XIV School on Synchrotron Radiation:
*Fundamentals, Methods and Applications*
Muggia, Italy / 18-29 September 2017

SILS
SOCIETA' ITALIANA DI LUCE DI SINCROTRONE

Elettra Sincrotrone Trieste

# Photoemission Spectroscopy: Fundamental Aspects

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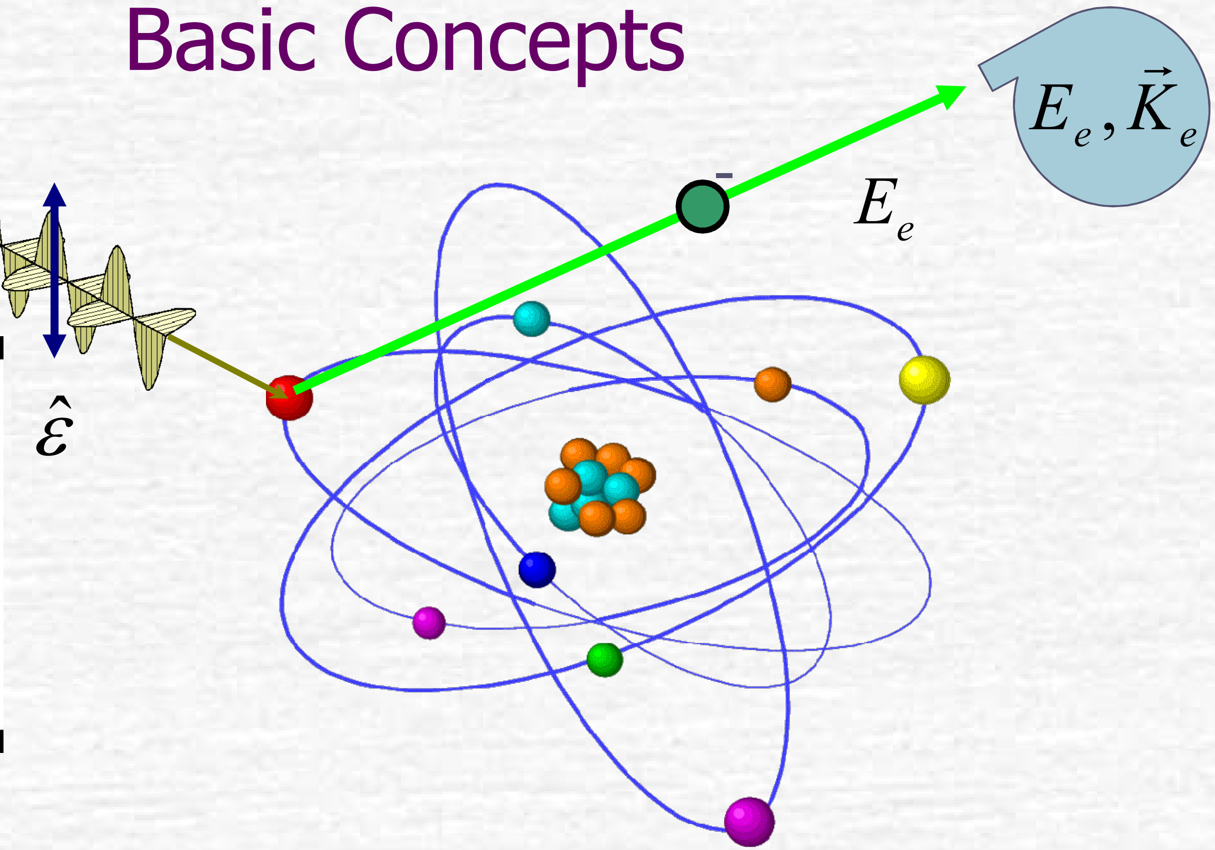
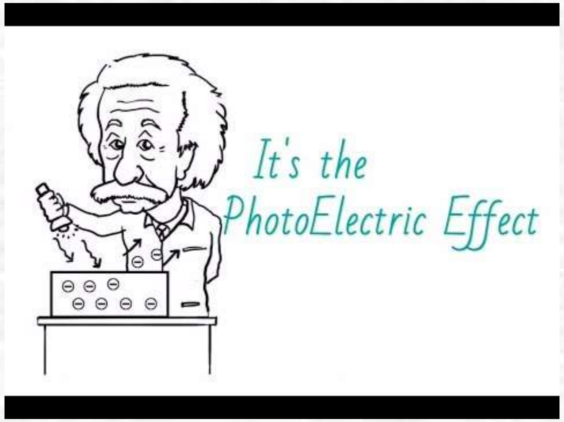
CNISM Unita' di Ricerca di Roma 3

EUSpec

# Basic Concepts





$$E_e^{MAX} = h\nu - \Phi$$

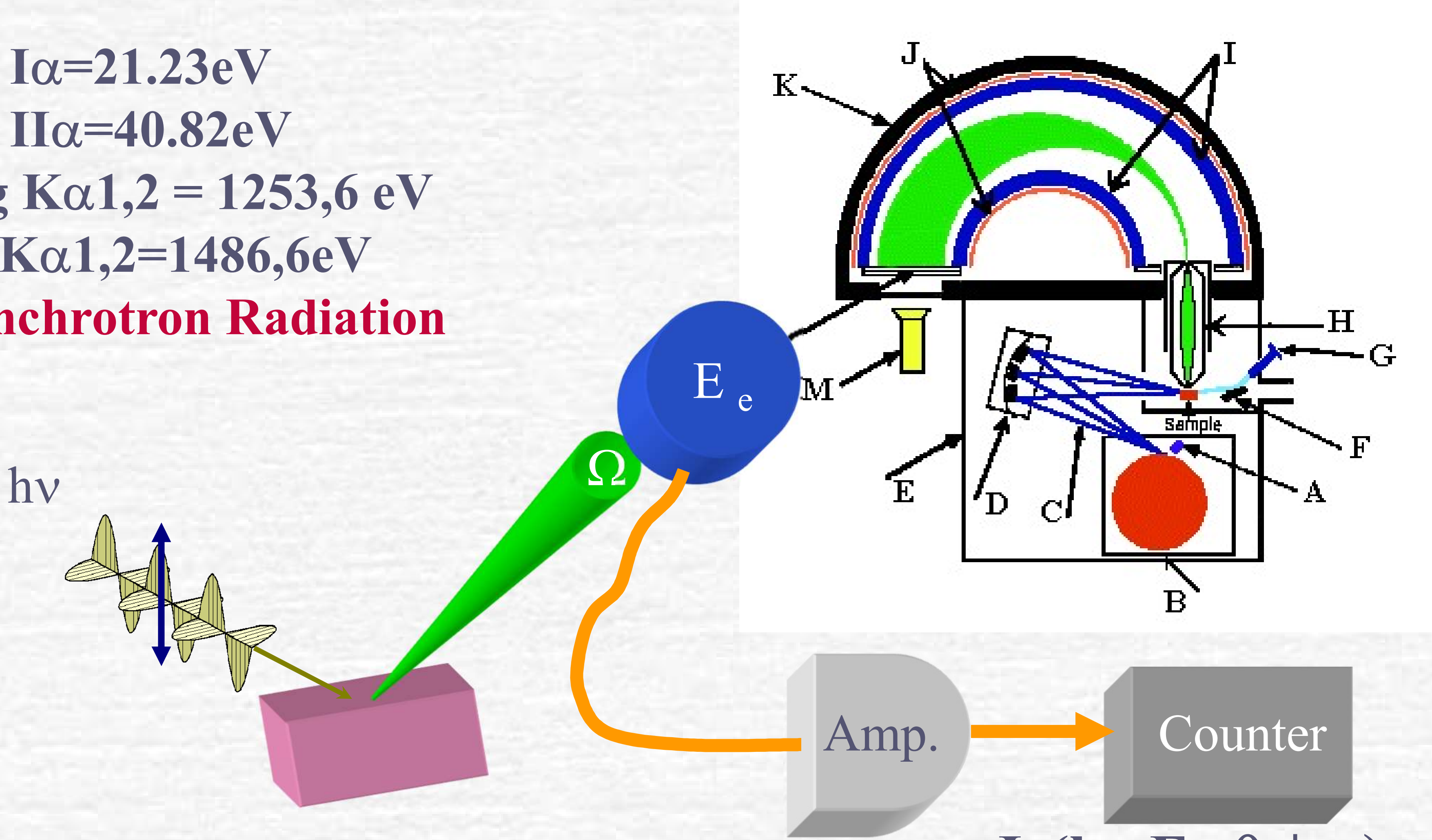
$$E_e = h\nu - \Phi - \Delta energy$$

# Outline

1. Photoelectron energy and bound state energy
2. Satellite structures and multiplet splitting
3. Chemical shift
4. Molecular photoelectron spectra
5. Photoelectron angular distributions
6. Hole state relaxation
7. Photoemission in solids
8. EDC and core ionization
9. Angular resolved PES
10. High energy photoemission HAXPES

# Photoemission Schematics:

**He Iα=21.23eV**
**He IIα=40.82eV**
**Mg Kα1,2 = 1253,6 eV**
**Al Kα1,2=1486,6eV**
**Synchrotron Radiation**



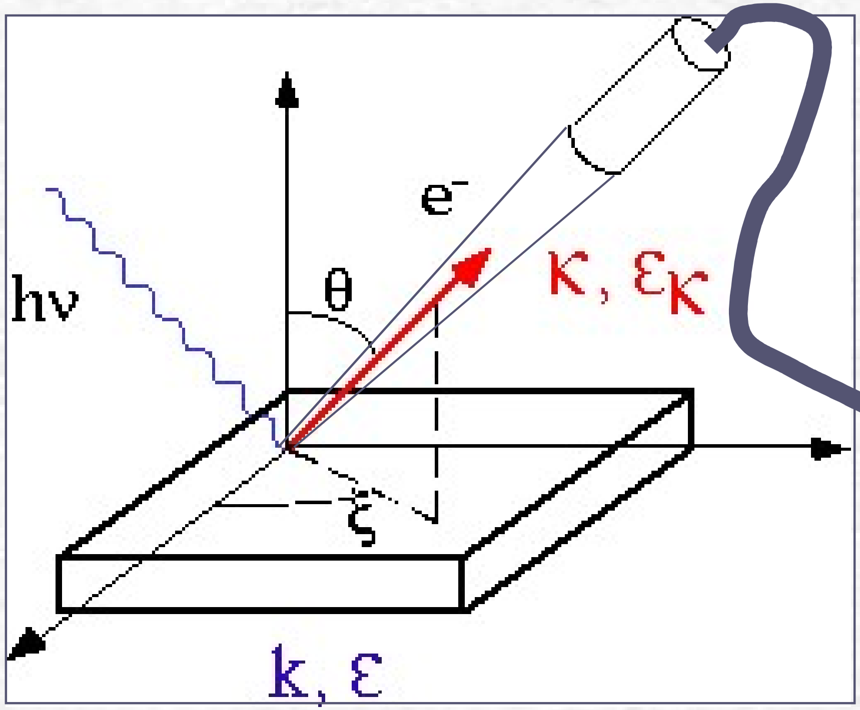
$$J_e(h\nu, E_e, \theta, \phi, \sigma)$$

