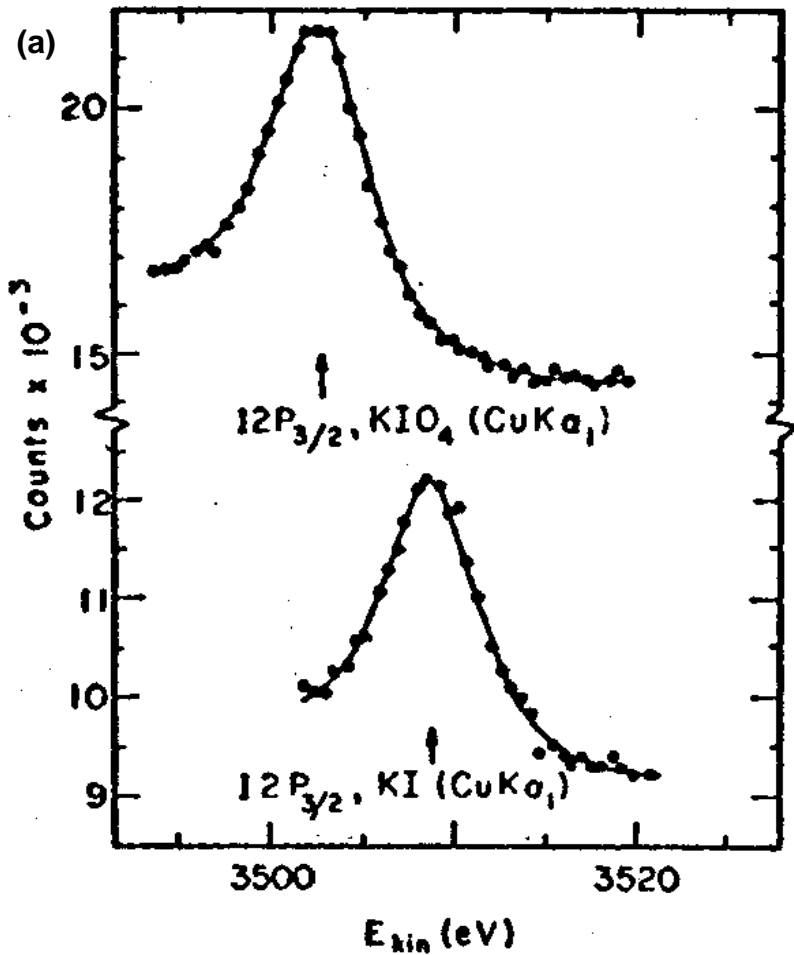
hν

Metal-vapor oven

# Photoelectron spectroscopy: the various dimensions



# Chemical shifts



Potential model for chemical shifts

Fadley, Hagstrom, Hollander, Klein, Shirley,  
*Science* **157**, no. 3796, 1571 (1967)



# Multiplet splittings in molecules and solids → Net spin moment

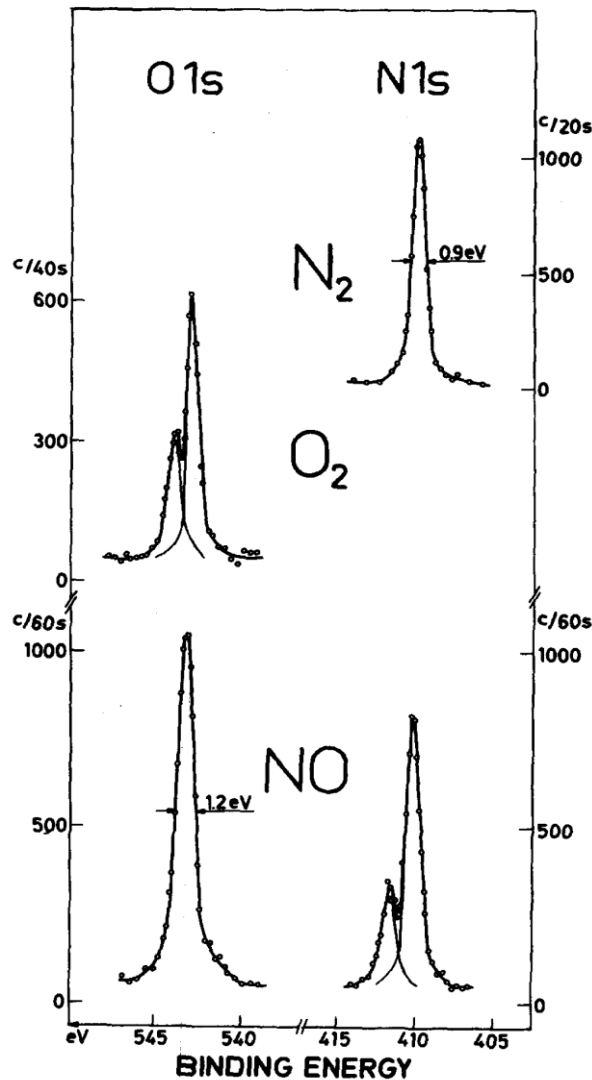
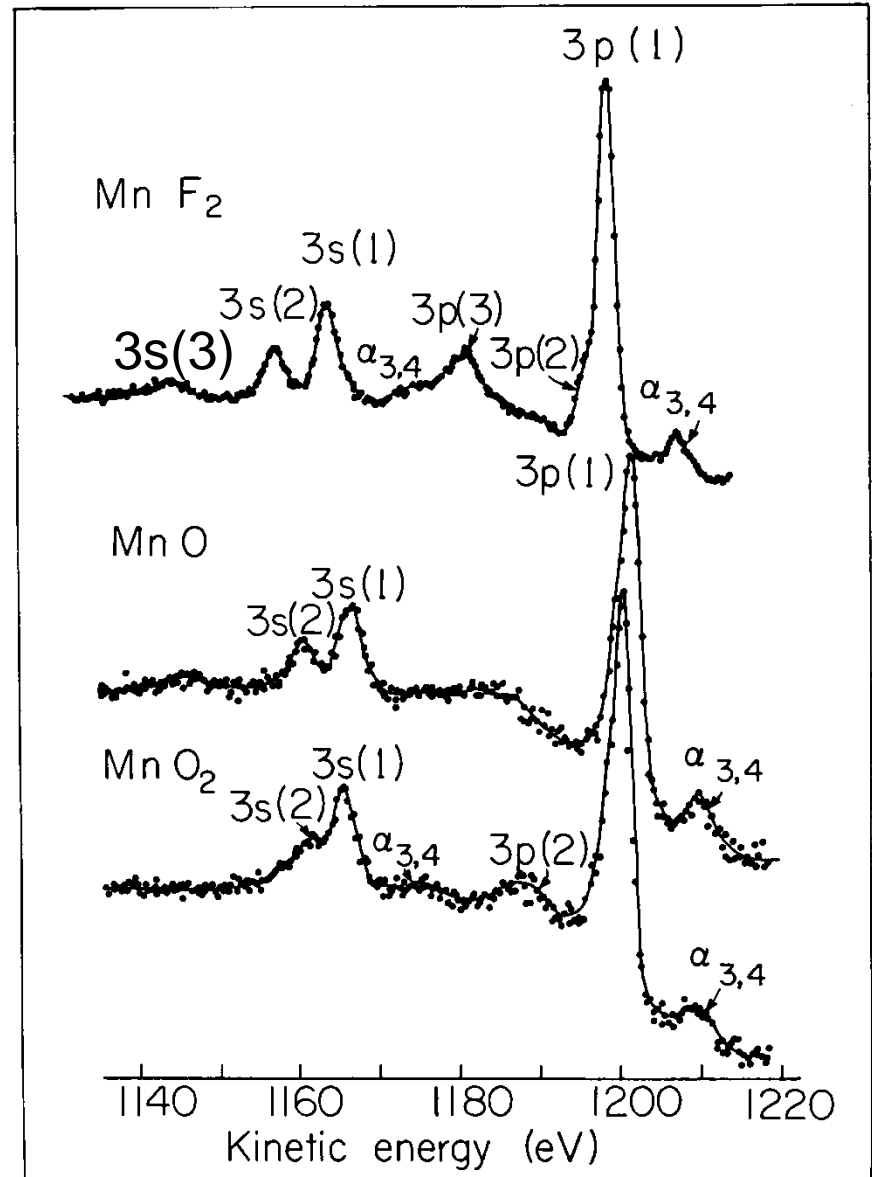
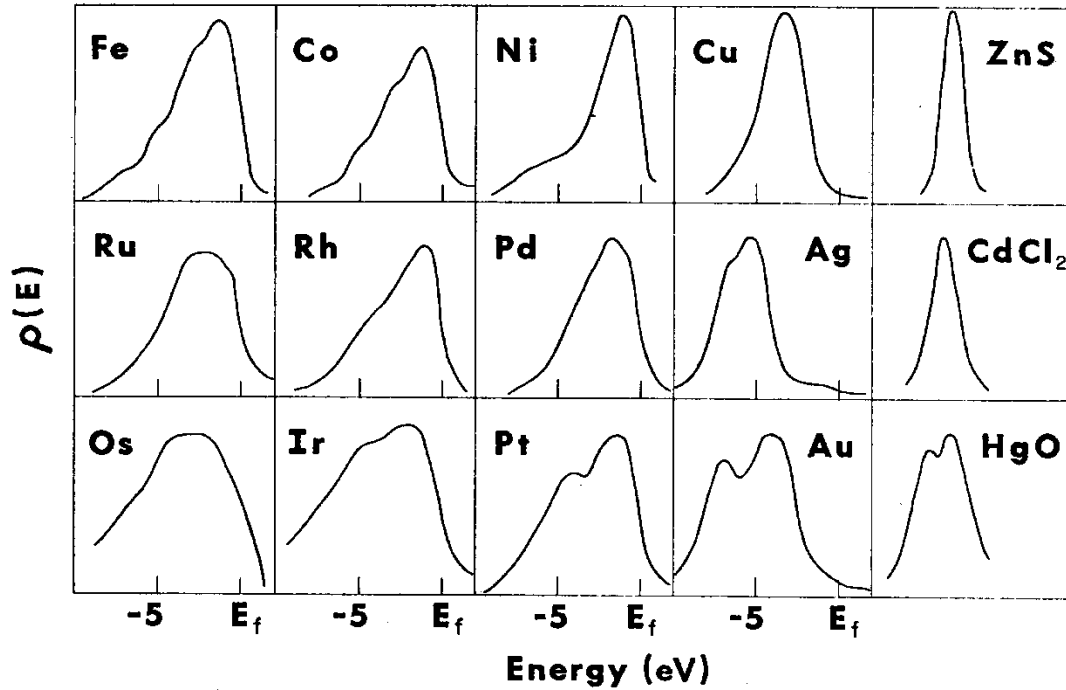


Fig. 1. ESCA spectra of core electron levels in N<sub>2</sub>, O<sub>2</sub>, and NO. Paramagnetic splitting is observed for the 1s levels in the O<sub>2</sub> and NO molecules.



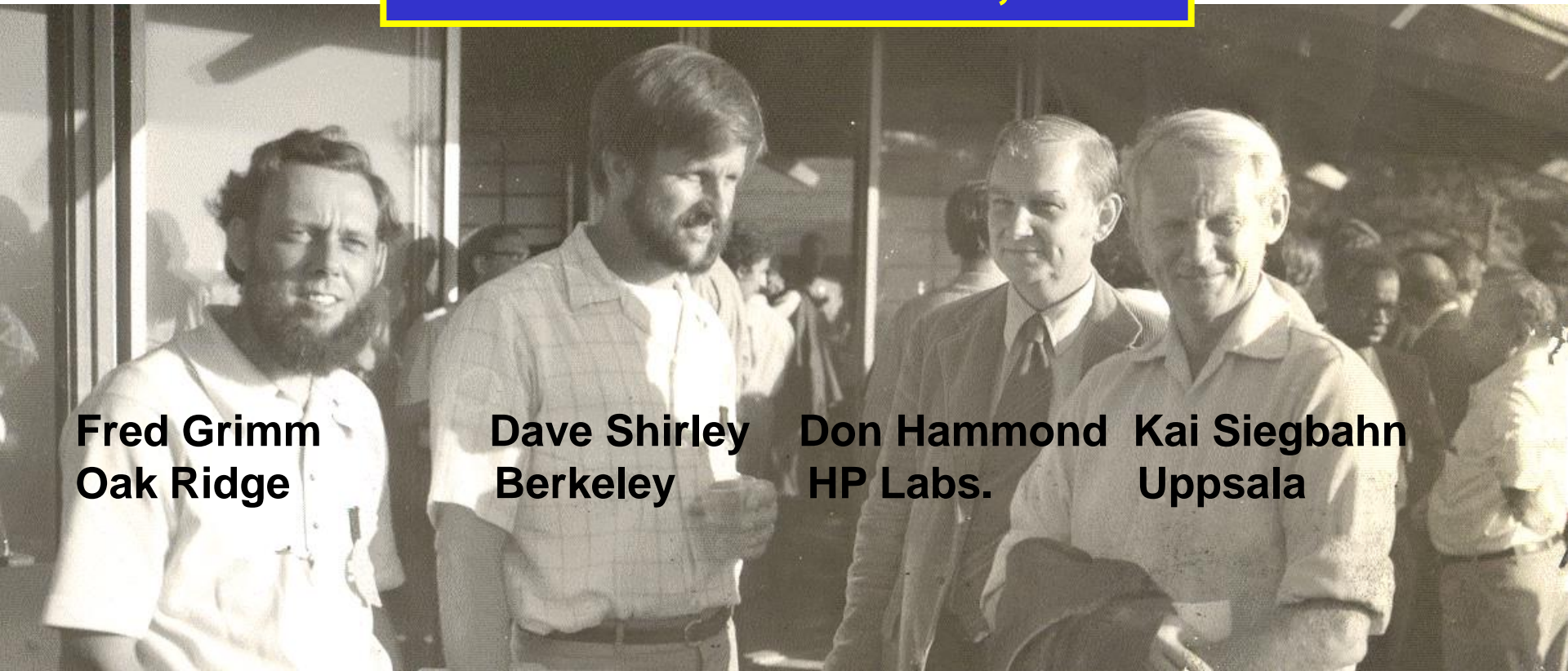
# Densities of state of solids



Fadley, Shirley, Phys. Rev. Letters,  
Phys. Rev. Letters 21, 980 (1968)



# “ICISS-1”--Asilomar, 1971



**Fred Grimm**  
**Oak Ridge**

**Dave Shirley**  
**Berkeley**

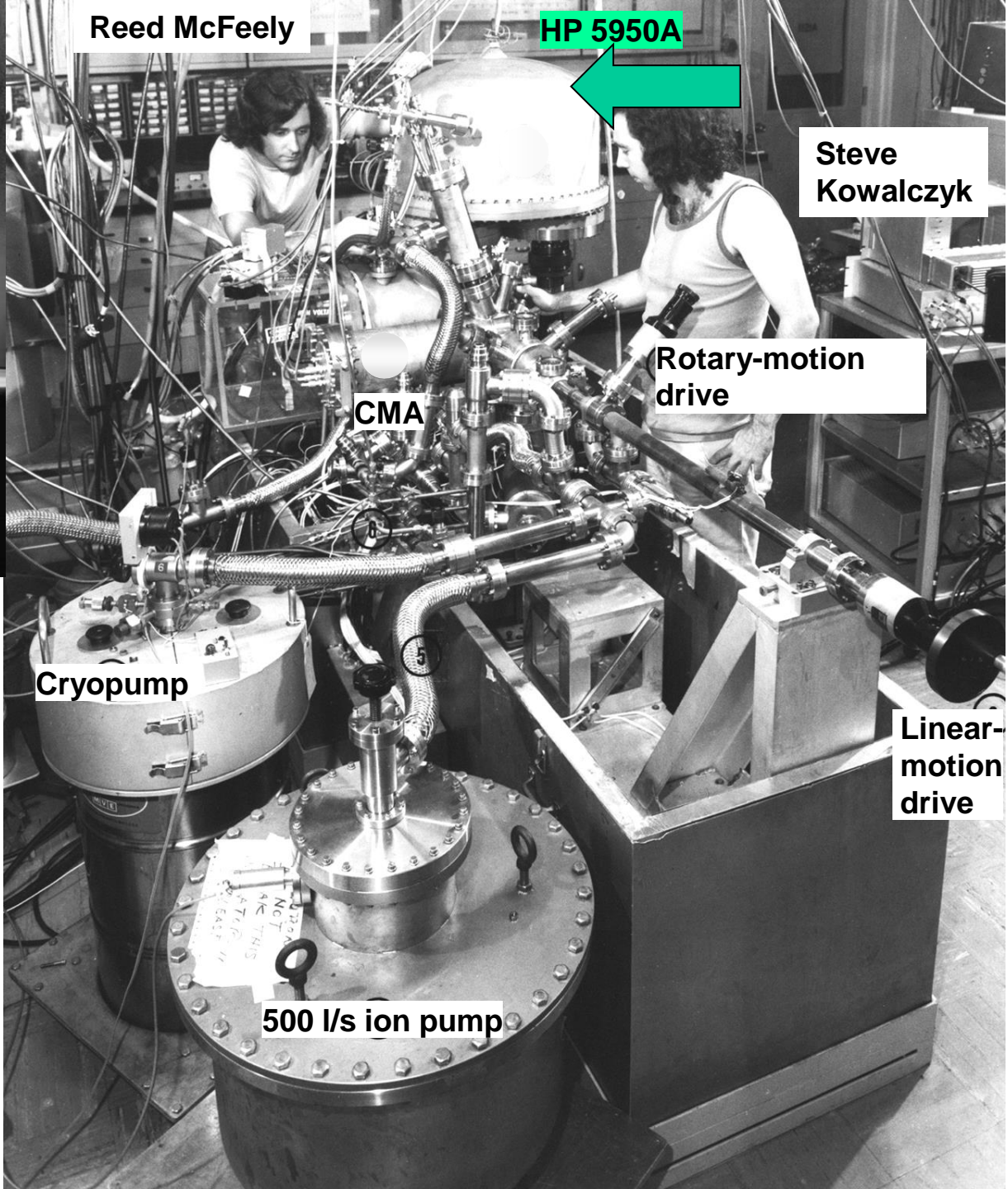
**Don Hammond**  
**HP Labs.**

**Kai Siegbahn**  
**Uppsala**

**Chalmers Fysikum, '71**



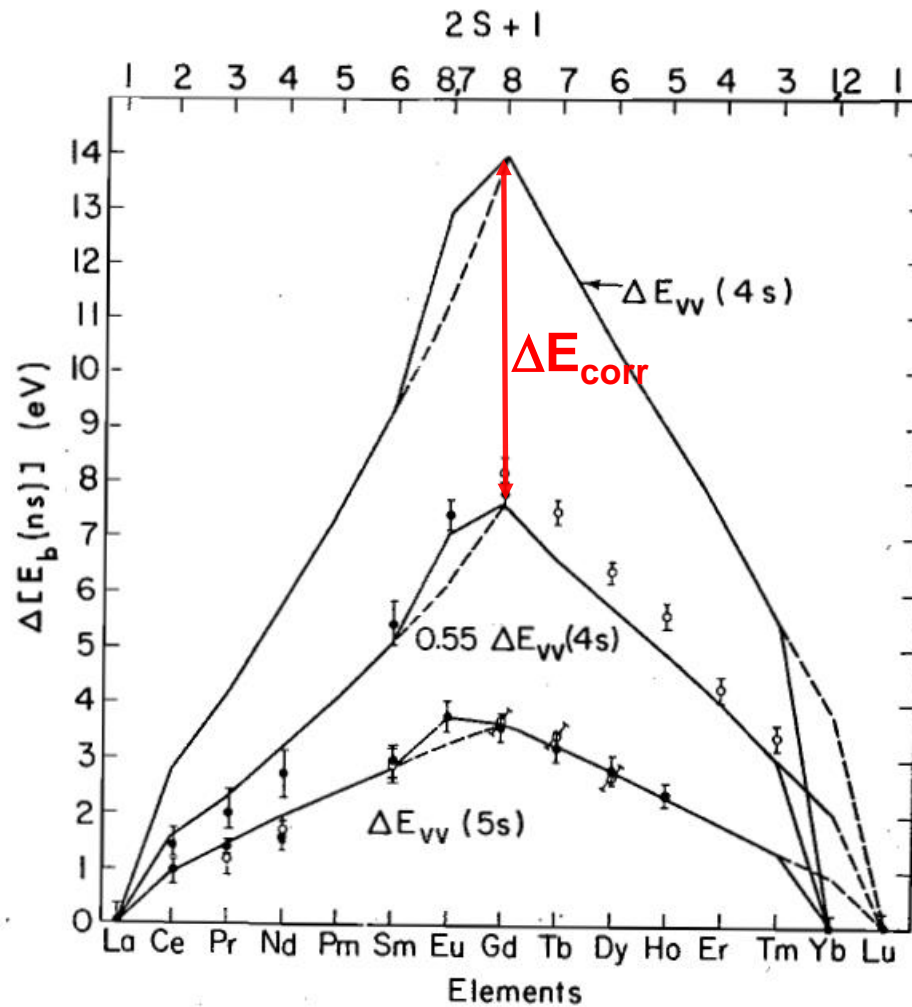
**The HP 5950 Spectrometer**



**The Berkeley electron spectroscopy lab. -ca. 1972**



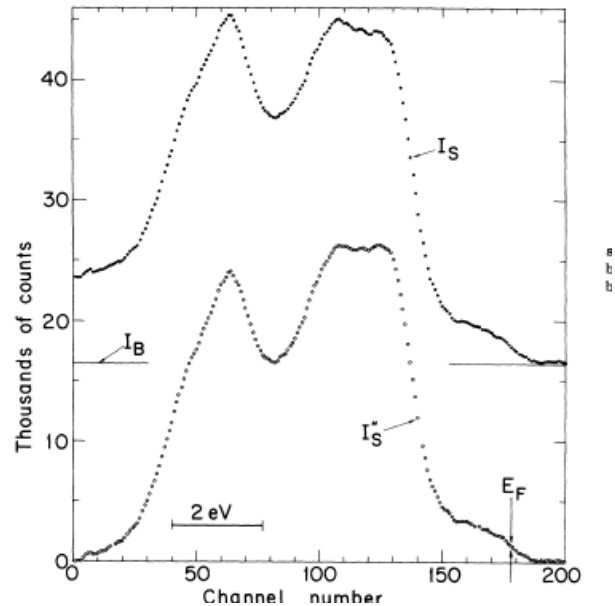
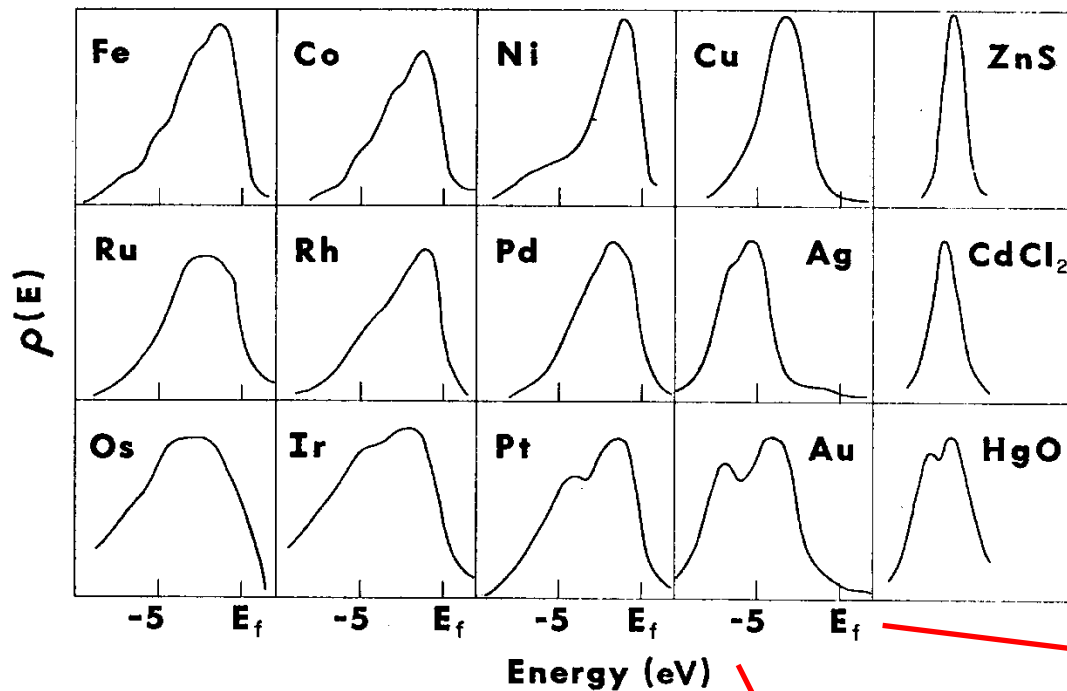
# Multiplet splittings and intrashell correlation effects



F.R. McFeely, S.P. Kowalczyk, L. Ley, D.A. Shirley, Physics Letters A4 49, 301 (1974)