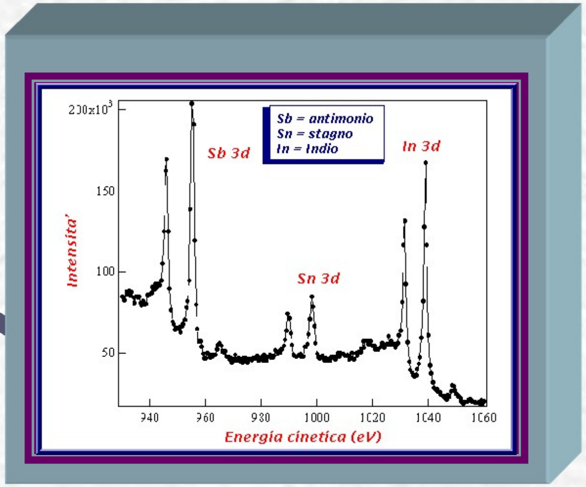
# ENERGY CONSERVATION, BINDING ENERGY AND PHOTOELECTRON ENERGY

$$E_{kin} = \hbar\omega - \phi - |E_b|$$

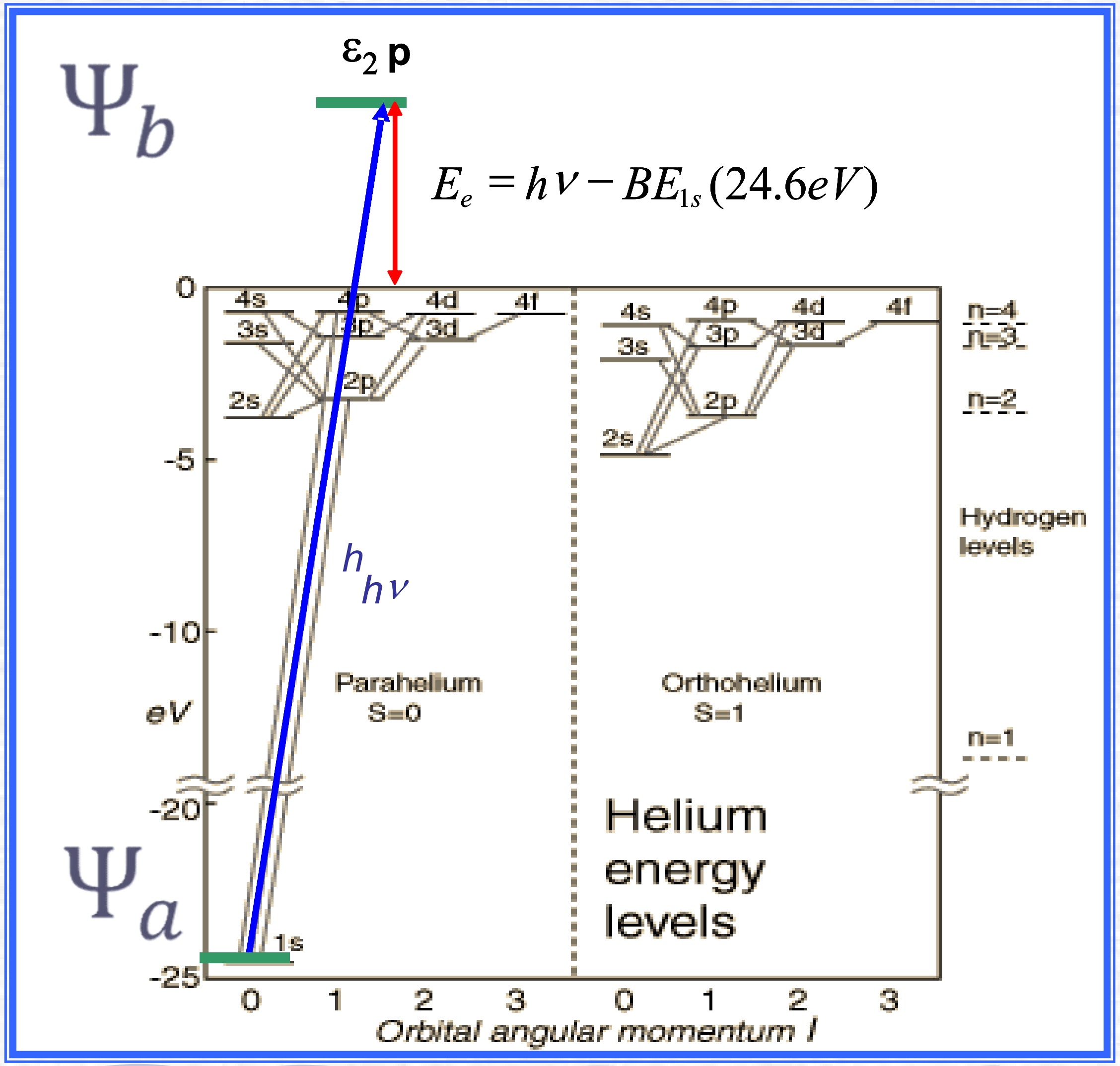
$$E_{kin} = \frac{p^2}{2m}$$

$$p = \sqrt{2mE_{kin}}$$





# The photoemission process



$$E_e = h\nu - BE_{1s}(24.6eV)$$

$$\left|\Psi_a\right\rangle$$

$$1s^2$$

$$^1S_0$$

# Interaction radiation matter and transition probability

$$\frac{d\sigma}{dh\nu} = 4\pi^2 \alpha h\nu \sum_B \left| \hat{\varepsilon} \bullet \left\langle \Psi_B \middle| \sum_i \vec{r}_i \middle| \Psi_A \right\rangle \right|^2 \delta(E_B - E_A - h\nu)$$

Bertoni's lectures at this school

Initial state A = Neutral ground(excited) state
Final state B = Residual ion + free electron(s)

$$\frac{d\sigma}{dh\nu} = \int_E \int_\Omega \frac{d\sigma}{d\Omega dE} d\Omega dE$$

# X-section vs. Photoemission current

$$J_e(h\nu,\vartheta,\phi)=J_{h\nu}(\rho l)\int_{\Delta E}\int_{\Delta\Omega}\frac{d\sigma}{d\Omega dE}F_{an}(E,\Omega)\eta_{\det}(E)d\Omega dE$$

**Photoemission peak lineshape**

| | | |
|---|---|---|
| 1. | Photon monochromaticity | Gaussian |
| 2. | Electron analyzer resolution | Gaussian |
| 3. | Final state lifetime (uncertainty principle) | Lorentian |

**Lineshape =Convolution (1,2,3)**

# Energy balance for 2e atom

$$\boxed{E_B = E_A + h\nu}$$

$$\boxed{\Psi_A = \hat{A}\phi_1\phi_2}$$

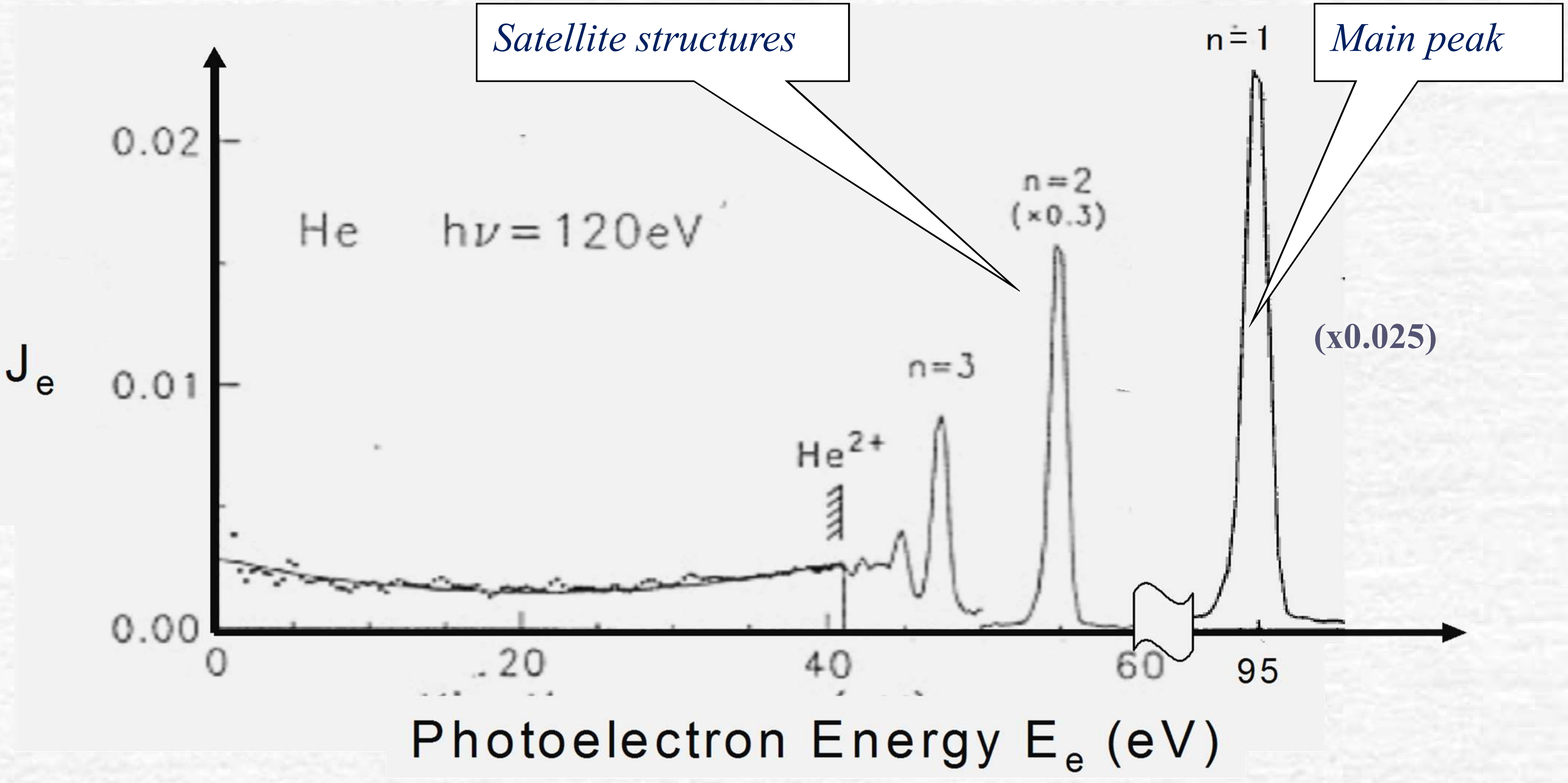
$$\boxed{\Psi_B = \hat{A}\phi_1\varepsilon_2}$$

$$\boxed{\cancel{E_{1s}} + E_e = \cancel{E_{1s}} + E_{1s} + h\nu}$$

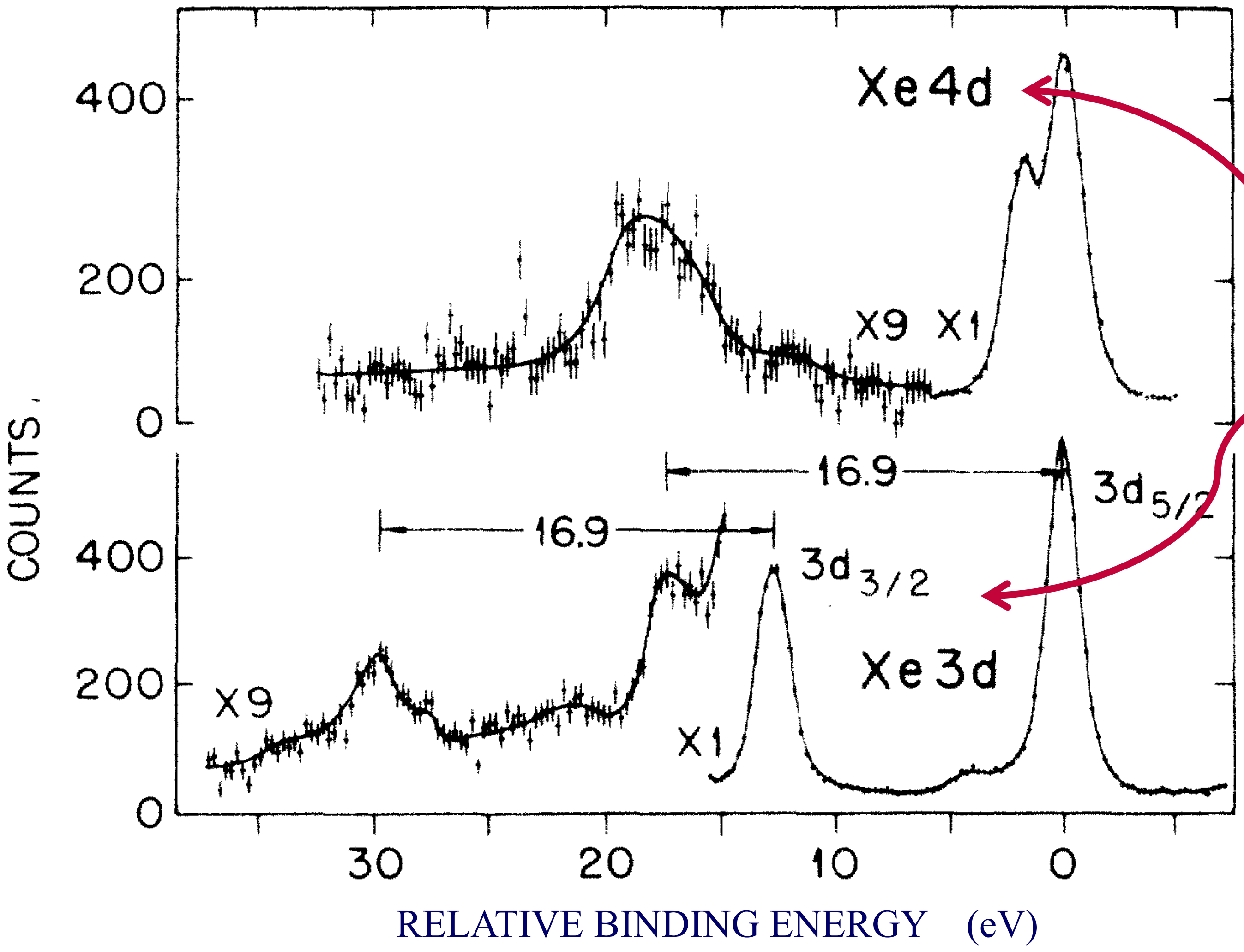
$$\boxed{E_e = h\nu - BE_{1s}(24.6eV)}$$