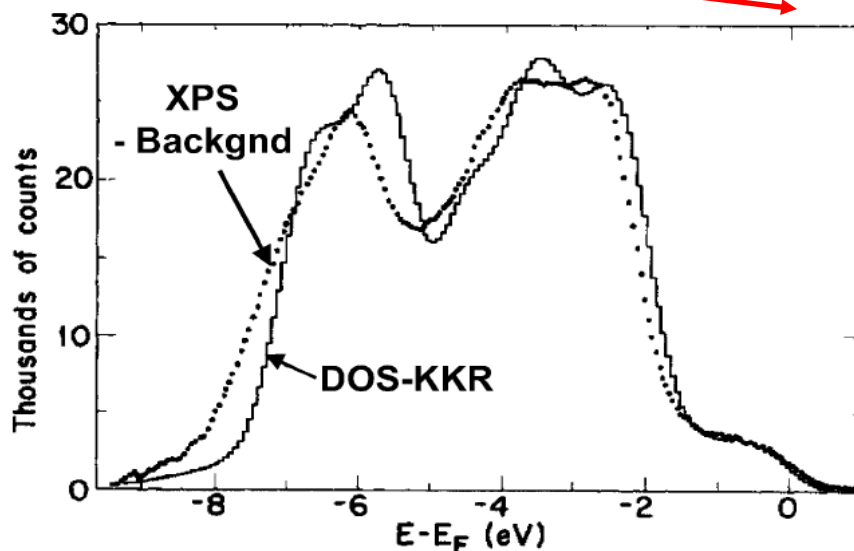
# Densities of state of solids

## The Shirley Background



$$I_S^{\#}(N) = I_S^{\#}(N) - I_S^{\#}(0) \left( \frac{\sum_{N' > N} I_S^{\#}(N')}{\sum_{N' > 0} I_S^{\#}(N')} \right)$$

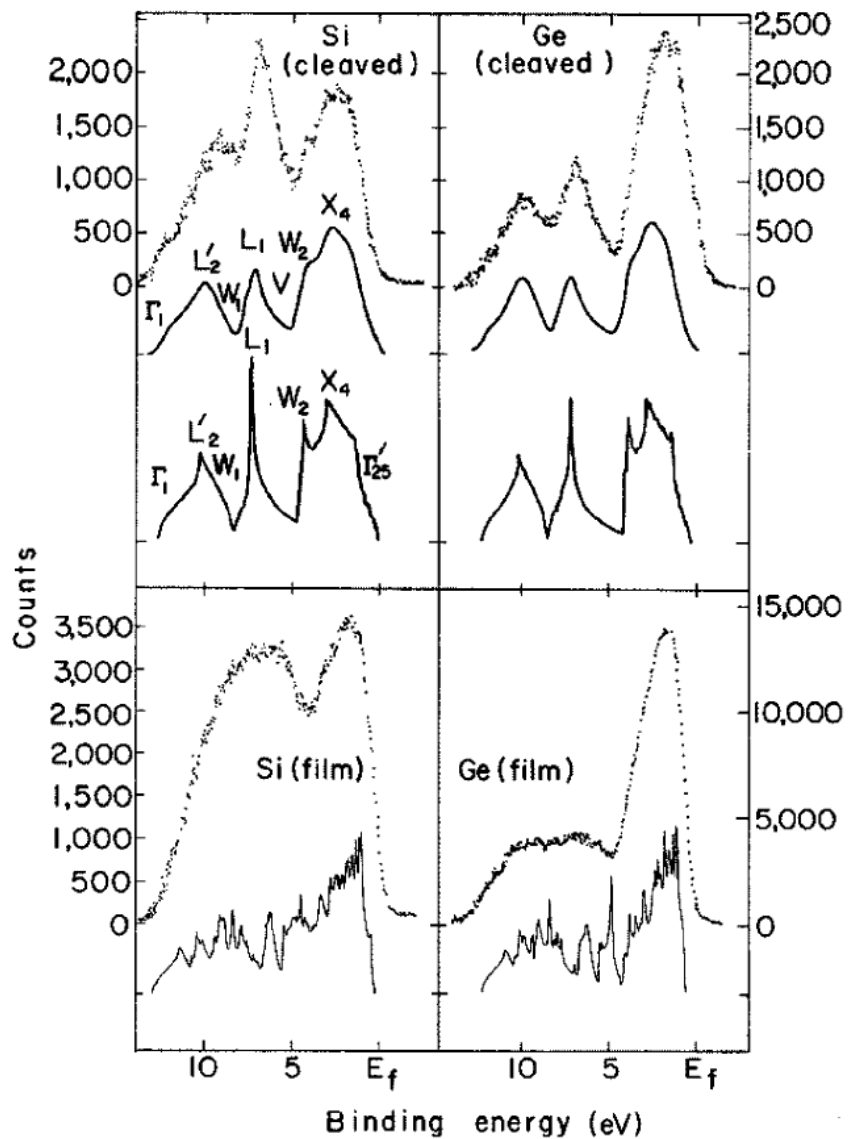
Fadley, Shirley, Phys. Rev. Letters, Phys. Rev. Letters 21, 980 (1968)



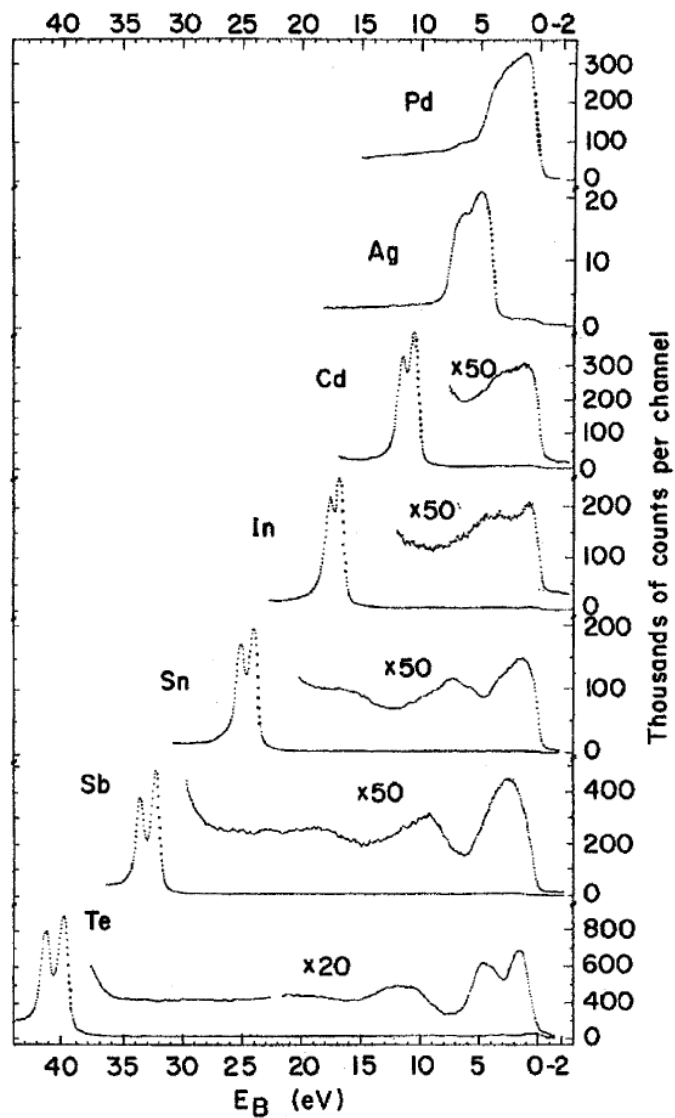
D.A. Shirley, Phys. Rev. B5 (1972) –3308 citations!



# Densities of state of solids



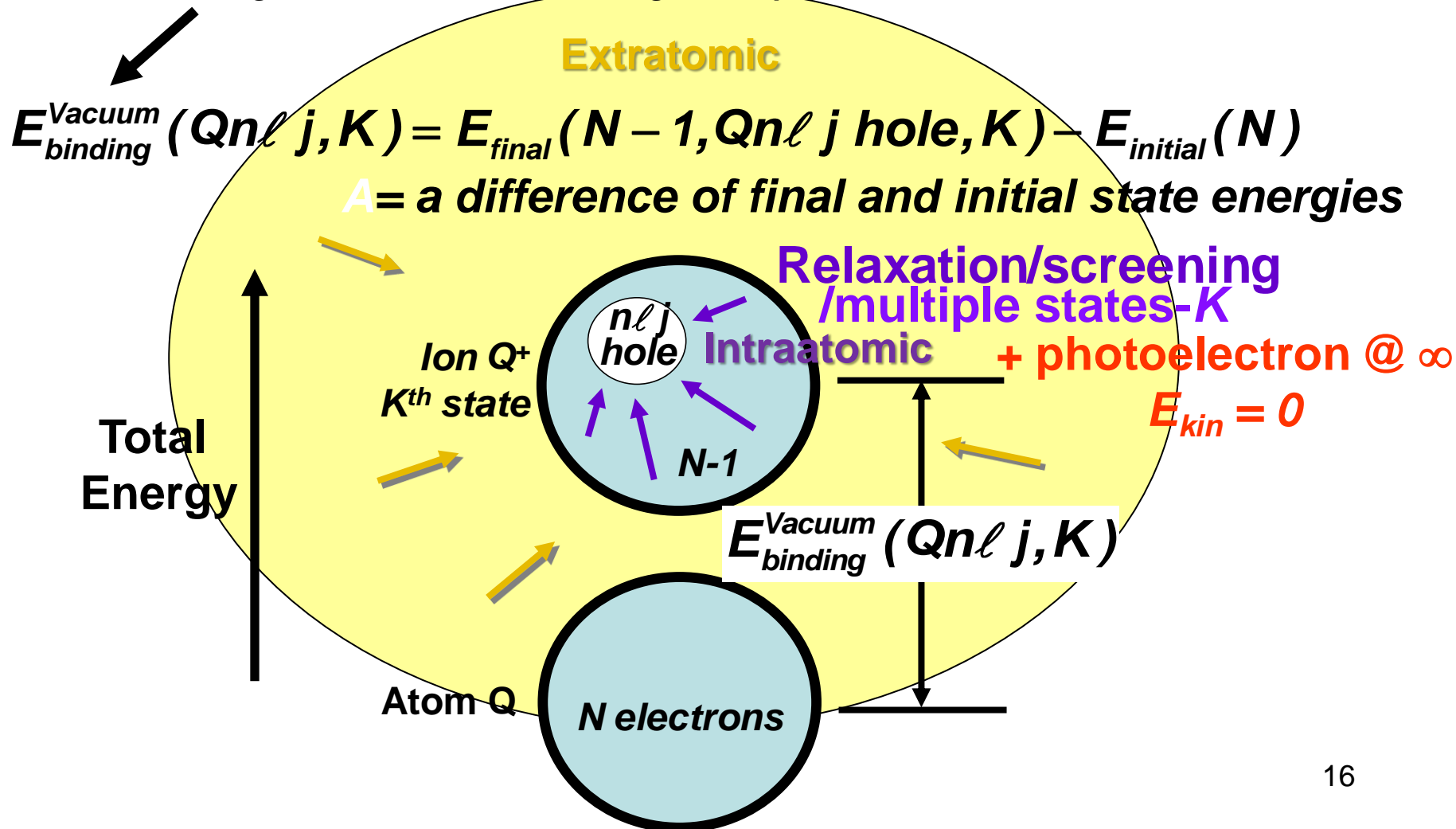
L. Ley, S. Kowalczyk, R. Pollak, and D. A. Shirley, Phys. Rev. Lett. 29, 1088 (1972)



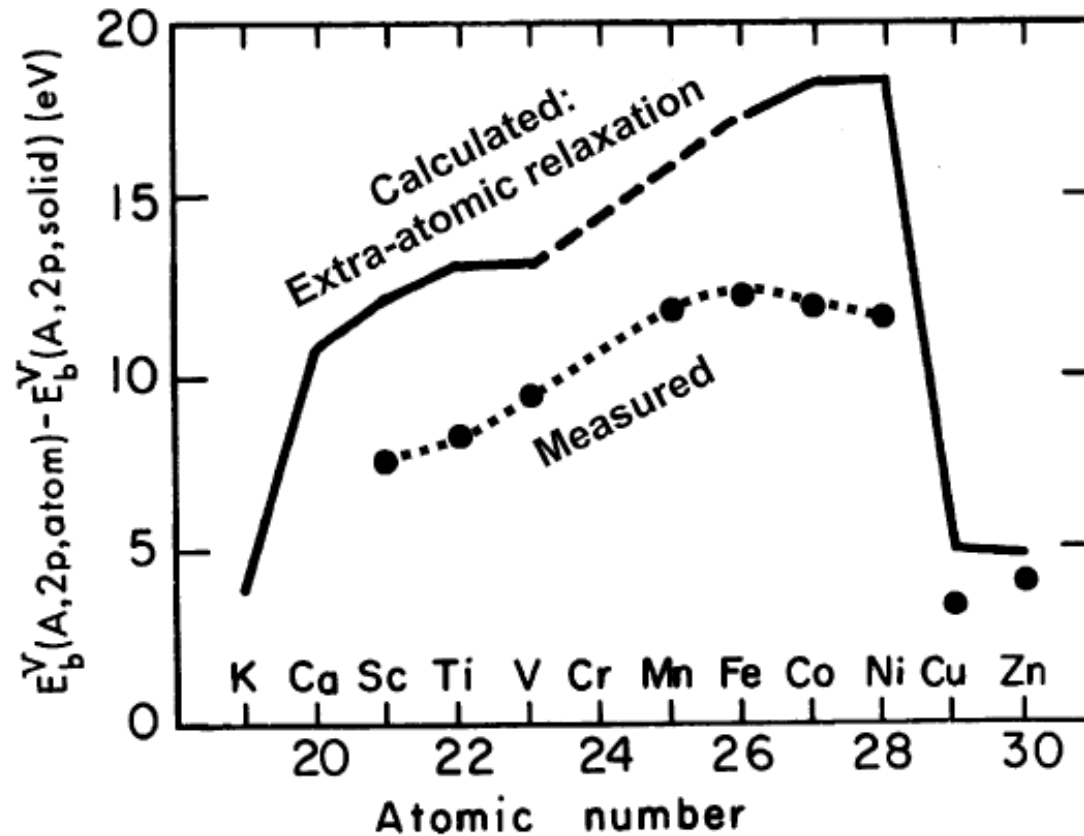
R. A. Pollak, S. Kowalczyk, L. Ley, and D. A. Shirley, Phys. Rev. Lett. 29, 274 (1972)