One single photoemission peak is expected
Energy and momentum are conserved

# Complexity of the photoemission spectrum



# How complex can it  be?

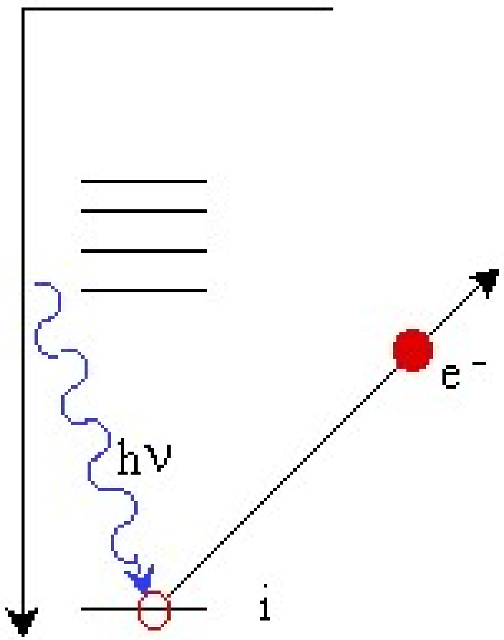


[Ar] 3d$^{10}$
4s$^{2}$ 4p$^{6}$ 4d$^{10}$
5s$^{2}$ 5p$^{6}$

PHYSICAL RE V IEW A VOLUME 9, NUMBER 4 APRIL 1974 1603

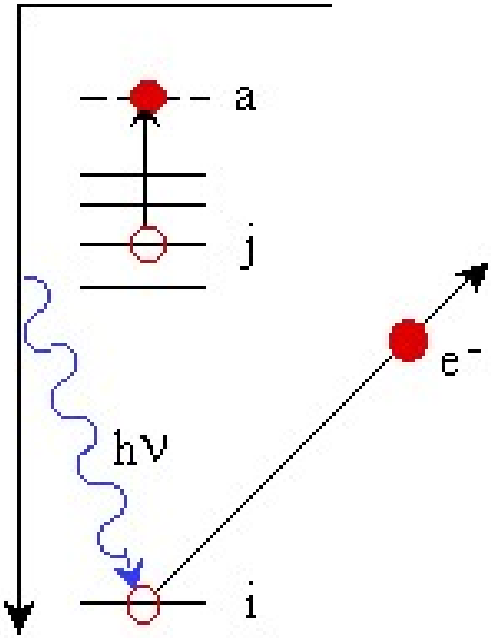
# Primary photoionization processes

MAIN PROCESS



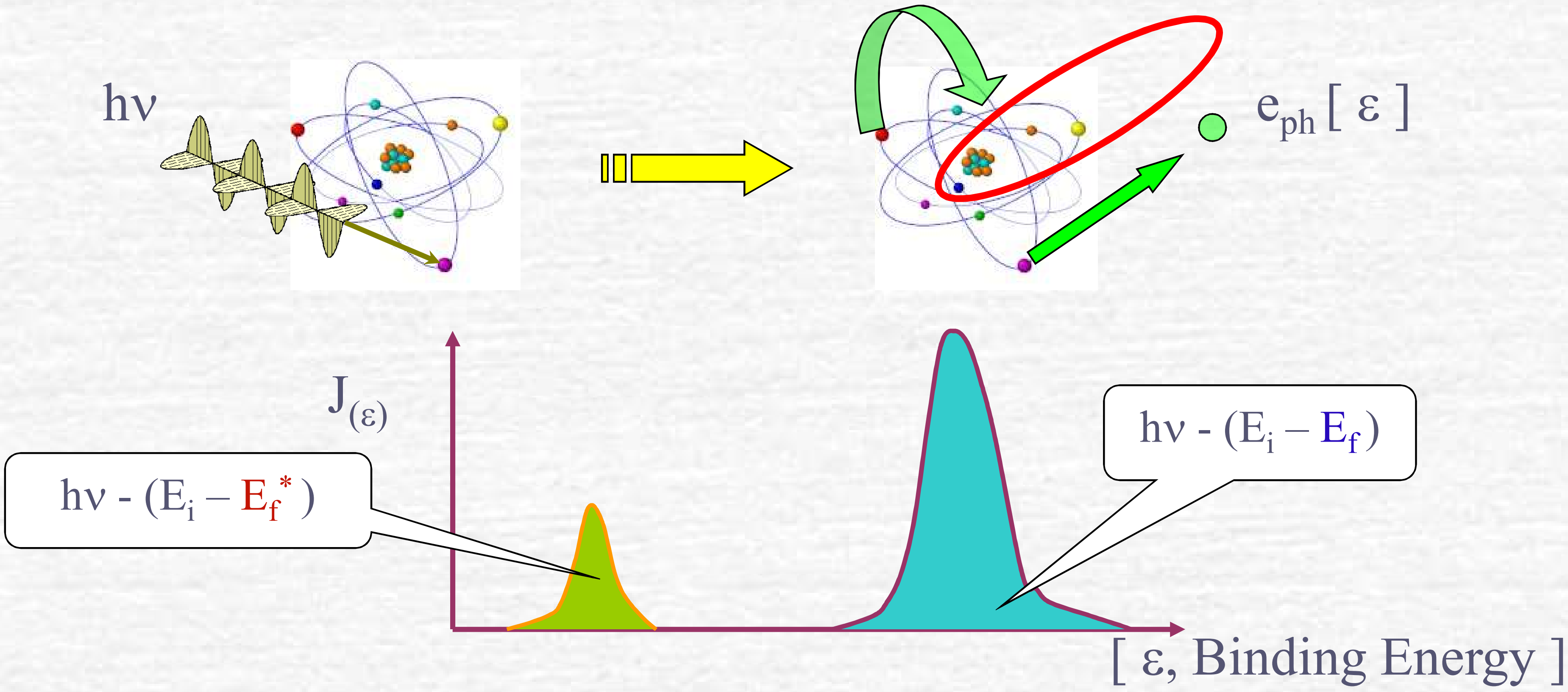
$M + h\nu \rightarrow M^{+} + e^{-}$

SATELLITE PROCESS

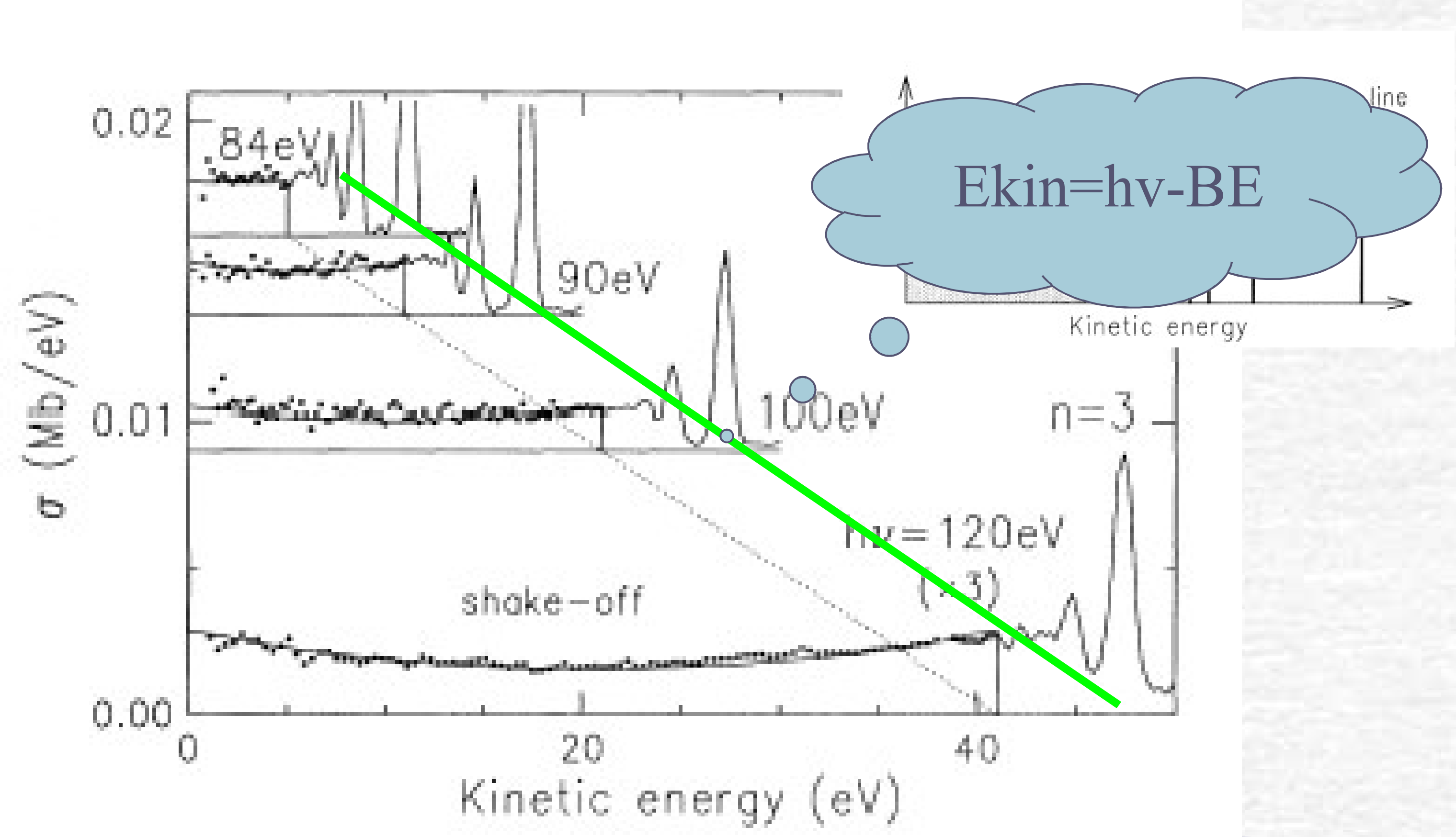


$M + h\nu \rightarrow M^{+*} + e^{-}$

- Photon = single particle operator
- 2 or more particles involved in final state = e-e correlation
- Relaxation & e-e correlation in photoemission = satellite



# The He satellite structure


Ekin=hv-BE

# A many electron atom

$$H_0\left|\Psi_A^{(N)}\right\rangle = E_A^{(N)}\left|\Psi_A^{(N)}\right\rangle$$

$$H_0 = H_0(kin) + H_0(e-n) + H_0(e-e) + H_0(s-o) =$$

$$= \sum_1^N \frac{p_i^2}{2m} + \sum_1^N -\frac{Ze^2}{r_i} + \sum_{i>j}^N \frac{e^2}{r_{ij}} + \sum_1^N \zeta(r_j)\vec{l}_i \bullet \vec{s}_i$$

$$\left|\Psi_A^{(N)}\right\rangle = \widehat{A}(\phi_j(\vec{r}_i,\sigma_i);\Psi_R^{(N-1)})$$

Single particle orbital

$$H_0^{'}\left|\Psi_B^{(N)}\right\rangle = E_B^{(N)}\left|\Psi_B^{(N)}\right\rangle$$

# sudden approximation

Neglect nucleus motion

$$\Psi_B^{(N)}\rangle = \hat{A}(\varepsilon_l ; |\Psi_B^{(N-1)}\rangle)$$

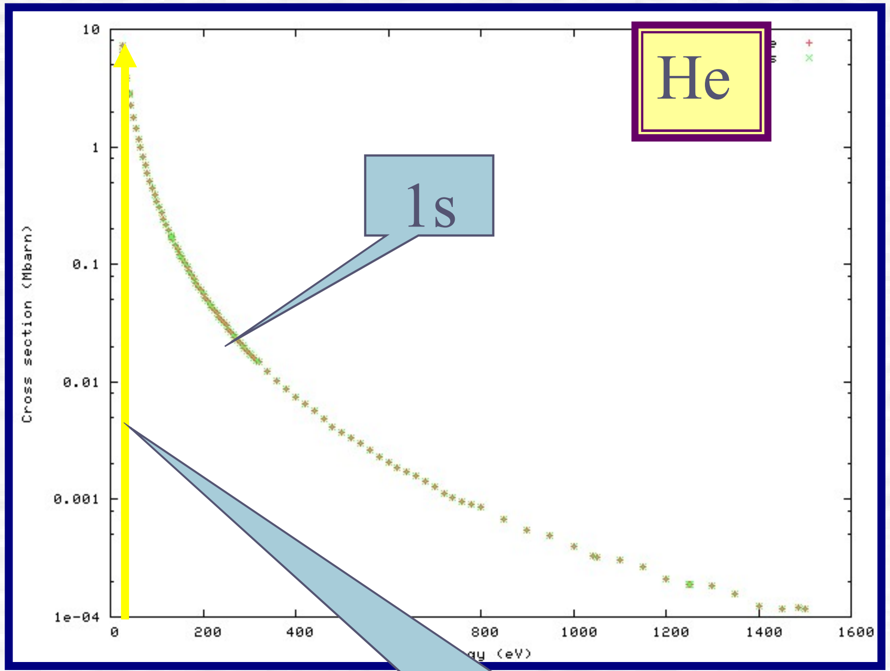
$$\frac{d\sigma}{d\Omega dE_e} \propto \frac{1}{h\nu}\sum_{A,B}\left|\hat{\varepsilon}\bullet\langle\varepsilon_l|\vec{r}_j|\phi_j(\vec{r}_j,\sigma_j)\rangle\langle\Psi_B^{(N-1)}|\Psi_R^{(N-1)}\rangle\right|^2 \delta(E_e + E_B^{(N-1)} - E_A - h\nu)$$

# frozen core approvimation

$$H_0^{'} = H_0$$

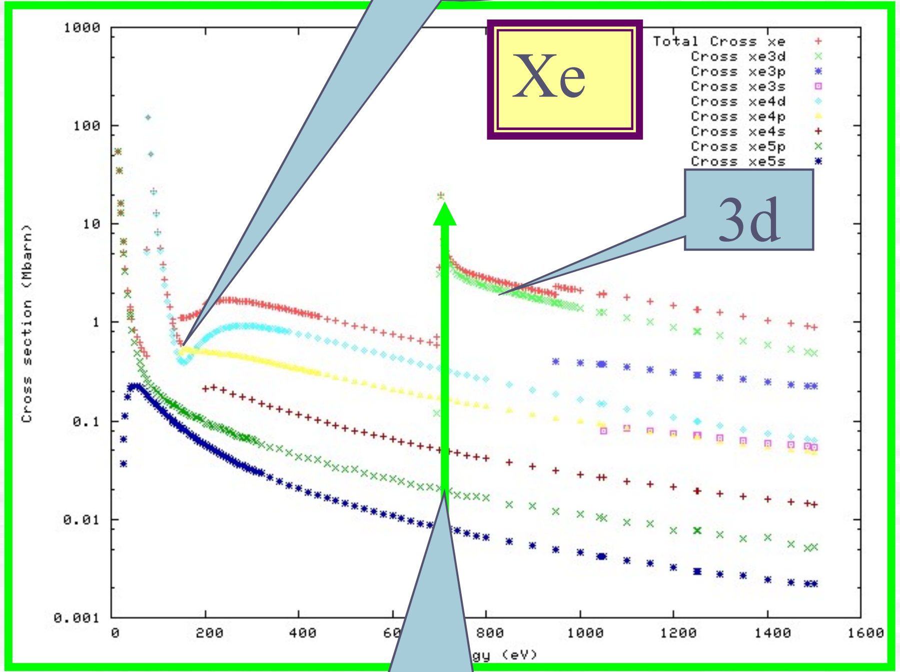
$$\frac{d\sigma}{d\Omega dE_e} \propto \frac{1}{h\nu}\sum_{A,B}\left|\hat{\varepsilon}\bullet\langle\varepsilon_l|\vec{r}_j|\phi_j(\vec{r}_j,\sigma_j)\rangle\right|^2 \delta(E_e + \varepsilon_j - h\nu)$$