# Photoemission: The correct energy picture

$$h\nu = E_{\text{binding}}^{\text{Vacuum}} + E_{\text{kinetic}} = E_{\text{binding}}^{\text{Fermi}} + \varphi_{\text{spectrometer}} + E_{\text{kinetic}}$$



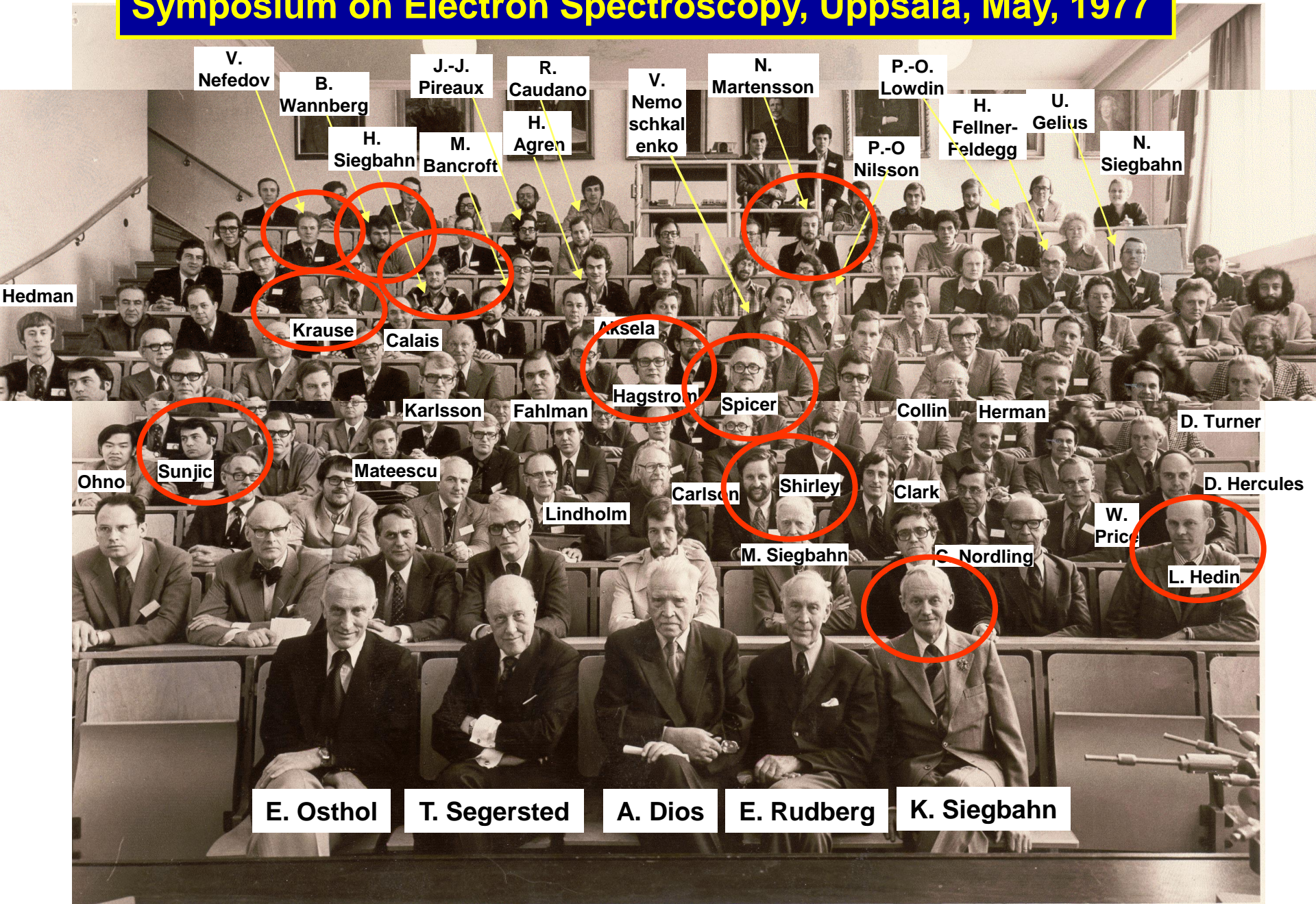
# Final-state relaxation/screening around a hole