# Total photoemission cross section



1s

1s Threshold

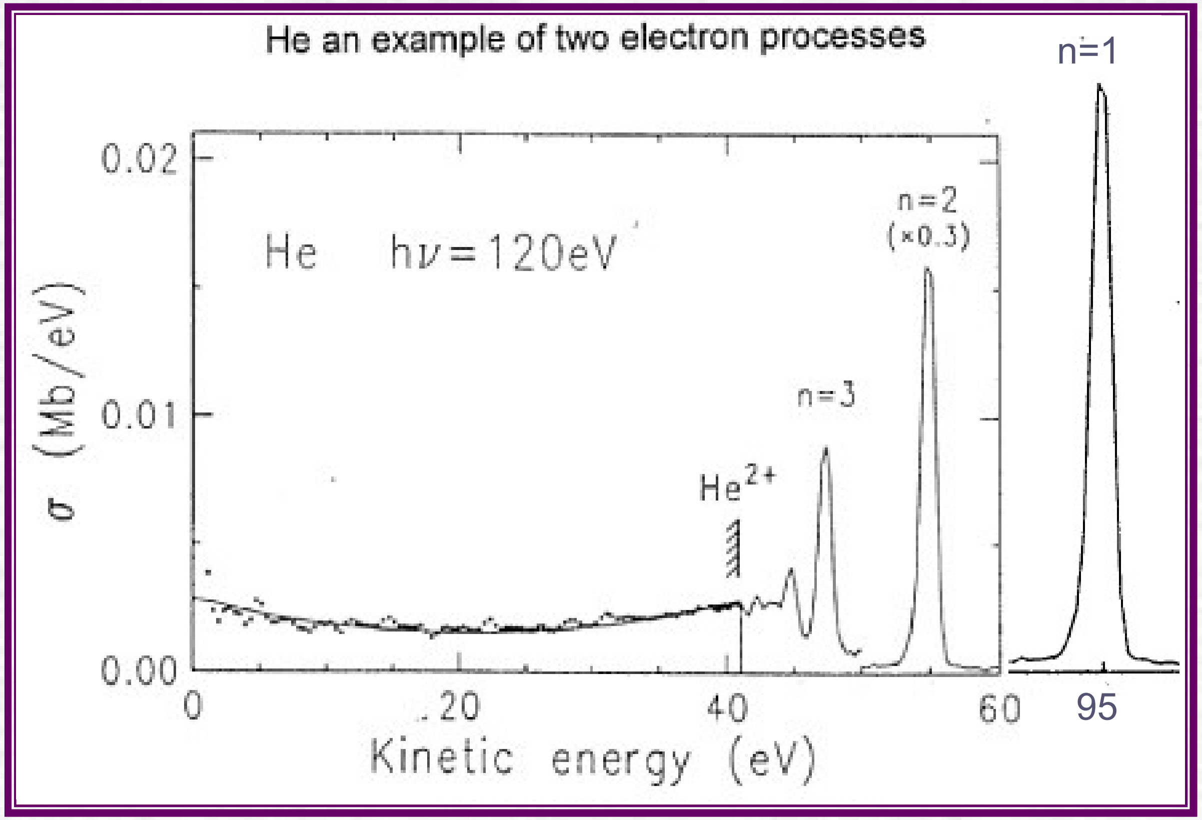


4d Cooper minimum

3d

3d Threshold

# Photoelectron current vs. photoelectron energy


He an example of two electron processes

Monopole and dipole selection rules

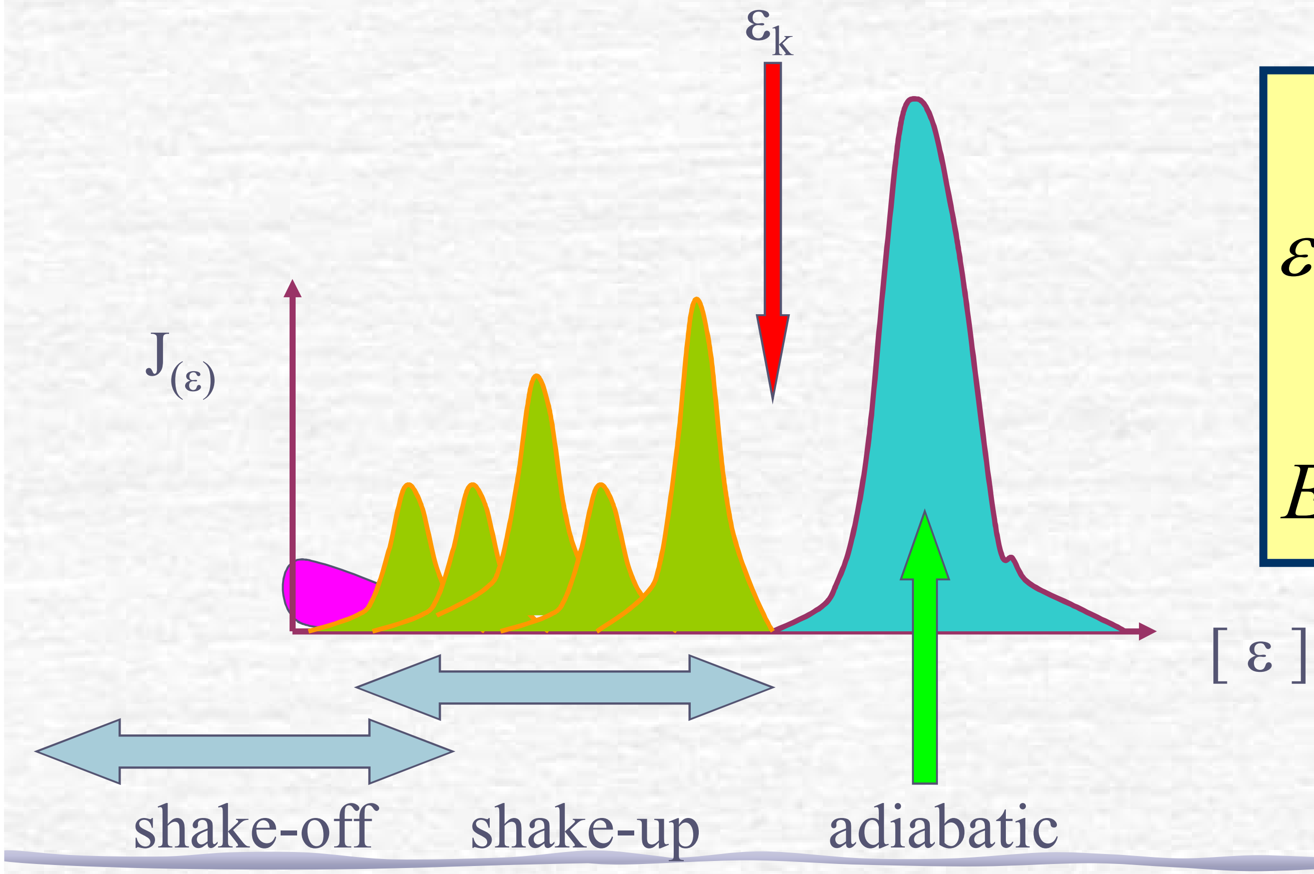
$$h\nu + He(1s^2) \rightarrow He^+(1s^1) + \varepsilon_{\ell=1}$$

$$h\nu + He(1s^2) \rightarrow He^+(2s^1) + \varepsilon_{\ell=1}, He^+(3s^1) + \varepsilon_{\ell=1}, He^+(4s^1) + \varepsilon_{\ell=1}, \ldots\ldots\ldots\ldots He^{++} + \varepsilon_{\ell} + \varepsilon_{\ell'}$$

$$h\nu + He(1s^2) \rightarrow He^+(2p^1) + \varepsilon_{\ell=0}, He^+(3p^1) + \varepsilon_{\ell=0}, He^+(4p^1) + \varepsilon_{\ell=0}, \ldots\ldots\ldots He^{++} + \varepsilon_{\ell} + \varepsilon_{\ell'}$$

# Koopmans energy vs. photoemission peaks

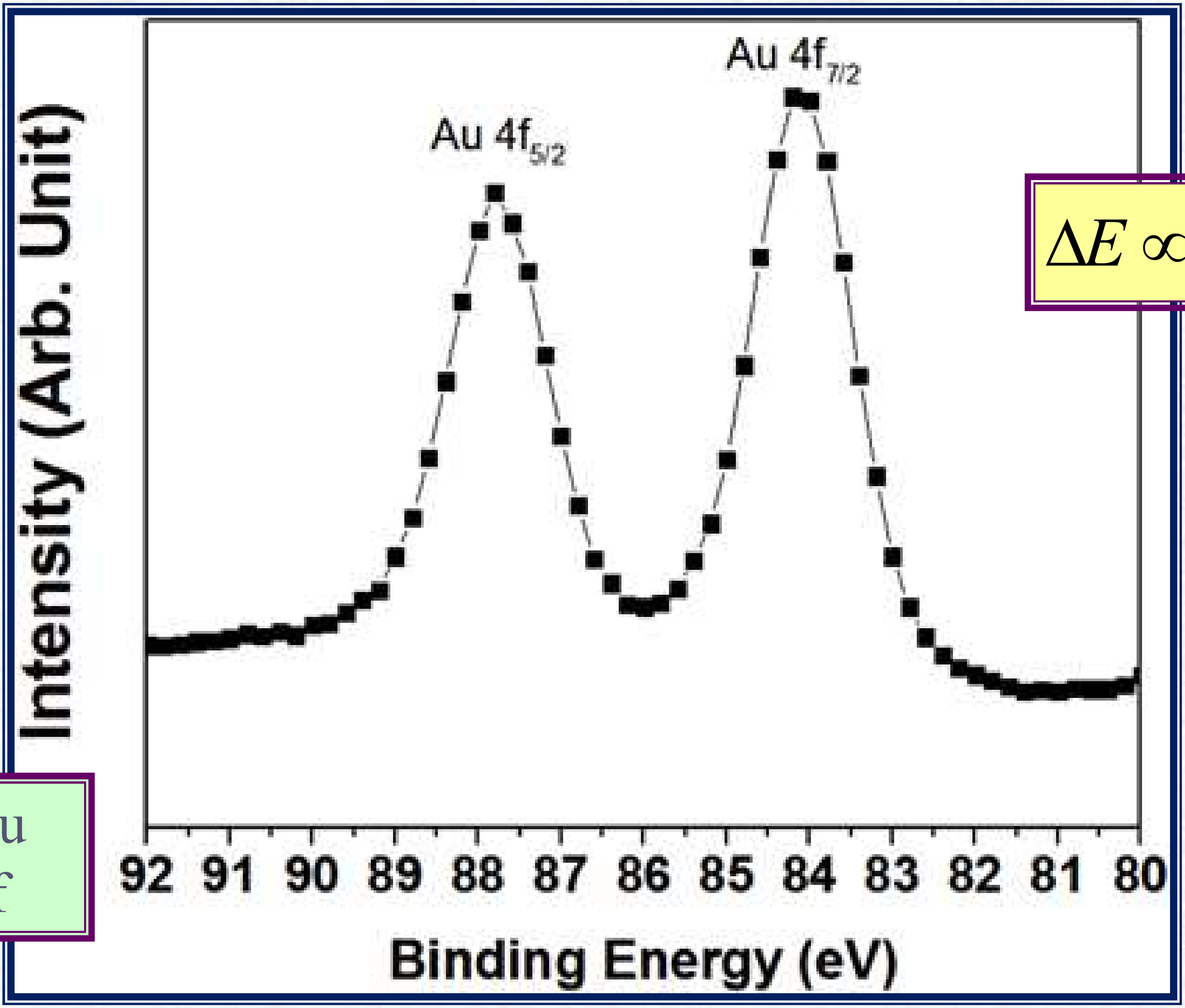
$$\frac{d\sigma}{d\Omega dE_e} \prec \frac{1}{h\nu}\sum_{A,B}\left|\hat{\varepsilon}\bullet\left\langle \varepsilon_l\left|\vec{r}_j\right|\phi_j(\vec{r}_j,\sigma_j)\right\rangle\left\langle \Psi_B^{(N-1)}\middle|\Psi_R^{(N-1)}\right\rangle\right|^2\delta(E_e+E_B^{(N-1)}-E_A-h\nu)$$



$$\varepsilon_k = \frac{\sum_i \varepsilon_i I_i}{\sum_i I_i}$$

$$E_{relax} = \varepsilon_{adiab} - \varepsilon_k$$

# Spin orbit splitting

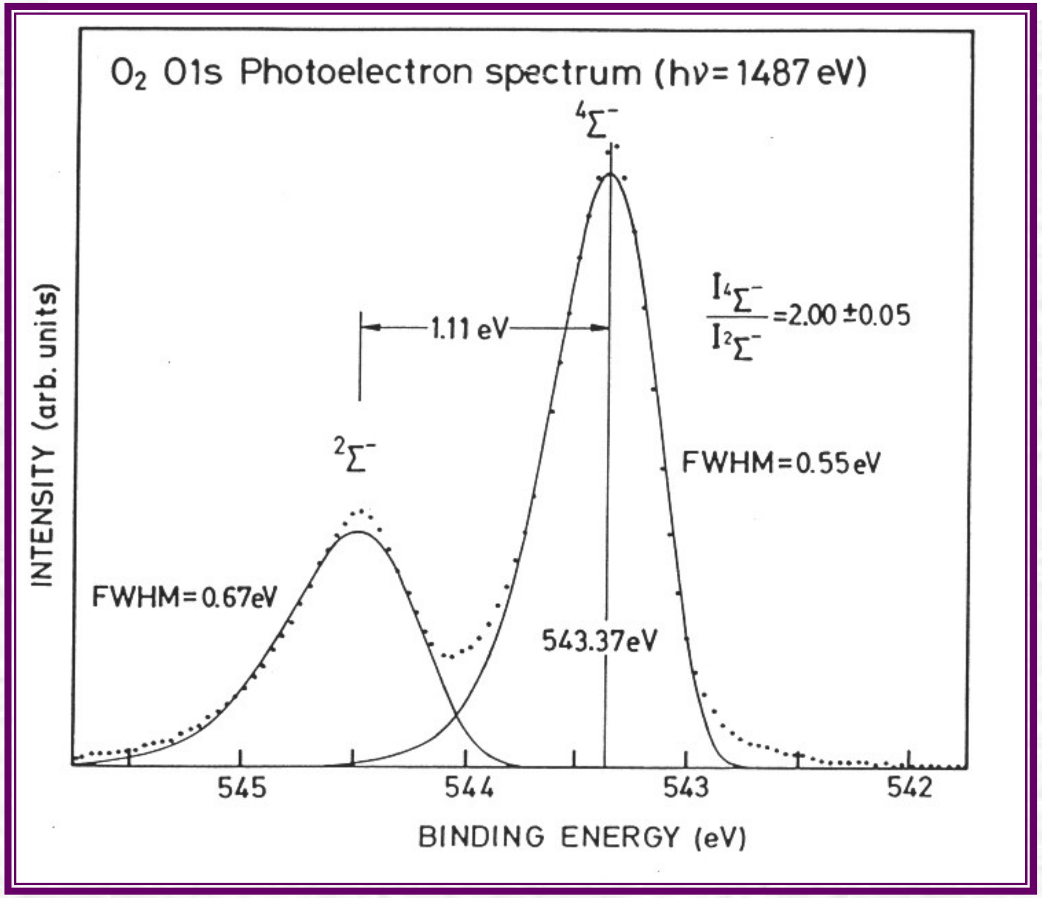


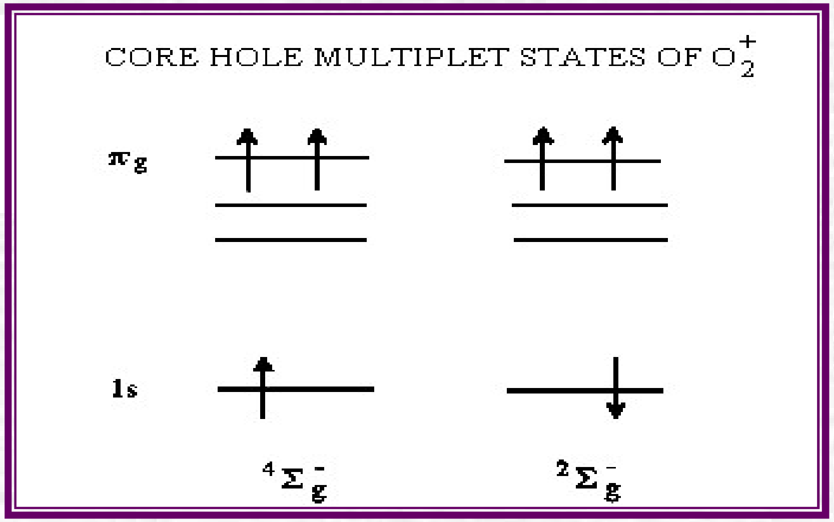
$$\Delta E \propto \vec{\ell}_i \bullet \vec{s}_i$$

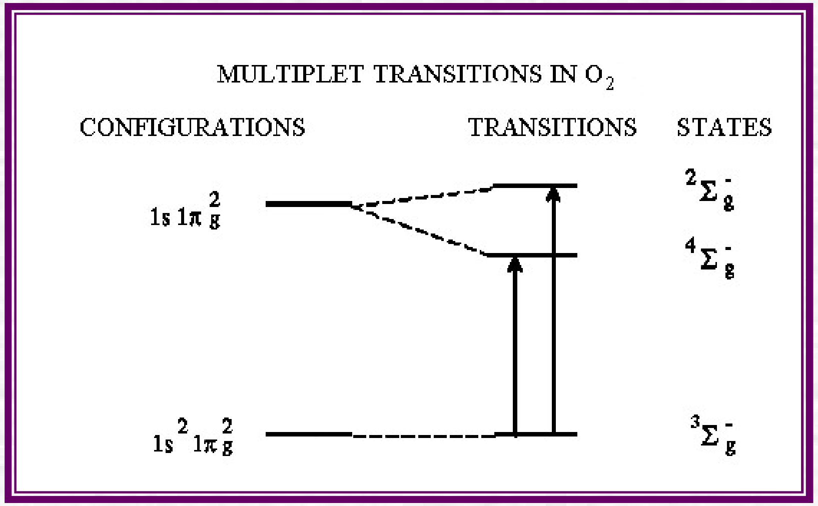
Au
4f

# Molecular multiplet splitting $O_2$

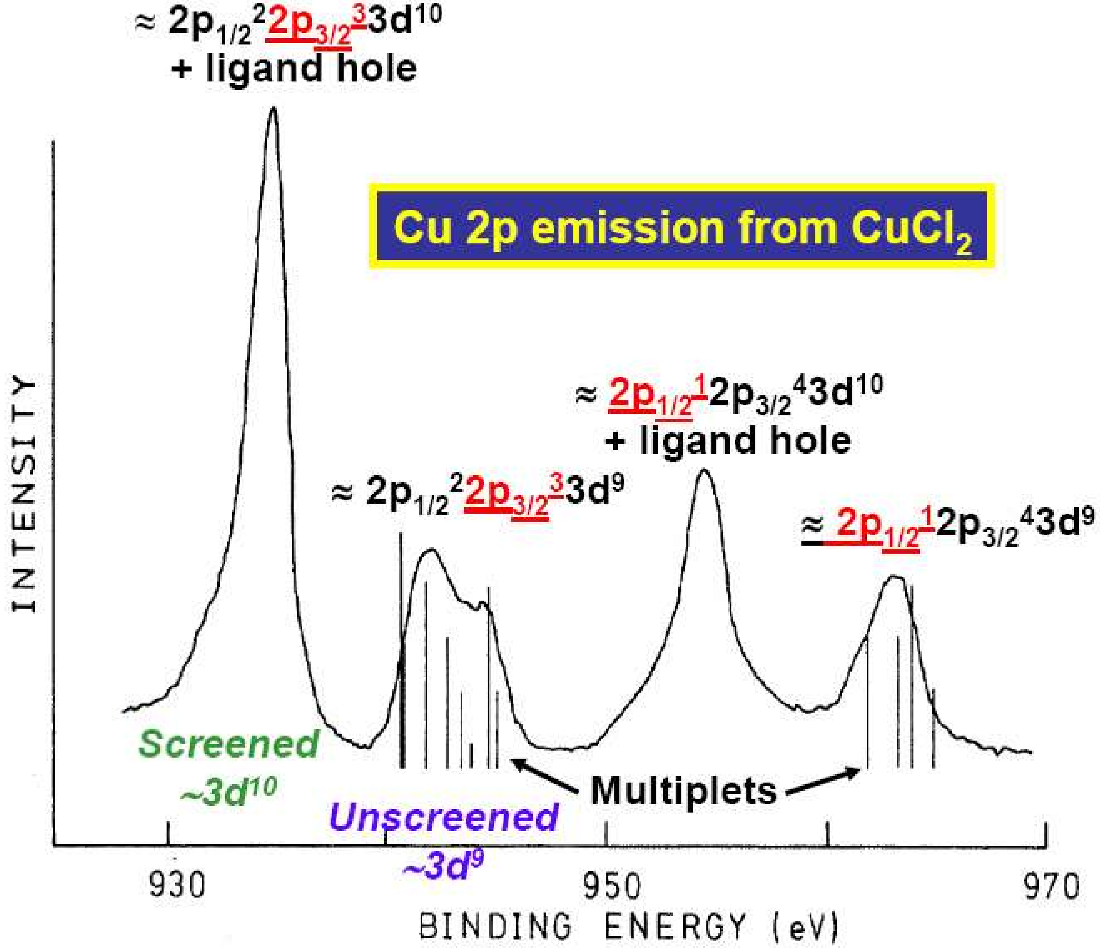
$$KK(\sigma_g 2s)^2\,(\sigma_u 2s)^2\,(\sigma_g 2p)^2\,(\pi_u 2p)^4\,(\pi_g 2p)^2\;\; {}^3\Sigma_g^-$$







# CuCl$_2$ multiplet & satellite

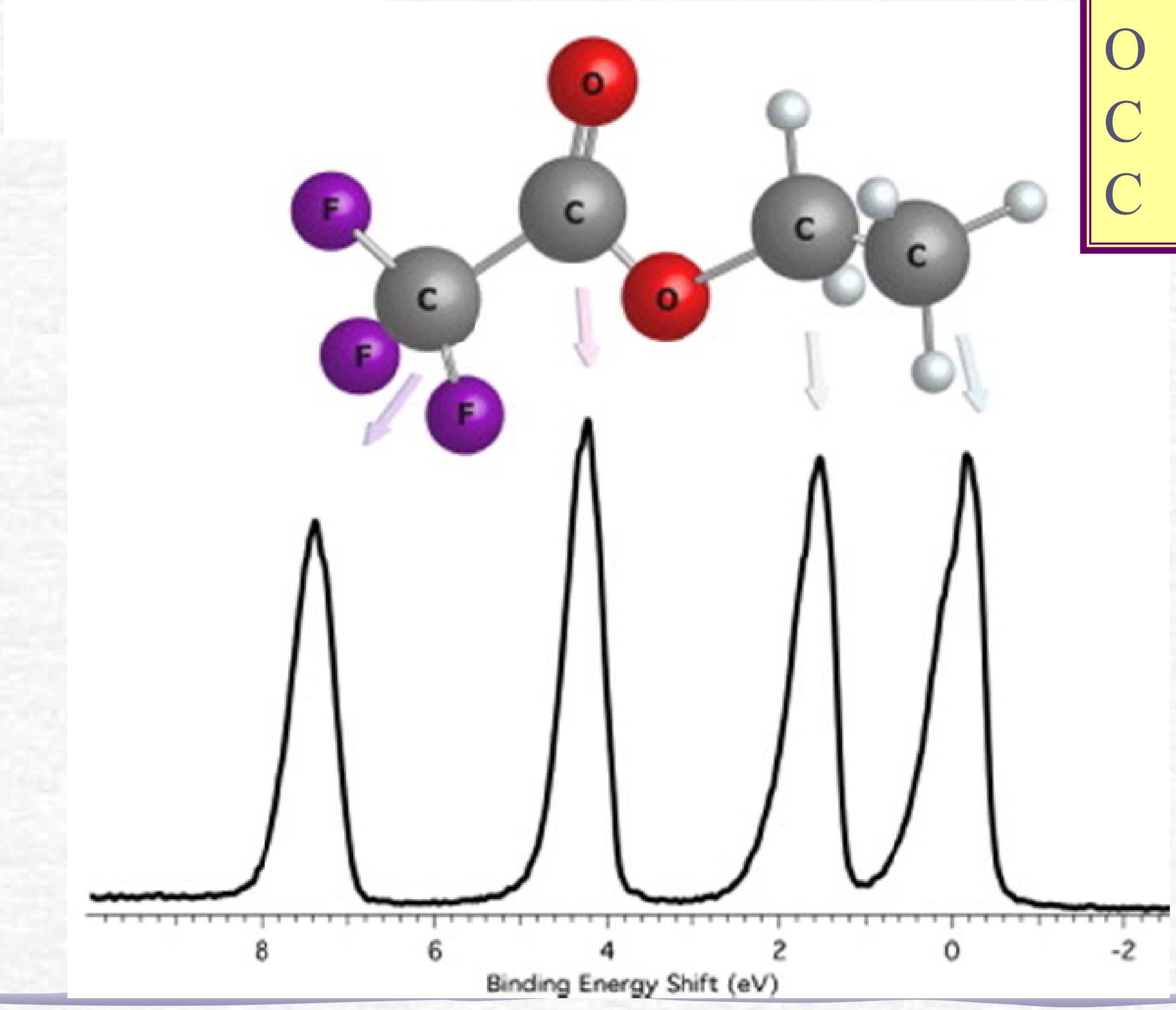


$$\Psi_{final,K}(N-1) = C_{1,K}(2p_{1/2}^2 2p_{3/2}^3 3d^{10} + C\ell\ \text{hole}) + C_{2,K}(2p_{1/2}^2 2p_{3/2}^3 3d^9)$$

Van der Laan et al., Phys. Rev. B 23 (1981) 4369

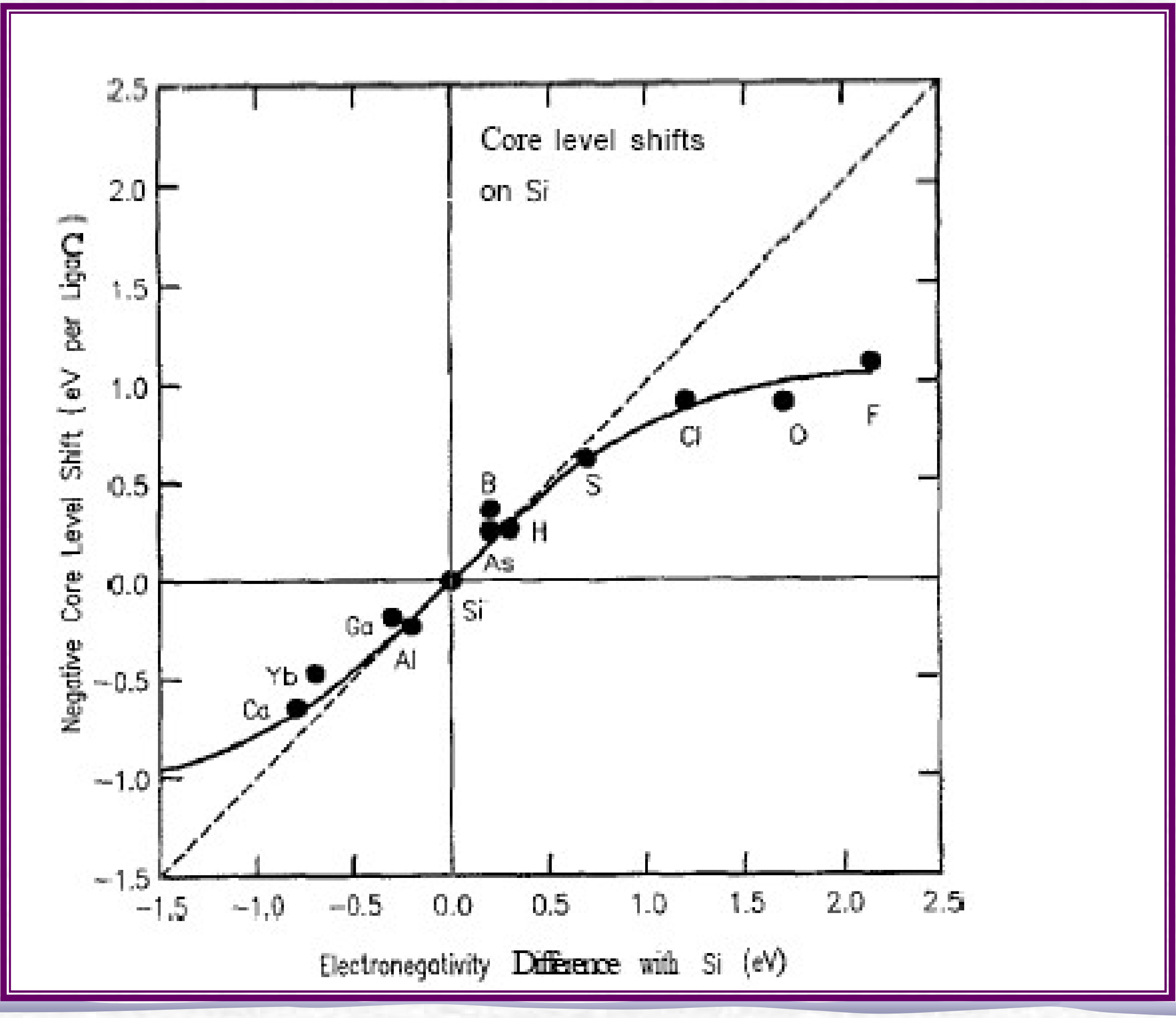
# Chemical shift

Journal of Electron Spectroscopy and Related Phenomena
Volume 185, Issues 8–9, September 2012, Pages 191–197