L. Ley, S. P. Kowalczyk, F. R. McFeely, R. A. Pollak, and D. A. Shirley  
Phys. Rev. B8 (1973) 2392



# Symposium on Electron Spectroscopy, Uppsala, May, 1977





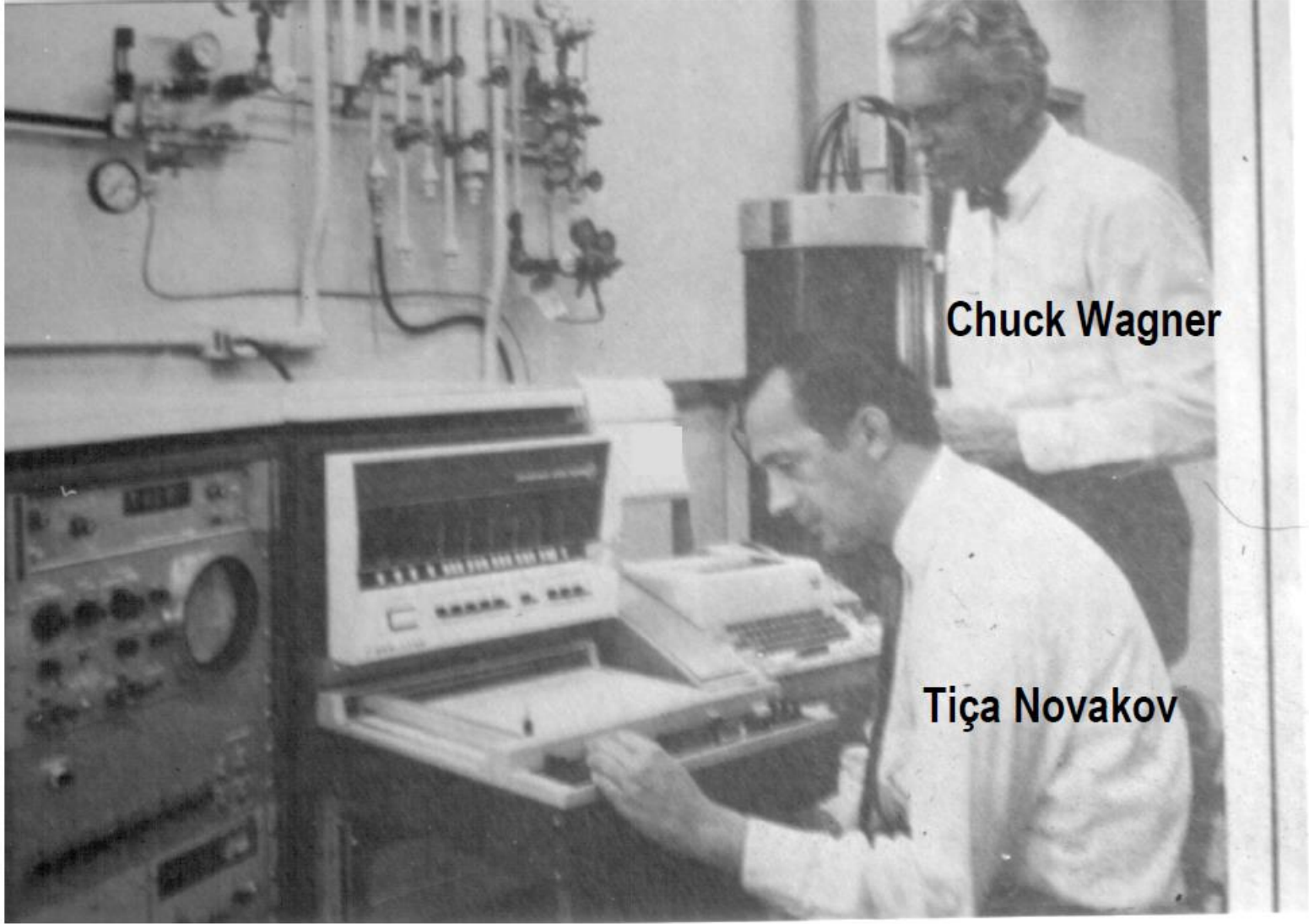
**Uppsala, May, 1977**

Dave Shirley

Vadim  
Nefedov

Hans  
Siegbahn





**Chuck Wagner**

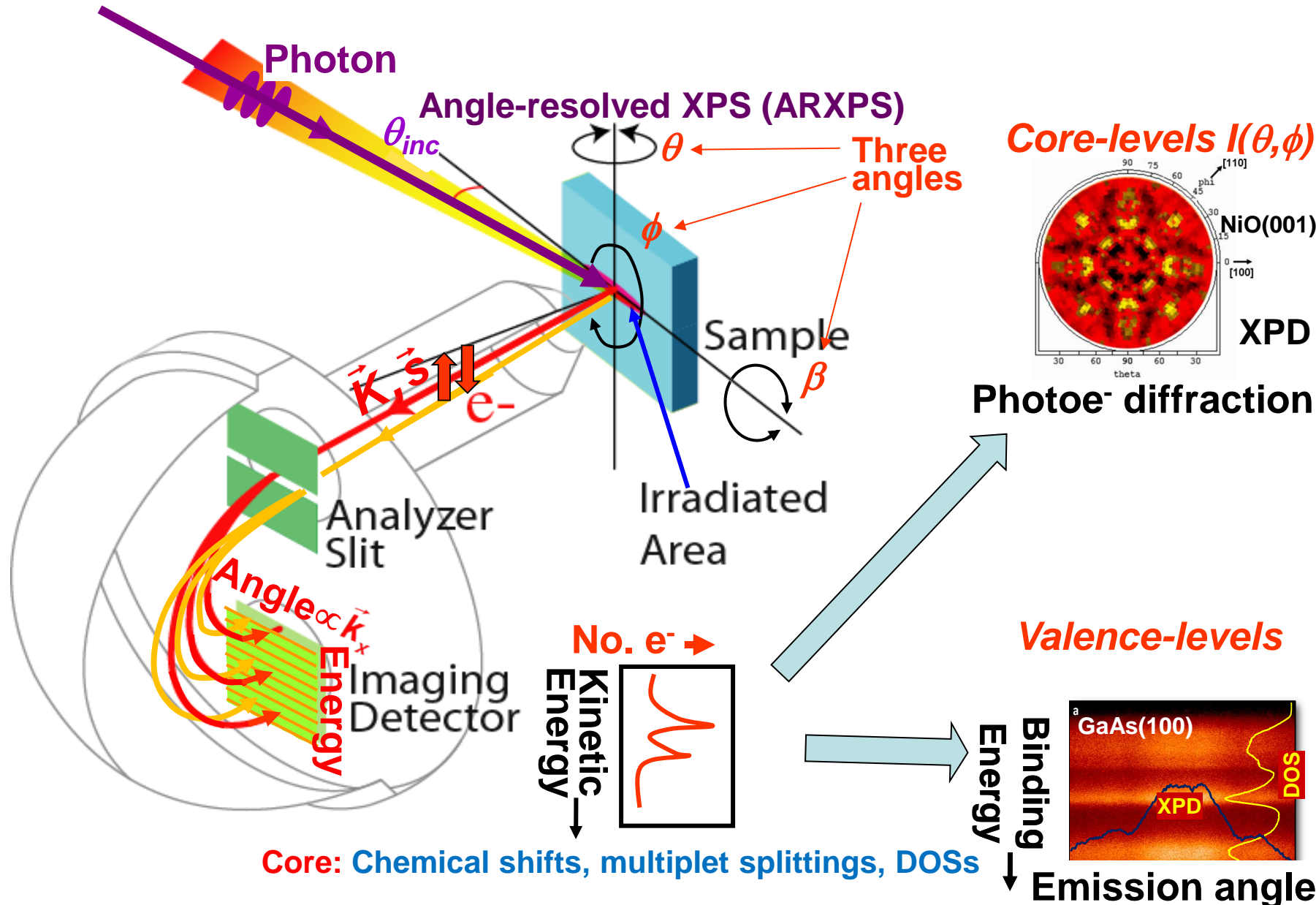
**Tiča Novakov**



# The Stanford Synchrotron Radiation Lightsource Ca. 1974 to 1993

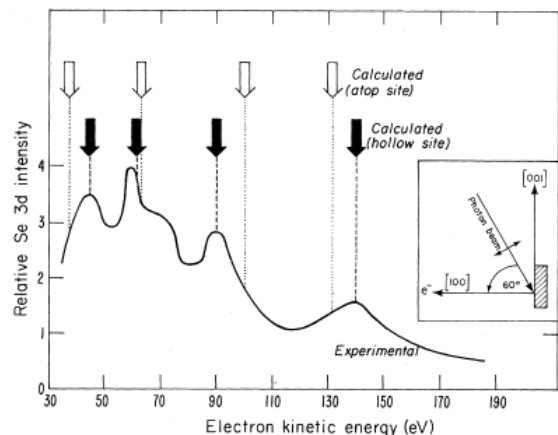


# Photoelectron spectroscopy: the various dimensions

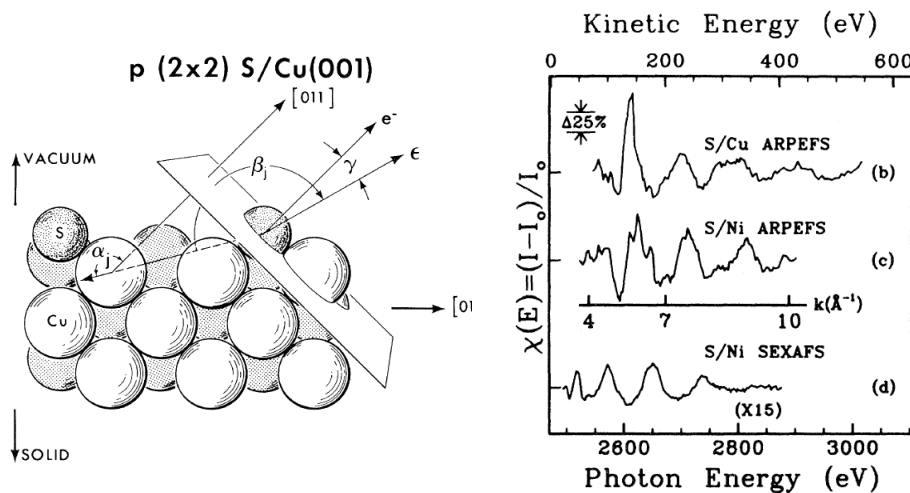


# Surface atomic structures from photoelectron diffraction and photoelectron holography

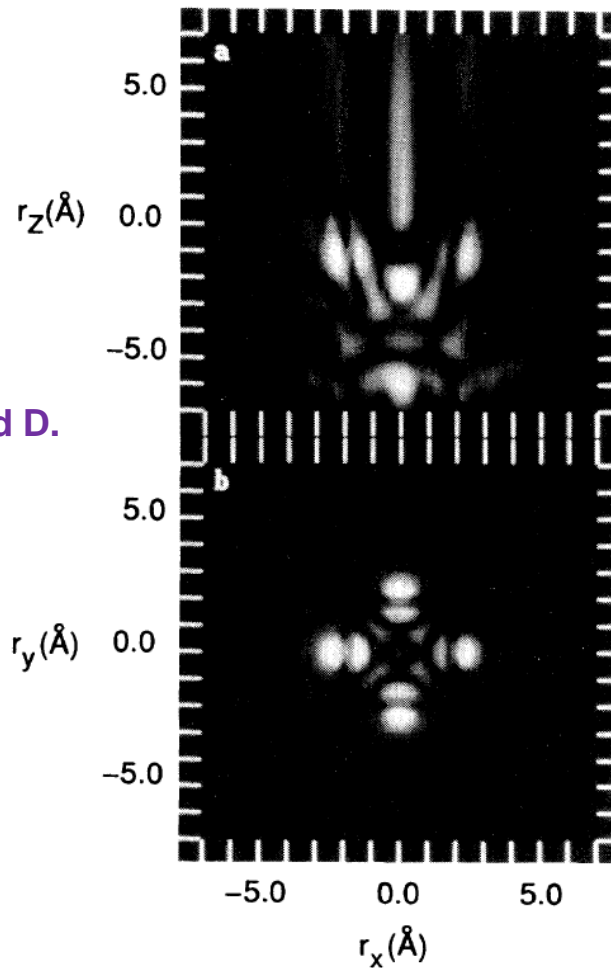
Se on Ni(001):



S. D. Kevan, D. H. Rosenblatt, D. Denley, B.-C. Lu, and D. A. Shirley, *Phys. Rev. Lett.* 41, 1566 (1978)



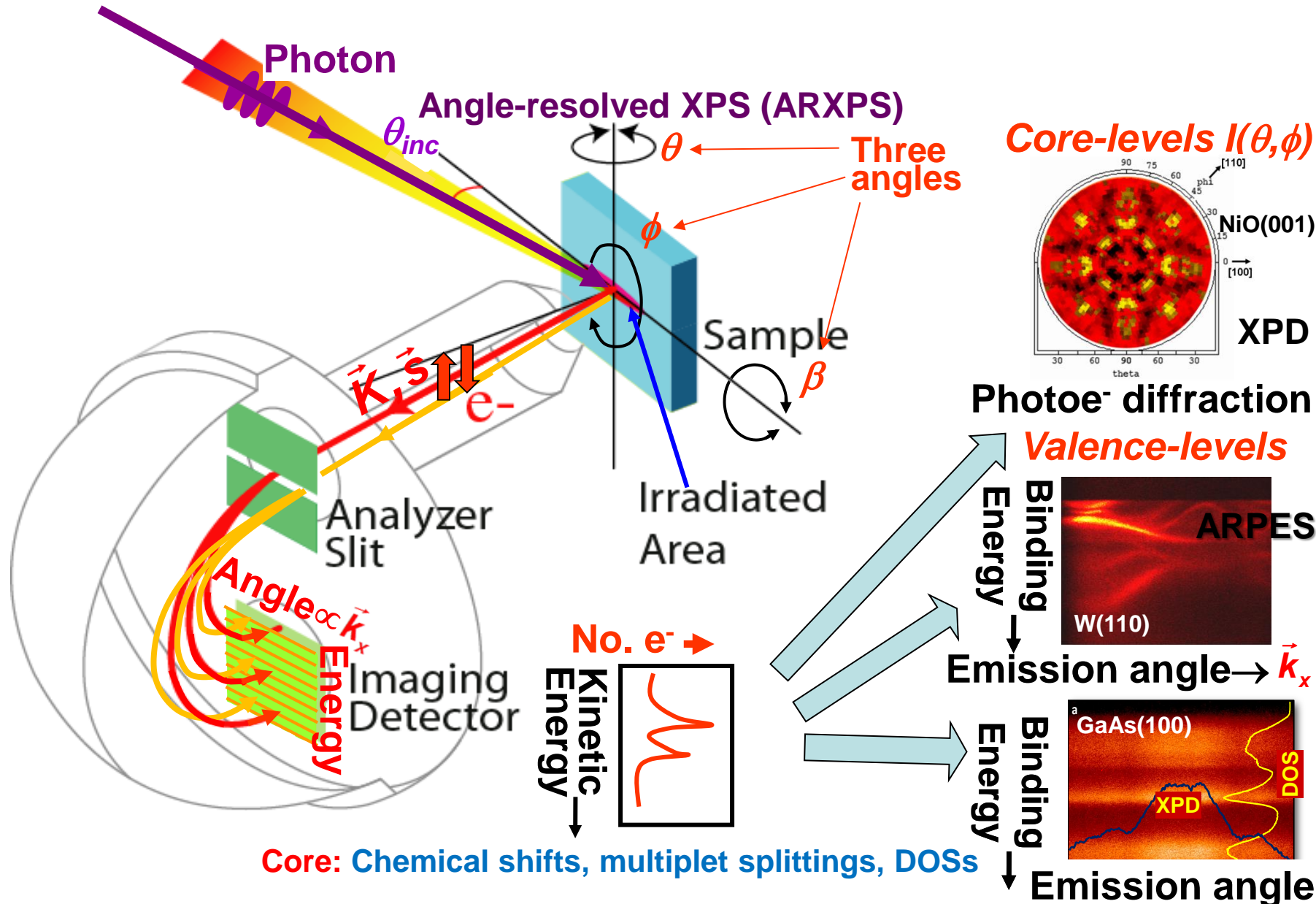
J. J. Barton, C. C. Bahr, Z. Hussain, S. W. Robey, J. G. Tobin, L. E. Klebanoff, and D. A. Shirley, *Phys. Rev. Lett.* 51, 272 (1983)