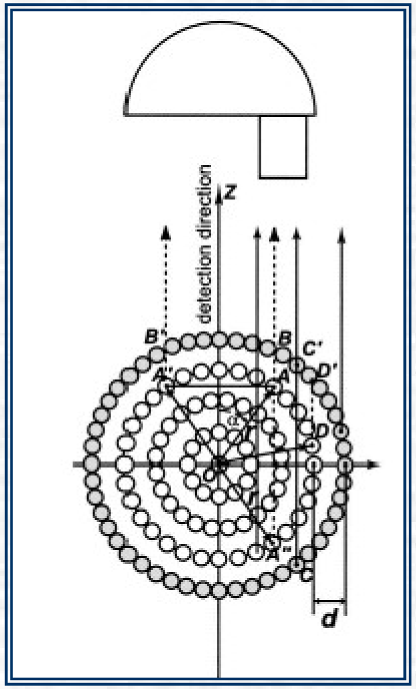


C 1s 285-300 eV
O 1s 530-540 eV
C 1s $CO_2$ 298 eV
C 1s $CH_4$ 291 eV

# Chemical shift vs.electronegativity



# Sensitivity to the local environment in free clusters



J. Chem. Phys.,
Vol. 120, No. 1, 1
January 2004

Tchaplyguine et al.

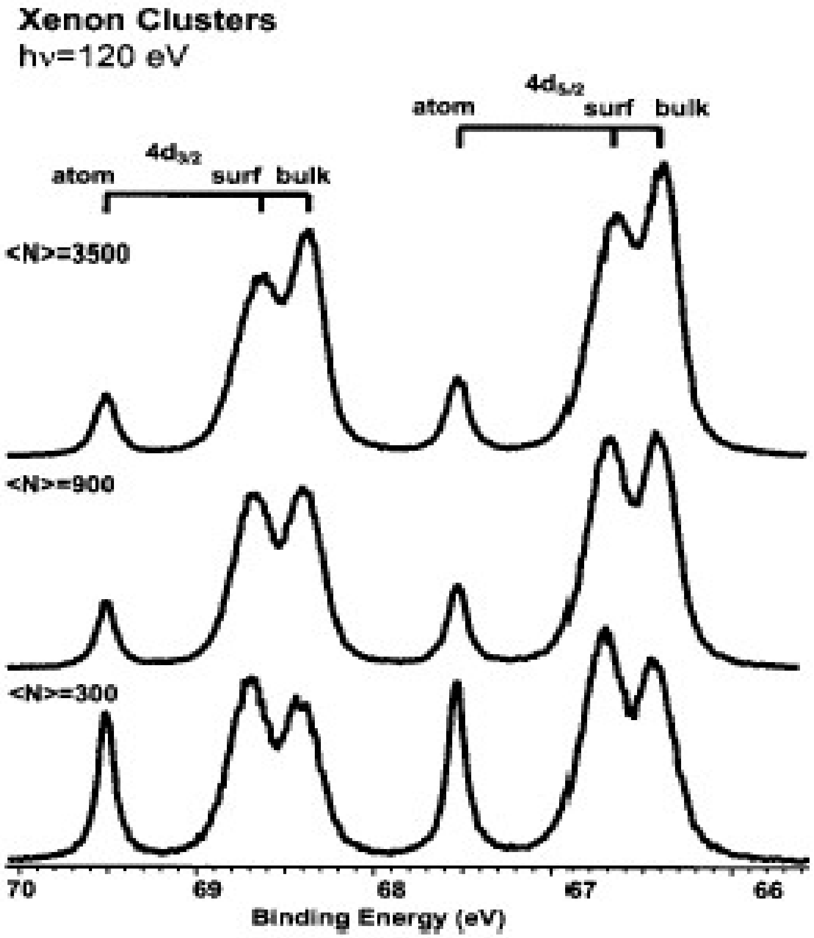
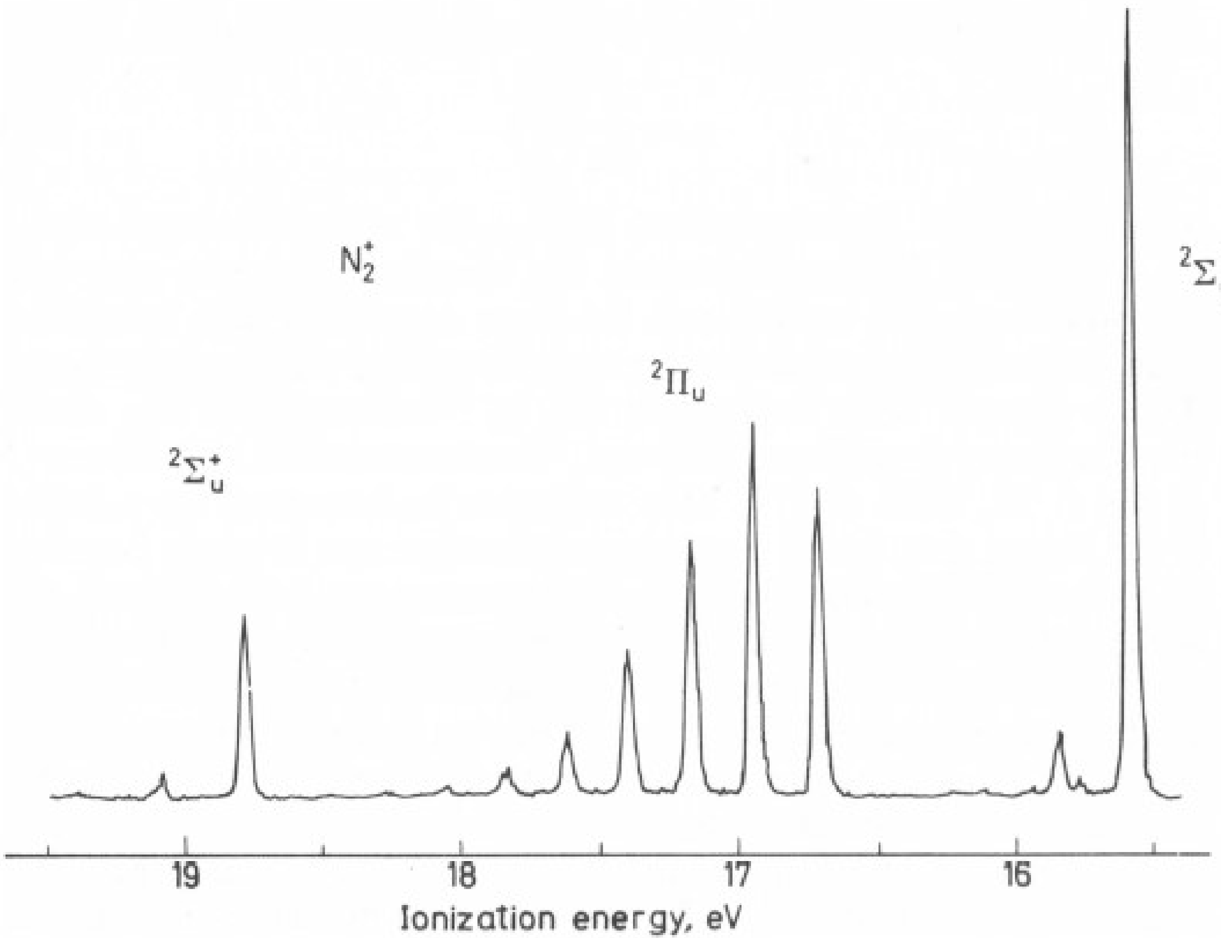
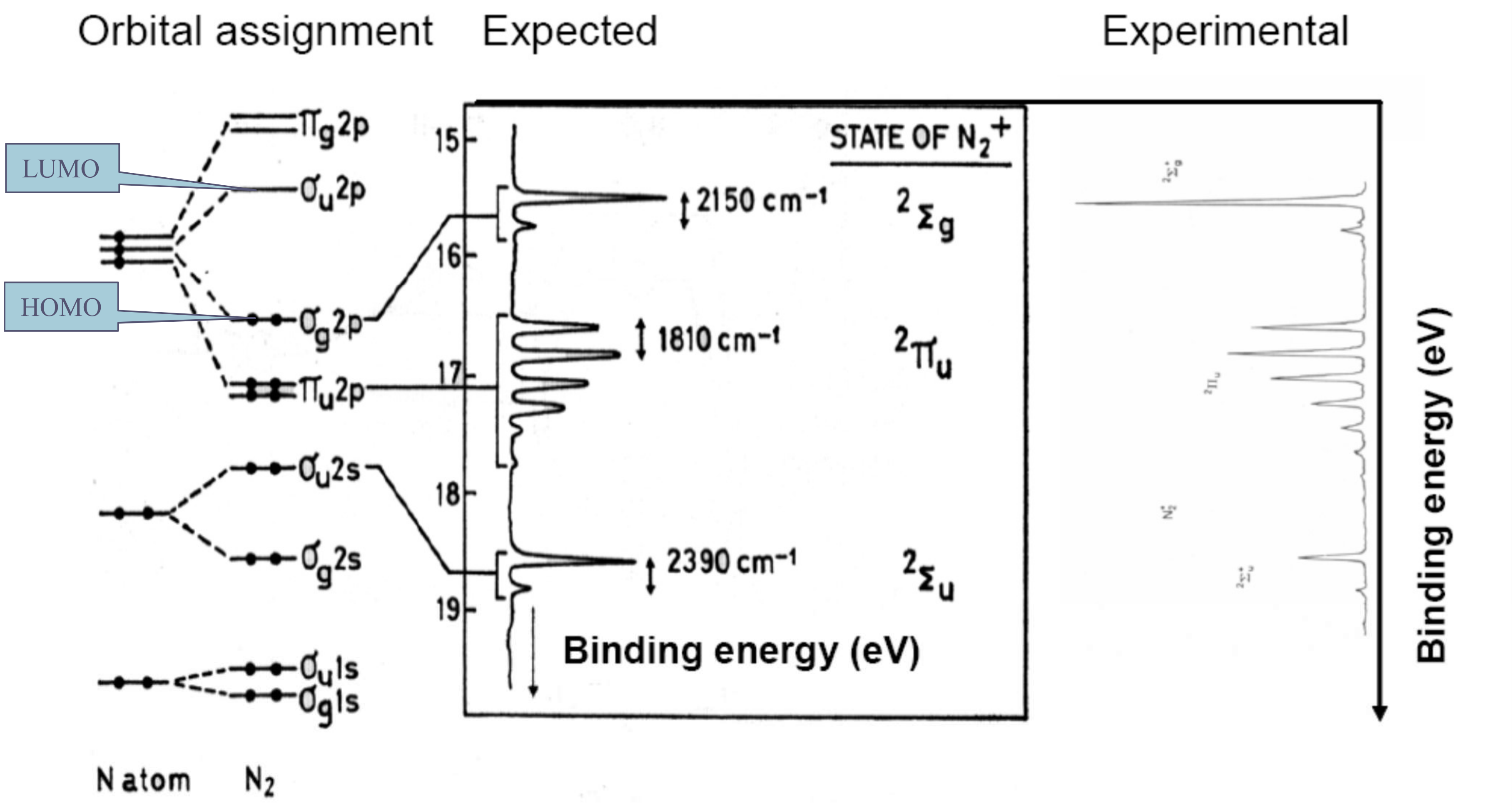


FIG. 3. 4*d* XPS spectra of xenon clusters of three mean sizes at 120 eV photon energy: $\langle N \rangle \approx 300$, 900, and 3500.