J. J. Barton, *Phys. Rev. Lett.* 67, 272 (1991)  
(By then at IBM Watson)

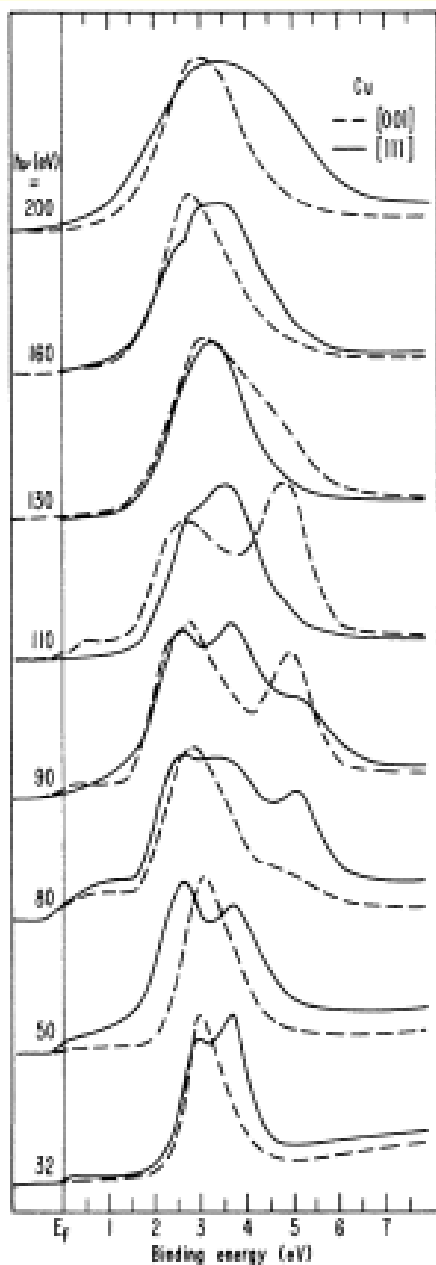


# Photoelectron spectroscopy: the various dimensions

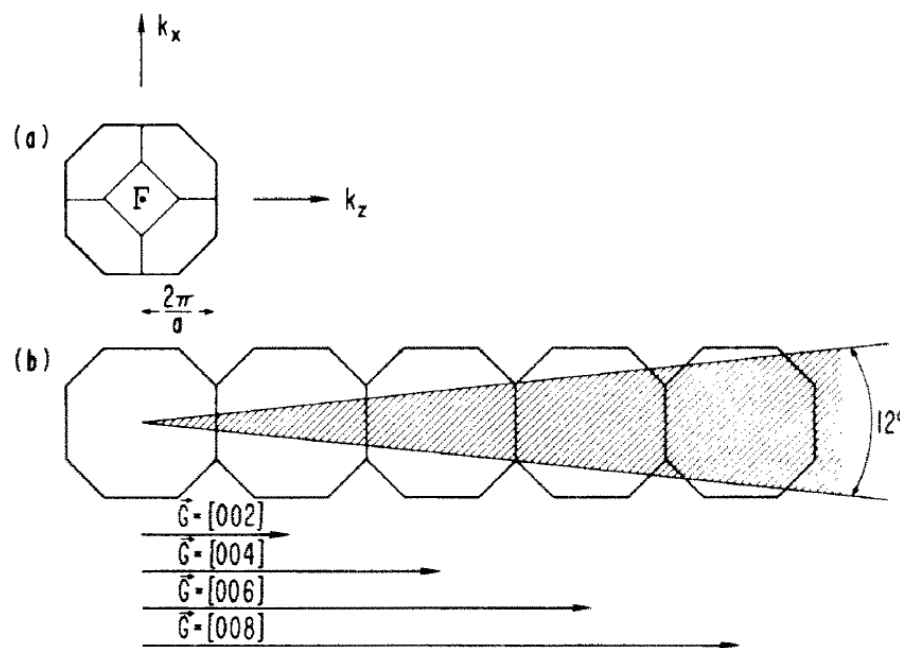


# Angle-resolved photoemission from valence bands: Cu

Increasing photon energy  $\rightarrow$

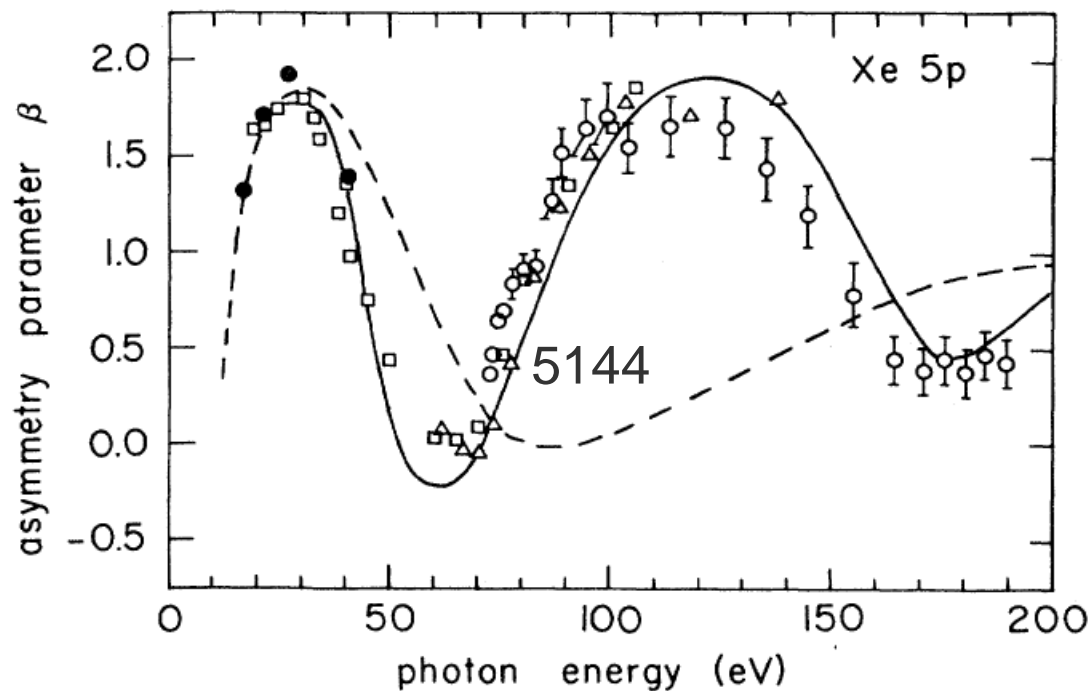


## Moving through k-space



J. Stöhr, G. Apai, P. S. Wehner, F. R. McFeely, R. S. Williams, and D. A. Shirley,  
 Phys. Rev. B 14, 5144 (1976)

# And gas-phase atomic and molecular studies: Differential photoelectric cross sections, the asymmetry parameter

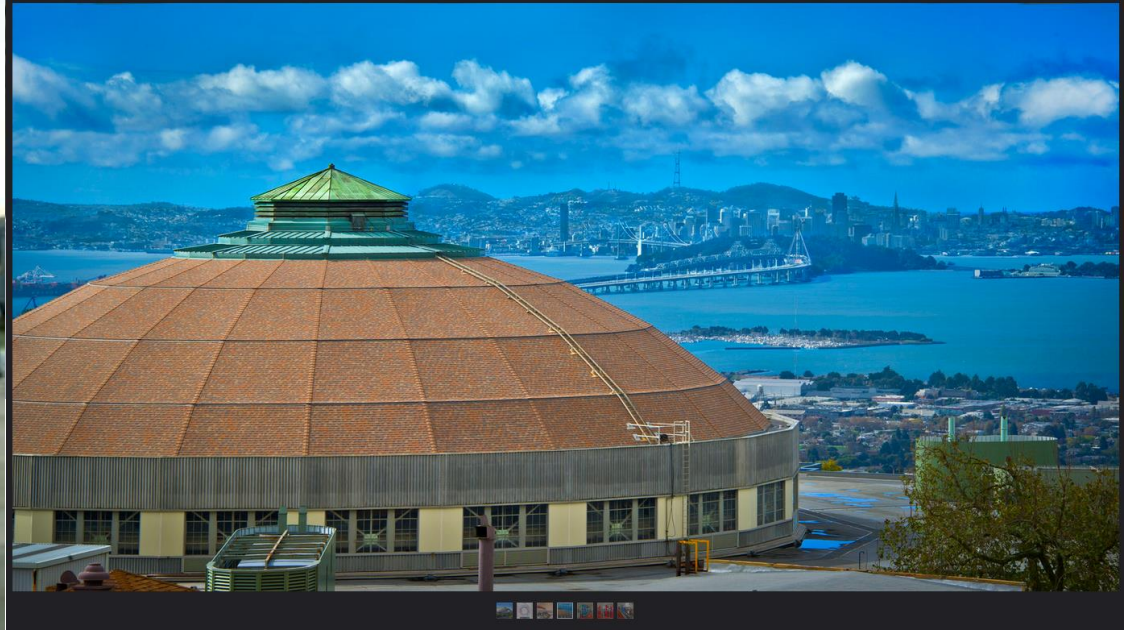


S. Southworth, U. Becker, C. M. Truesdale, P. H. Kobrin, D.  
W. Lindle, S. Qwaki, and D. A. Shirley  
Phys. Rev. A 28, 261-279 (1983)