# PES spectrum of $N_2$



# Experimental PE spectrum of $N_2$, and MOs



Molecular Nitrogen PES

# Molecular PE x-section

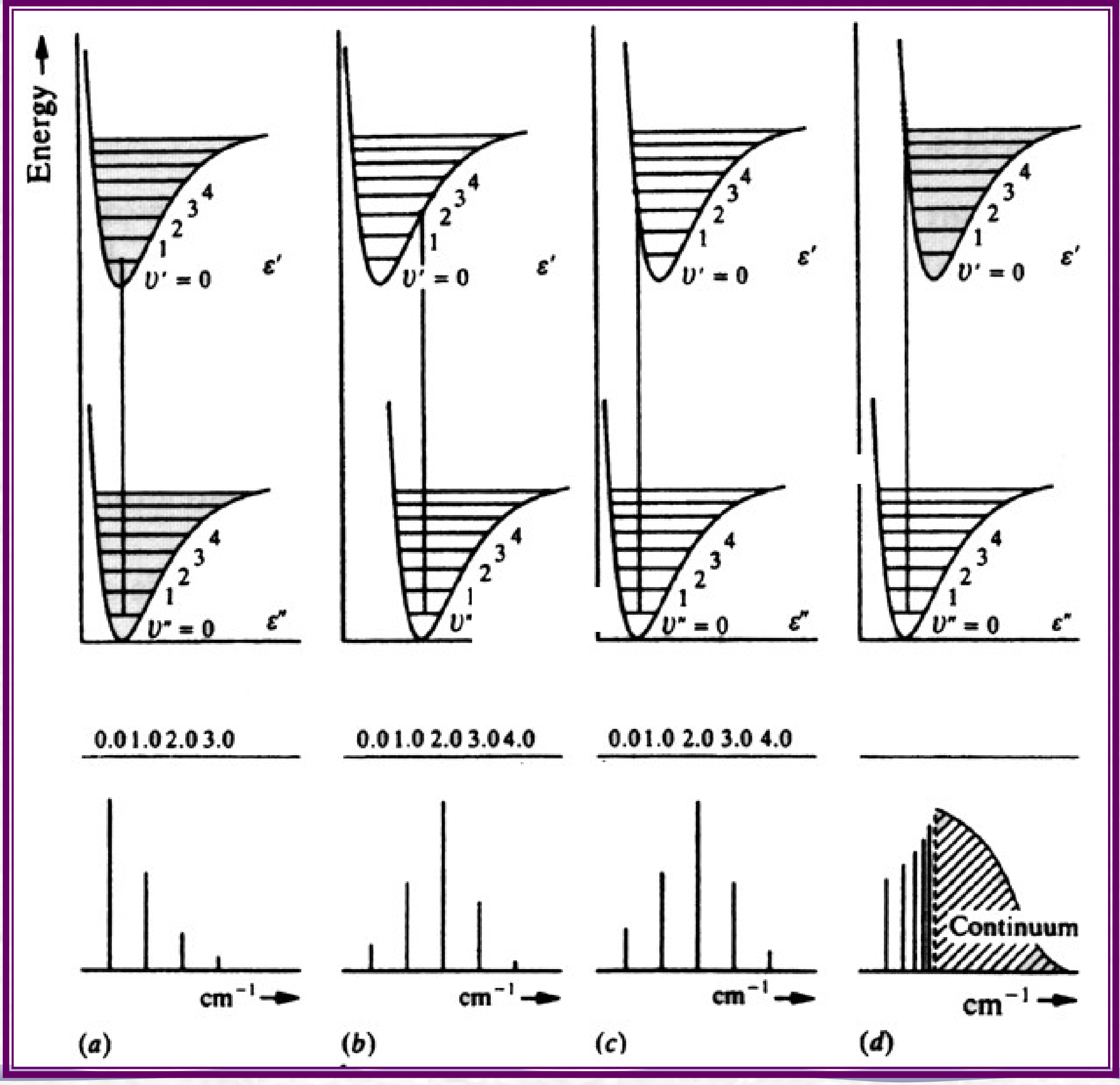
$$H_0 = H_0(kin) + H_0(e-n) + H_0(e-e) + H_0(s-o) + H_0(n-n) =$$
$$= \sum_1^N \frac{p_i^2}{2m} + \sum_1^N - \frac{Ze^2}{r_i} + \sum_{i>j}^N \frac{e^2}{r_{ij}} + \sum_1^N \zeta(r_j)\vec{l}_i \bullet \vec{s}_i + \sum_{i>j}^M \frac{e^2 Z_i Z_j}{r_{ij}}$$

Born Oppenheimer

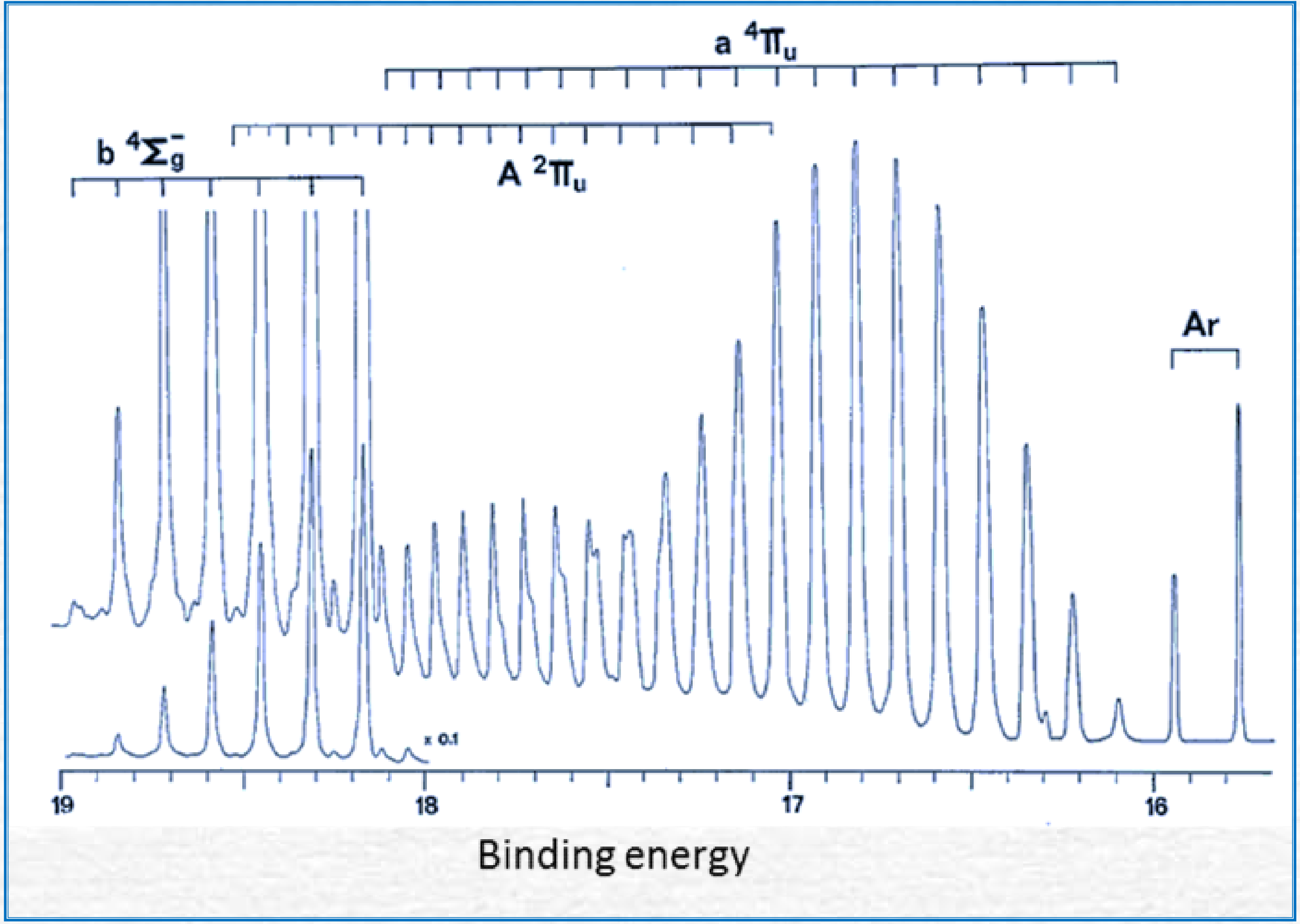
$$\left|\Psi_{A,B}^{(N)}\right\rangle = \left|\Psi_{A,B}^{(N)}\right\rangle \left|\Psi_{A,B}^{vib}\right\rangle$$

$$\frac{d\sigma}{d\Omega dE_e} \propto \frac{1}{h\nu} \sum_{A,B} \left| \hat{\varepsilon} \bullet \left\langle \varepsilon_l \middle| \vec{r}_j \middle| \sum_{A\lambda} C_{A\lambda}\phi_{A\lambda} \right\rangle \left\langle \Psi_B^{(N-1)} \middle| \Psi_R^{(N-1)} \right\rangle \right|^2$$
$$\left| \left\langle \Psi_B^{vib} \middle| \Psi_A^{vib} \right\rangle \right|^2 \delta(E_e + E_B^{(N-1)} - E_A - h\nu)$$