**LBL Director, 1980-89**

**The Advanced Light Source-1993 to present**

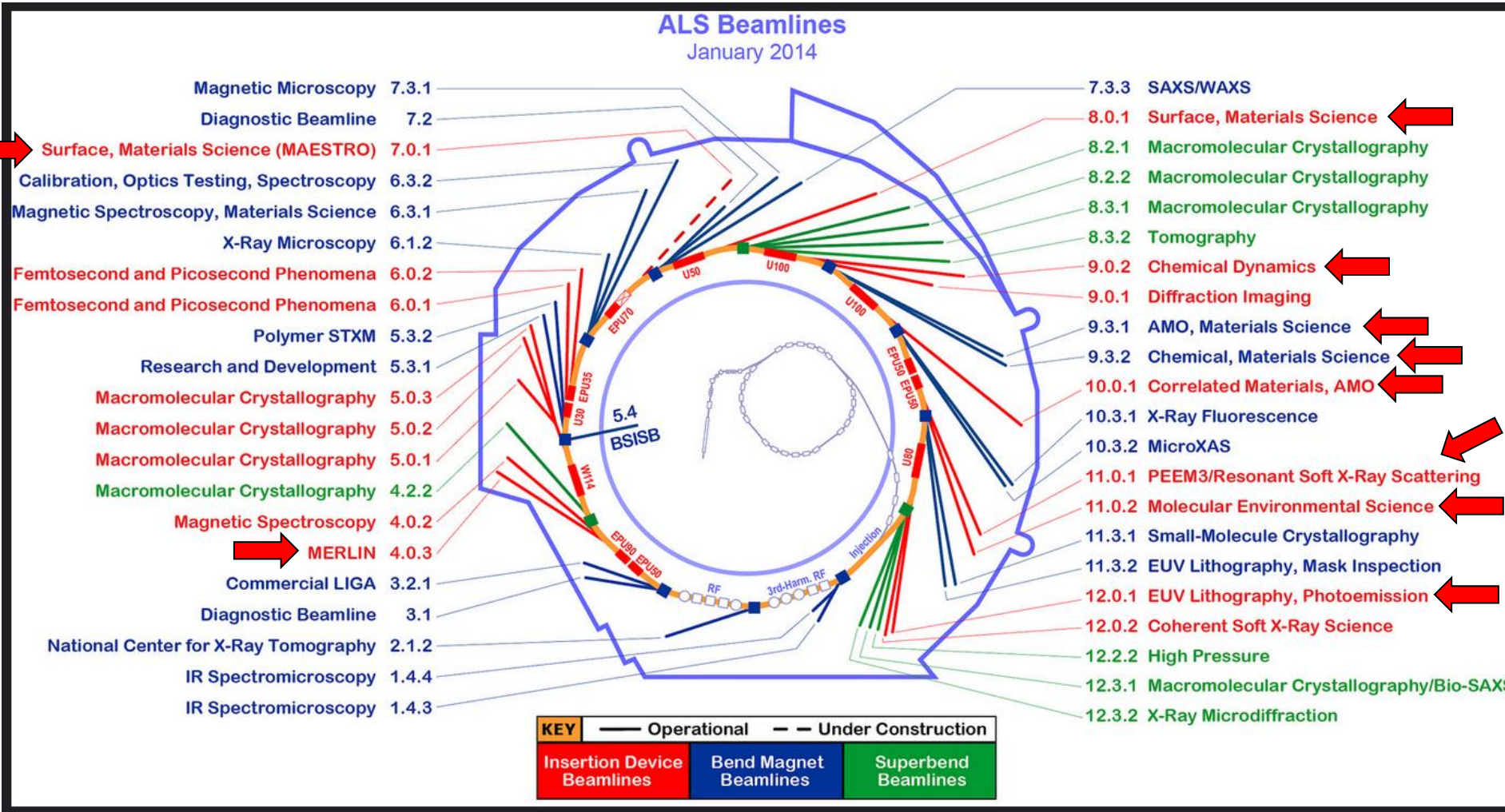


**The National Center for Electron Microscopy**

**The Center for X-Ray Optics**

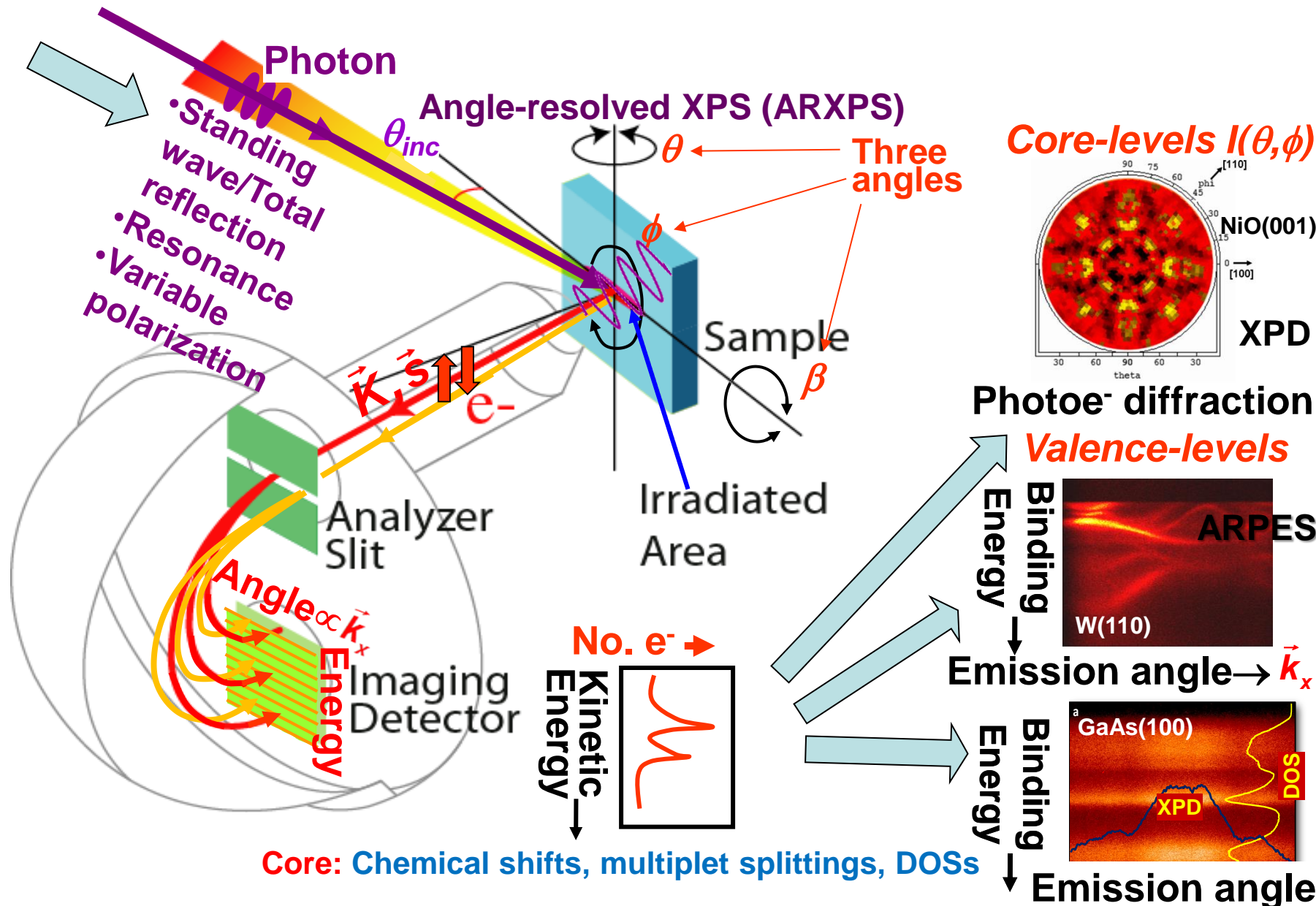
# The Advanced Light Source at 20 years

**→ = photoelectron spectroscopy/photoemission**



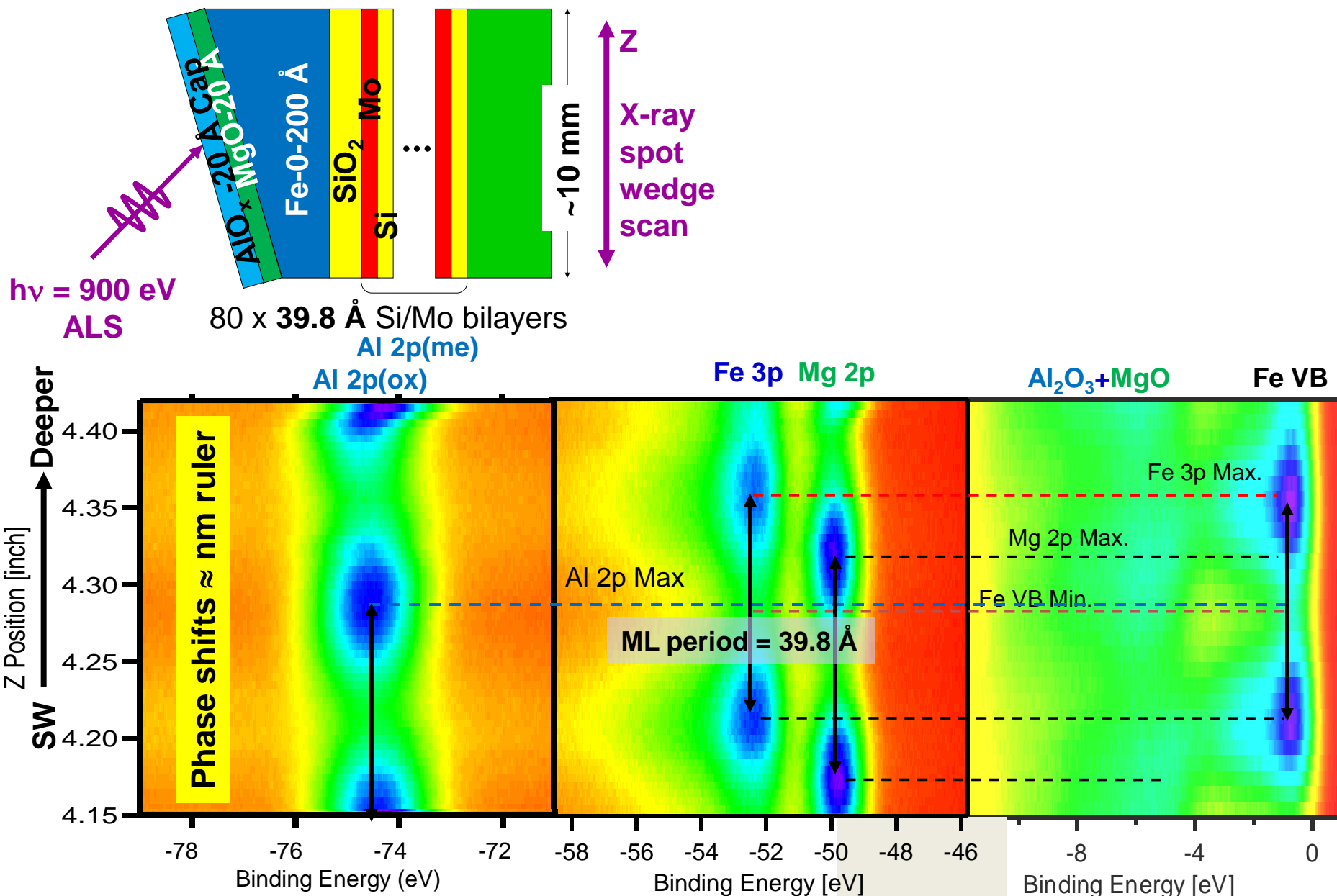


# Photoelectron spectroscopy: the various dimensions



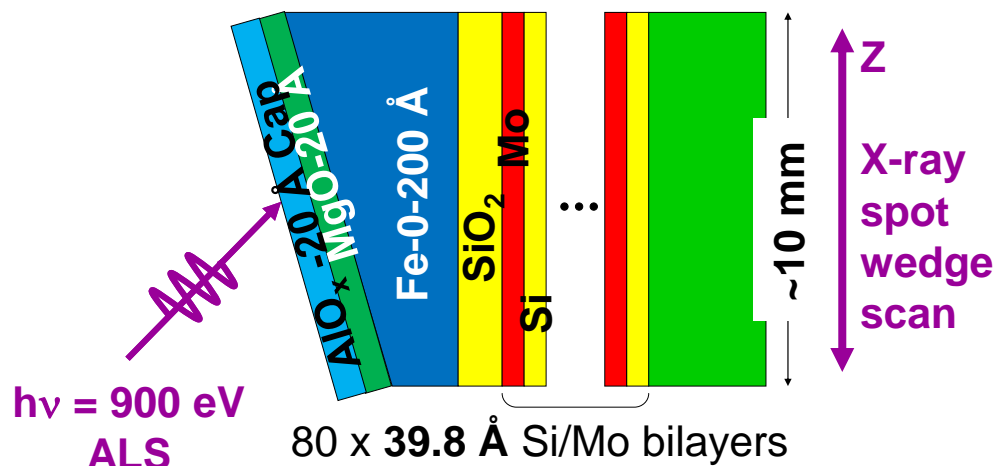


# Soft x-ray standing-wave wedge scans through a magnetic tunnel junction

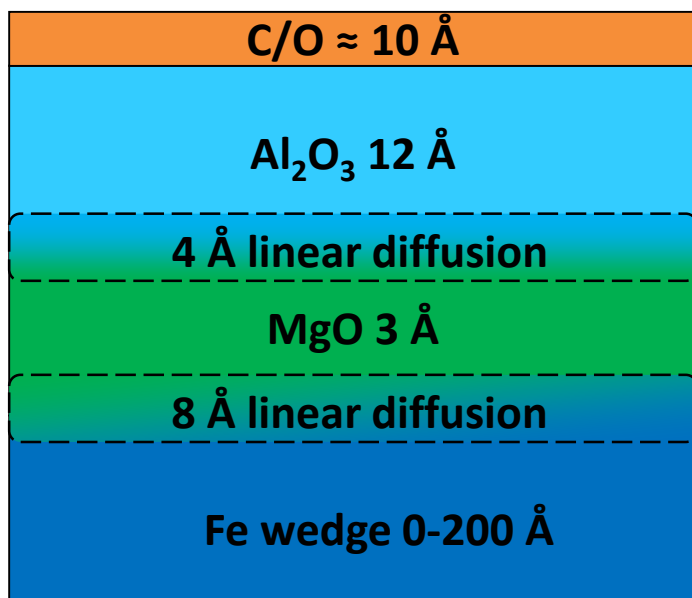


Balke, Yang et al., Phys. Rev. B 84, 184410 (2011)

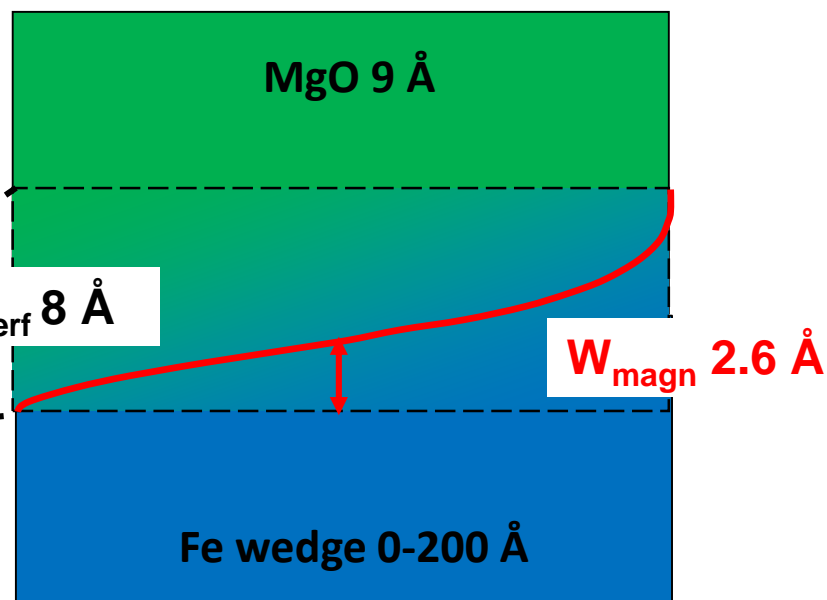
# Soft x-ray standing-wave wedge scans through a magnetic tunnel junction



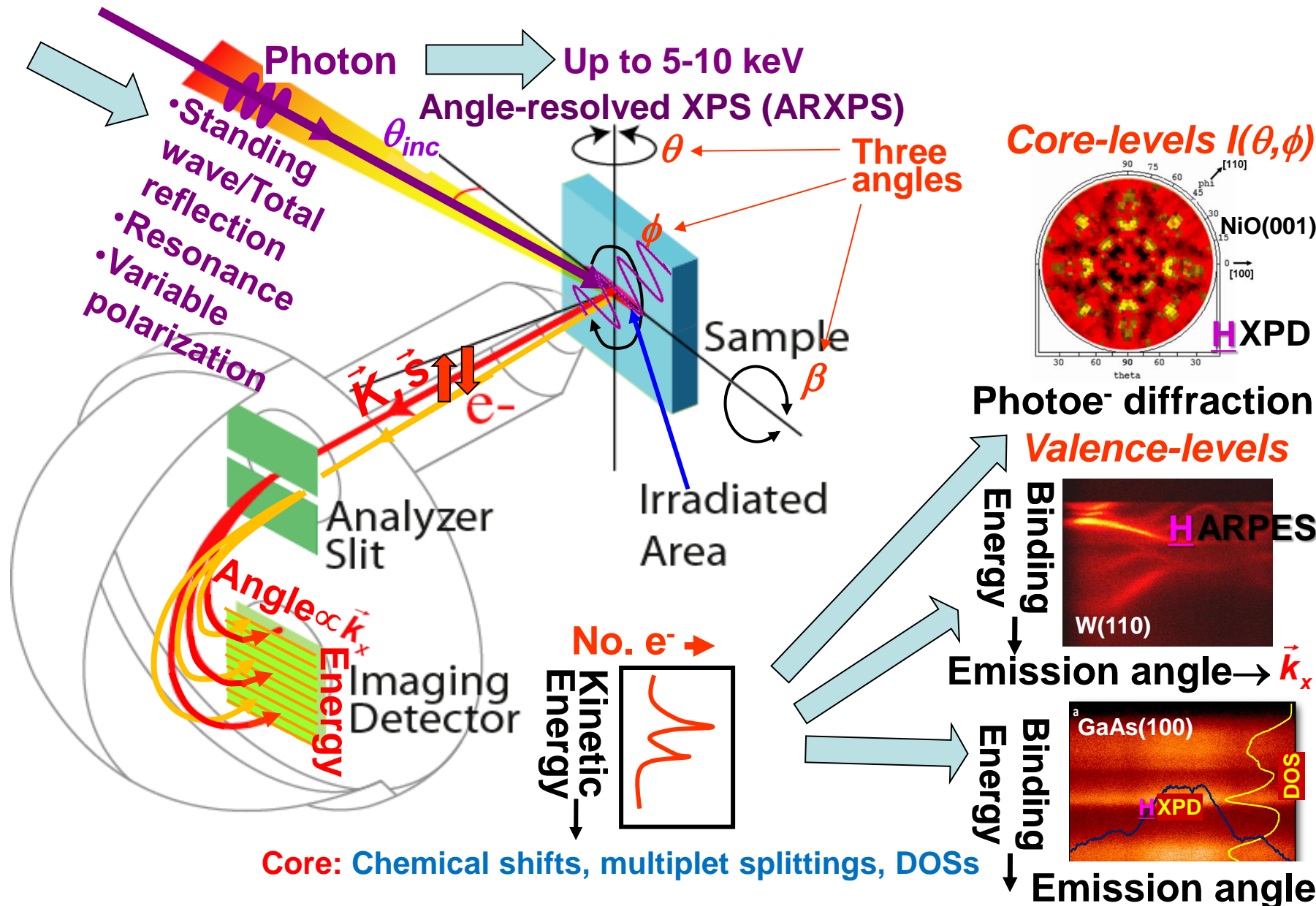
## Concentration



## Magnetization

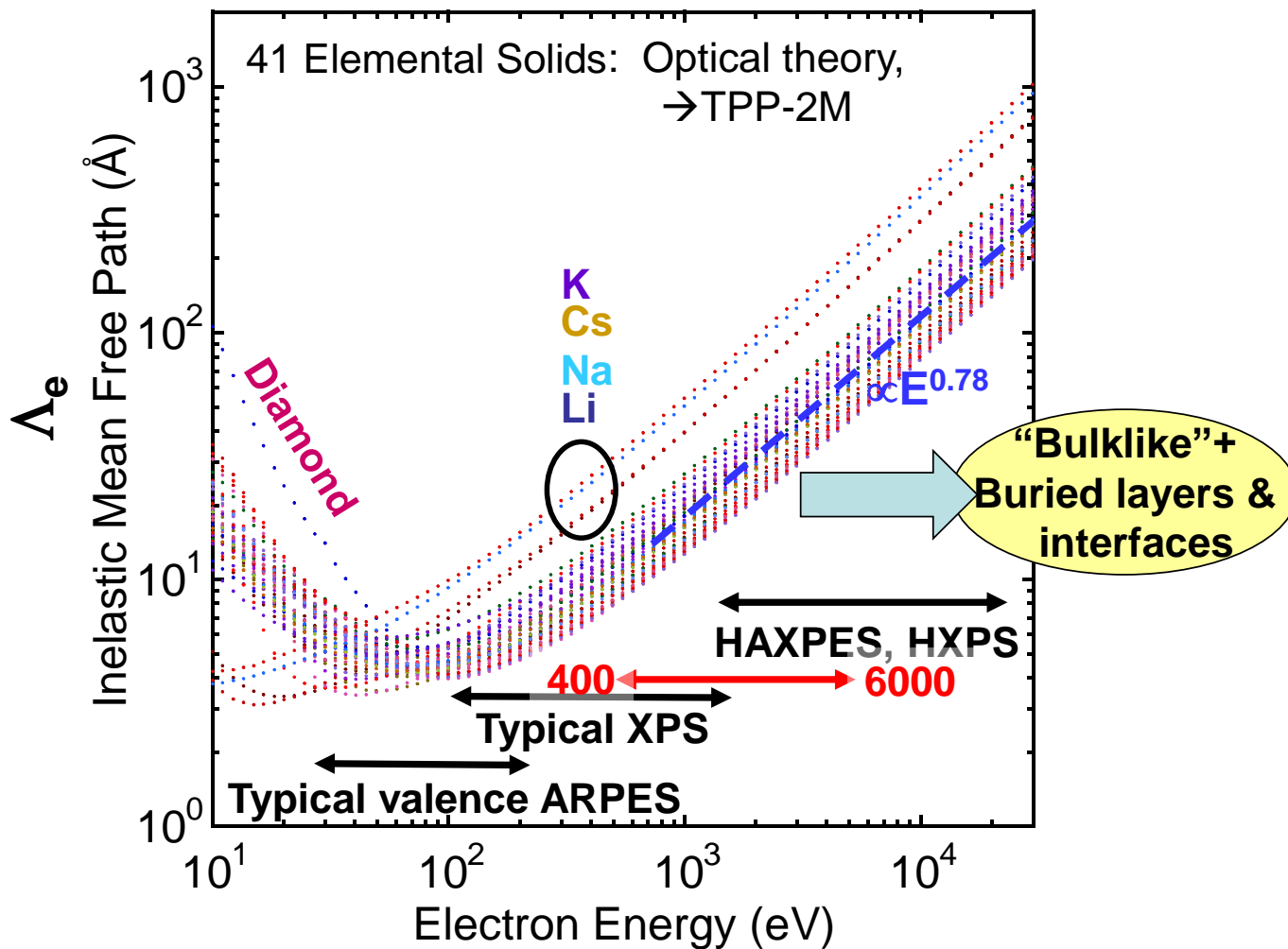


# Photoelectron spectroscopy: the various dimensions





# The reason for higher photon energies

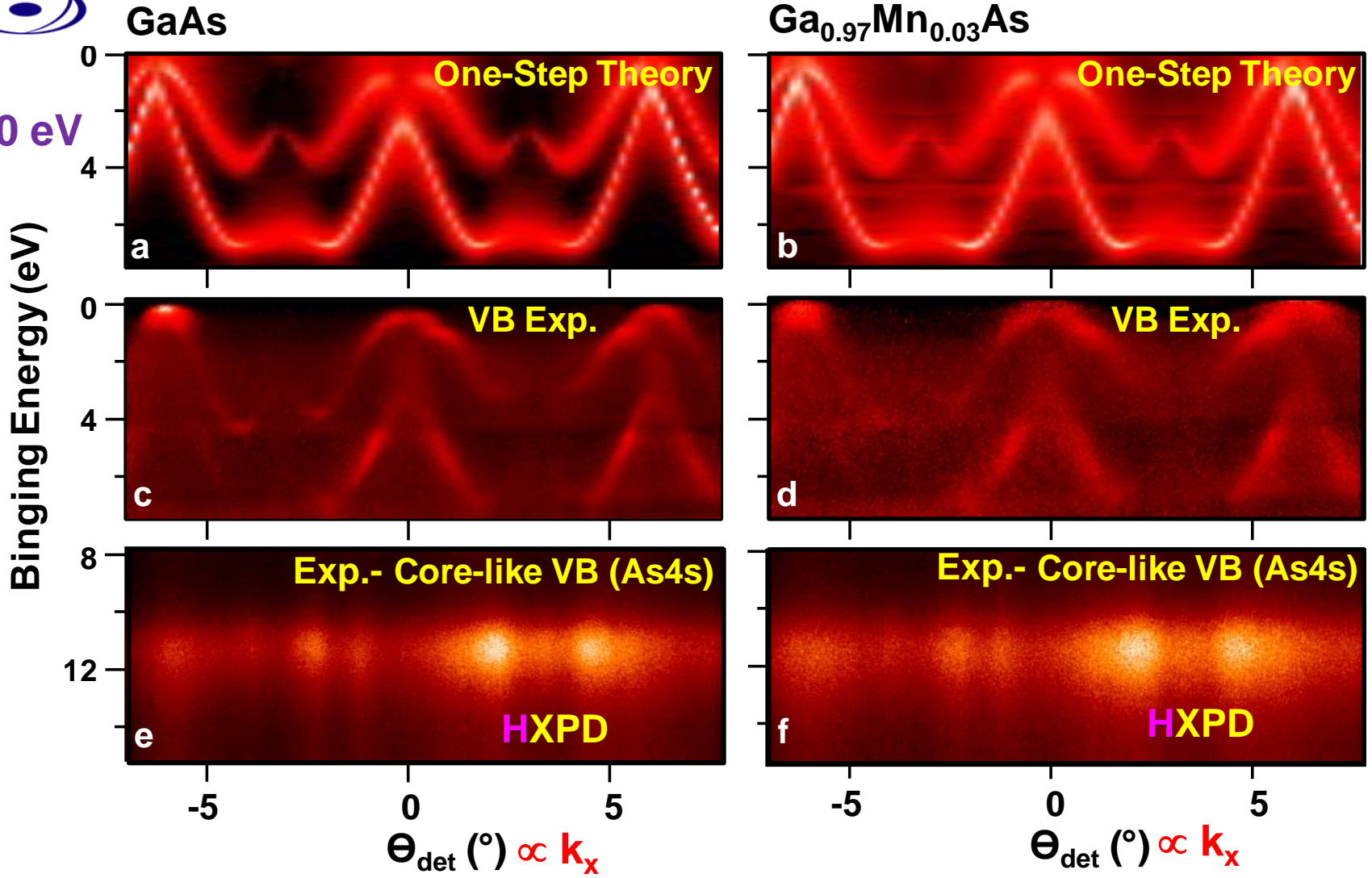


Tanuma, Powell, Penn, Surf. and Interf. Anal. 43, 689 (2011)

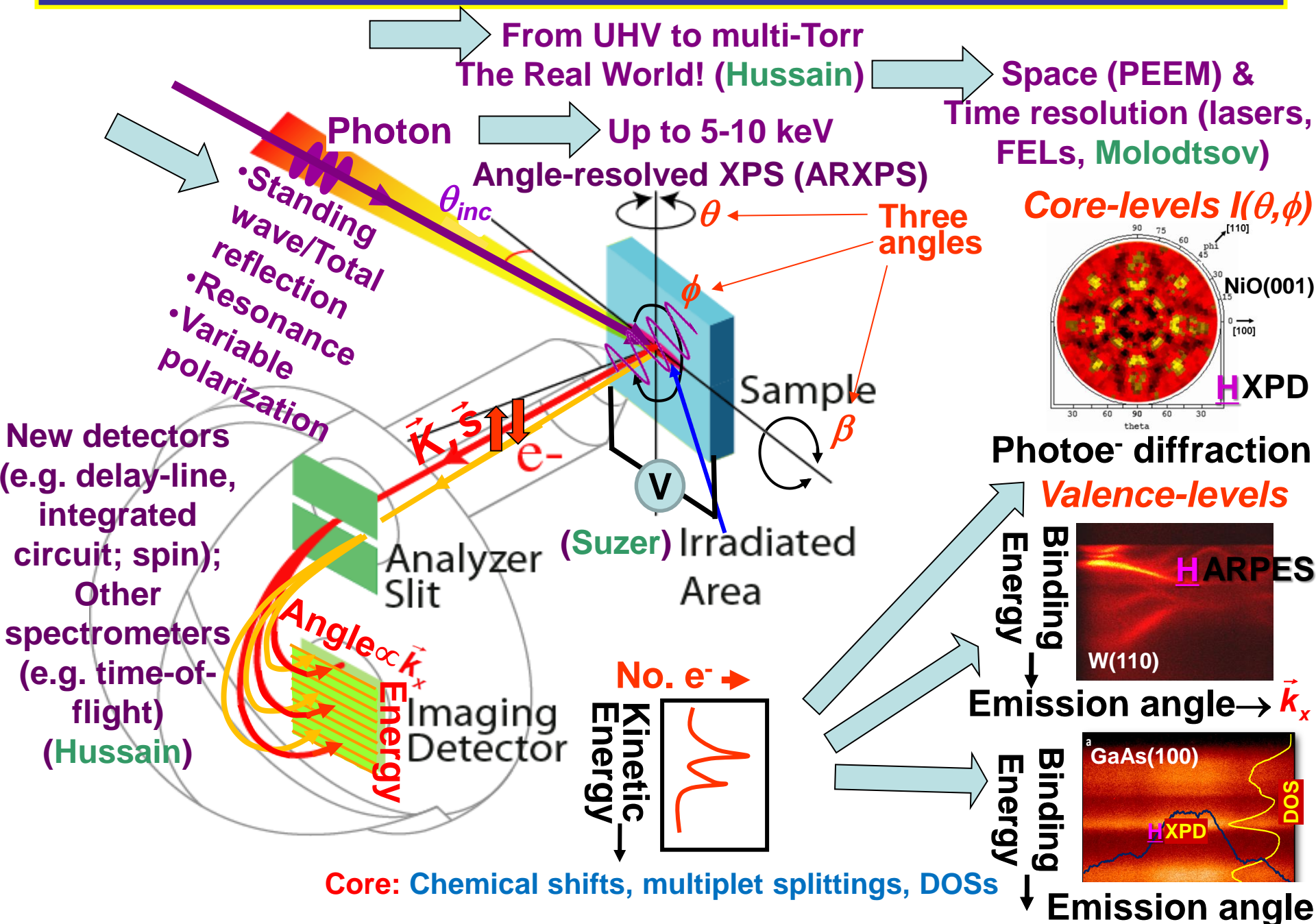
# Hard x-ray ARPES--GaAs and DMS $\text{Ga}_{0.97}\text{Mn}_{0.03}\text{As}$ Comparing Experiment and One-Step KKR Theory



3,200 eV



# Photoelectron spectroscopy: the various dimensions





**Thank you Dave, for many creative ideas, your vision of the future, your good advice on many matters, and all that you have contributed to us, to UCB, LBNL, FUB, and the scientific community at large.**