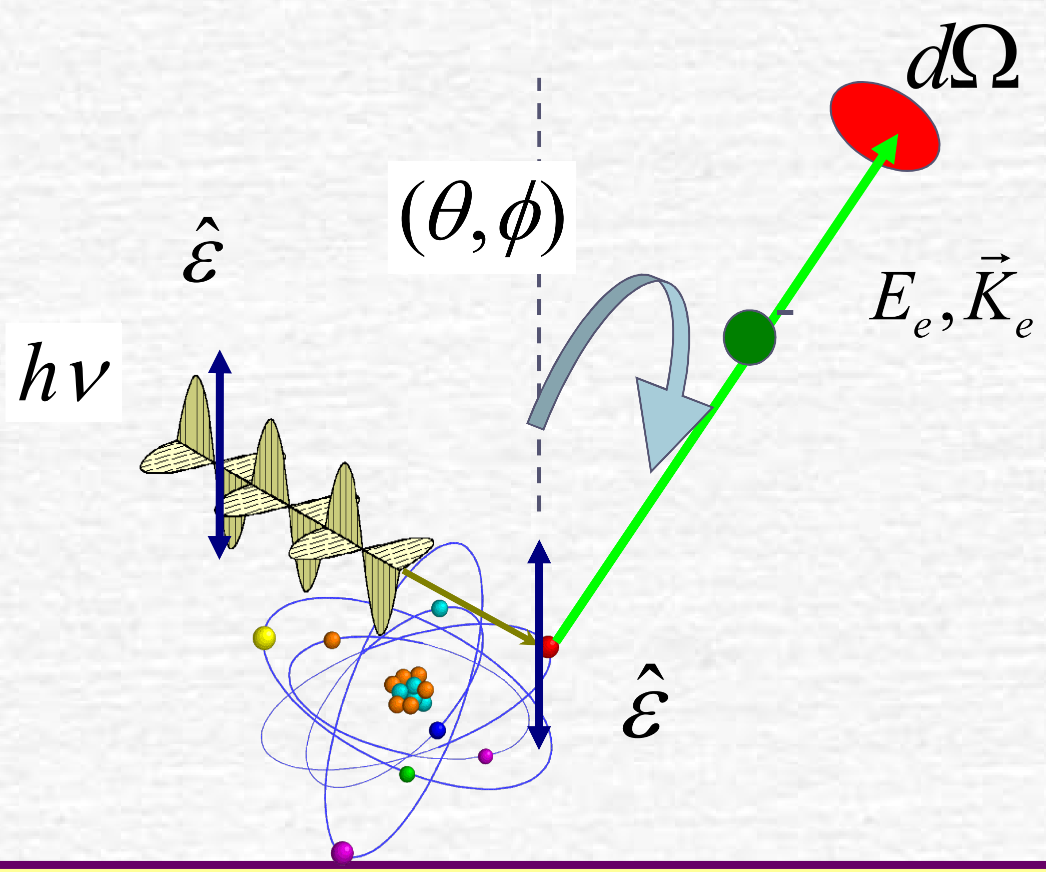
# Frank Condon Factors



# PES $O_2$ vibrational and multiplet splitting

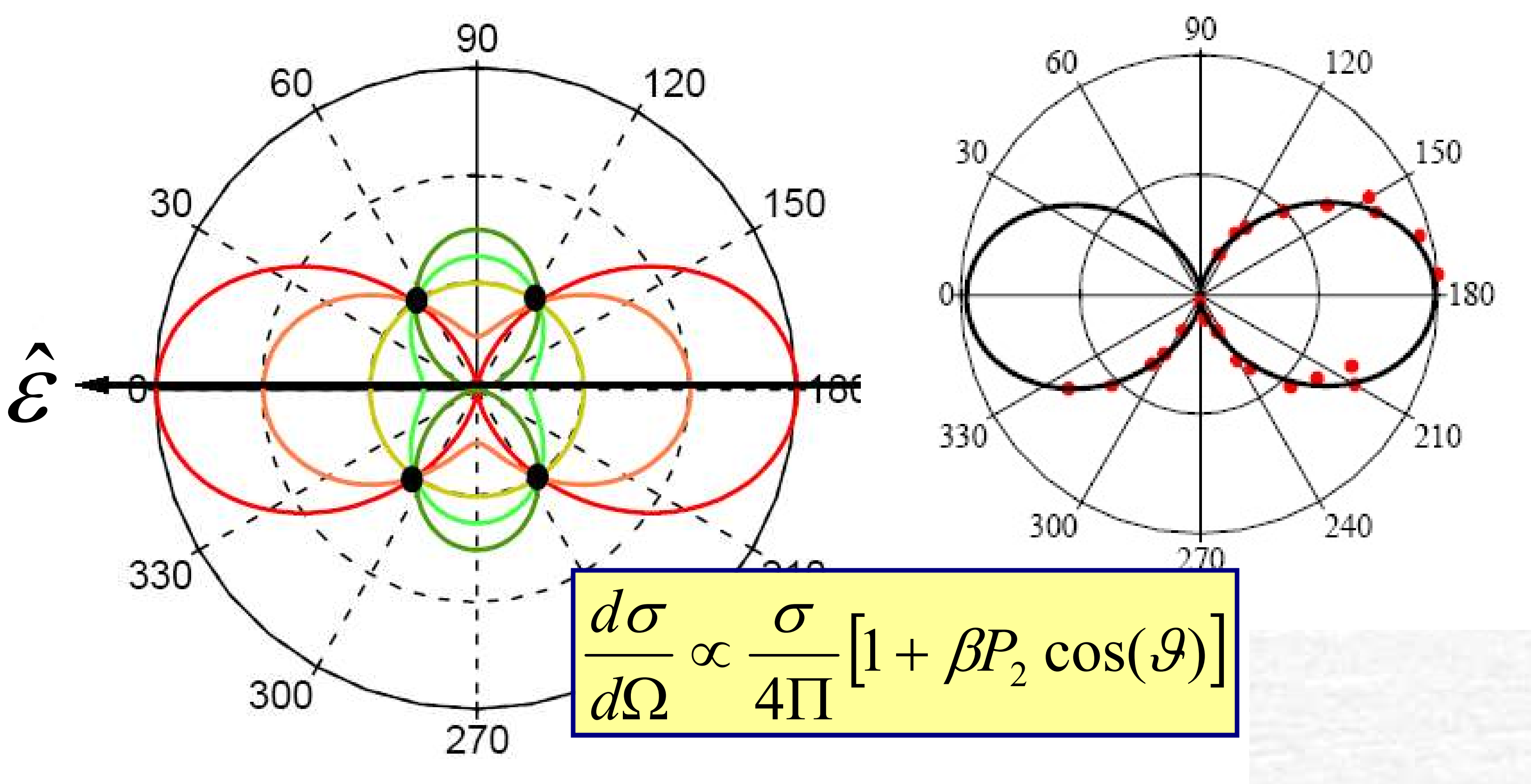


# PE angular distribution



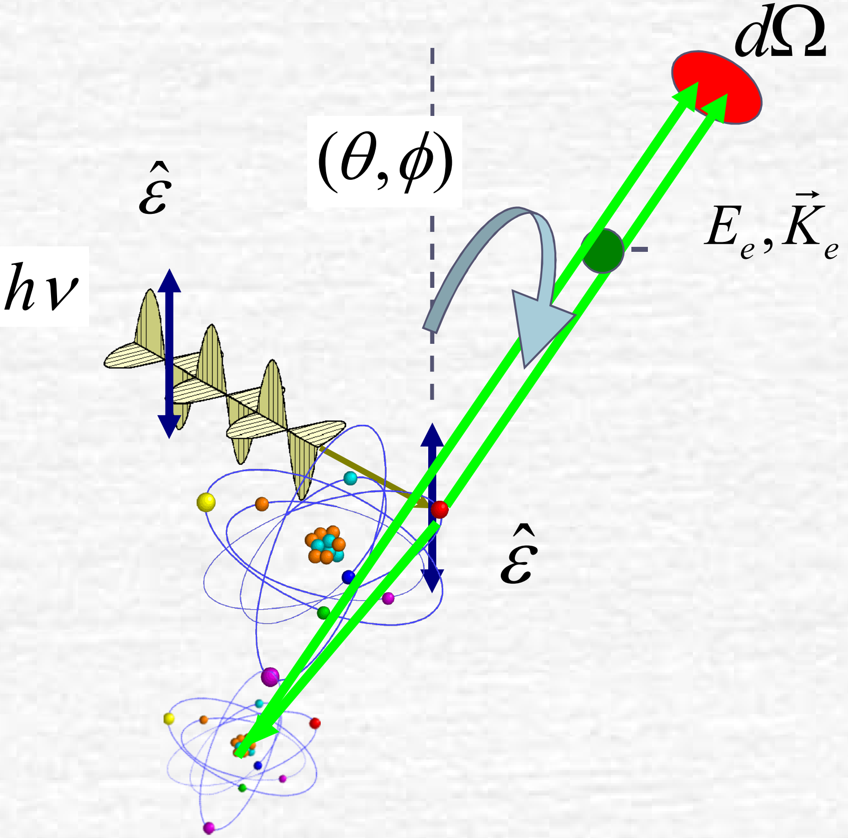
$$\frac{d\sigma}{d\Omega} \propto \frac{1}{h\nu} \sum_{A,B} \left| \hat{\varepsilon} \bullet \left\langle \varepsilon_l \middle| \vec{r}_j \middle| \phi_j(\vec{r}_j, \sigma_j) \right\rangle \left\langle \Psi_B^{(N-1)} \middle| \Psi_R^{(N-1)} \right\rangle \right|^2$$

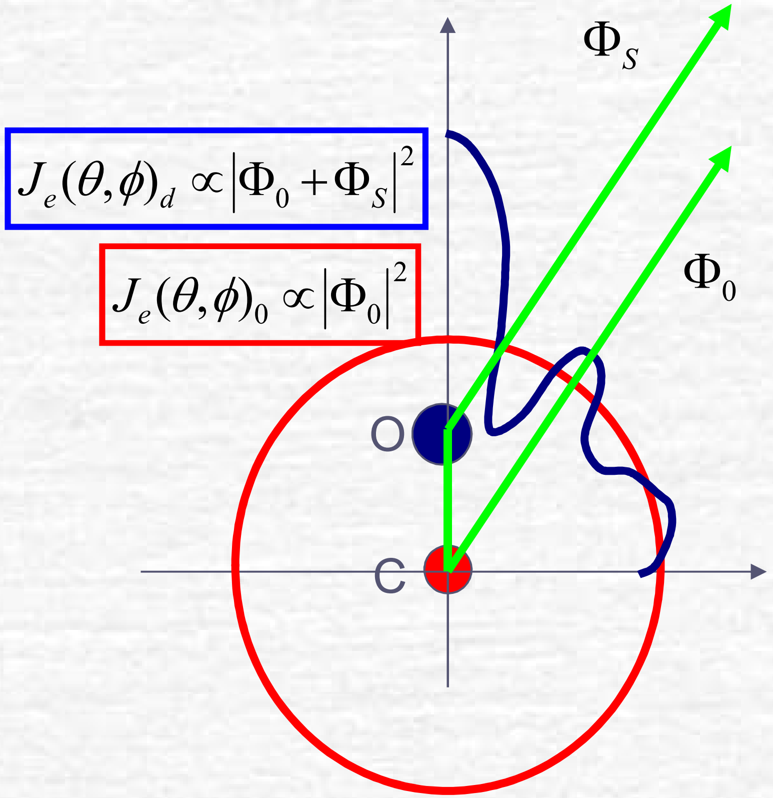
# Angular distributions



$$\frac{d\sigma}{d\Omega} \propto \frac{\sigma}{4\Pi}\left[1+\beta P_2\cos(\vartheta)\right]$$

$$\boxed{J_e \left| \Phi_{direct} + \sum_i \Phi^{i}_{scattered} \right|^2}$$

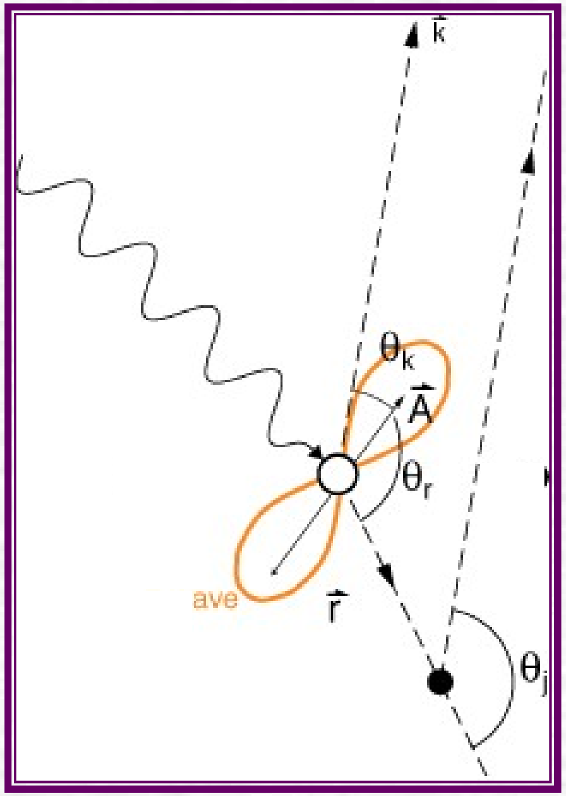


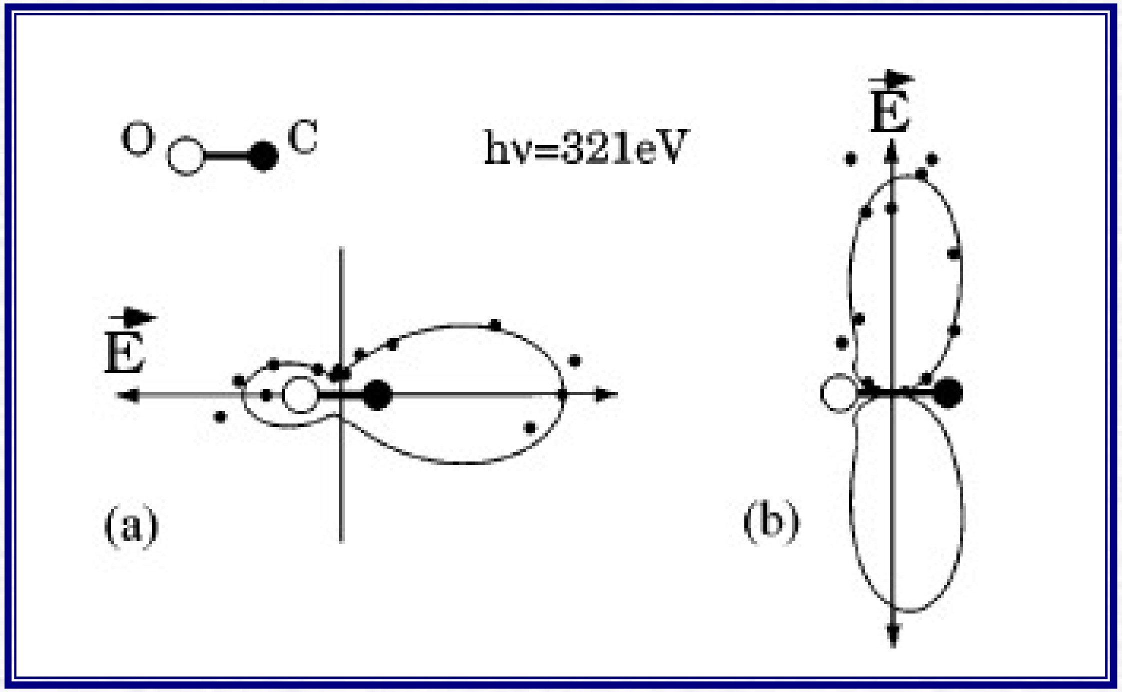


$$J_e(\theta,\phi)_d \propto \left|\Phi_0 + \Phi_S\right|^2$$

$$J_e(\theta,\phi)_0 \propto \left|\Phi_0\right|^2$$

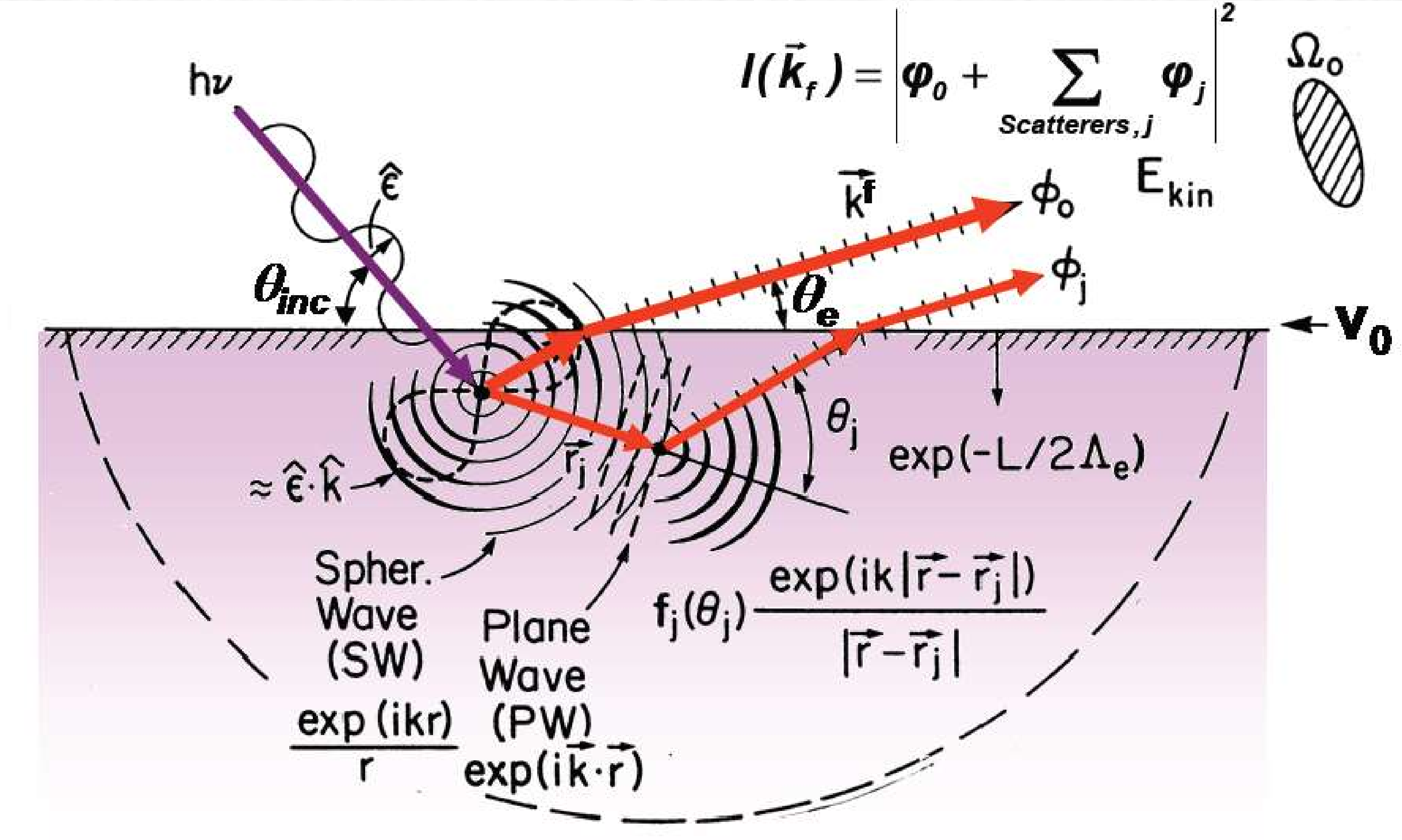
# Fixed in space molecules
# CO    C 1s



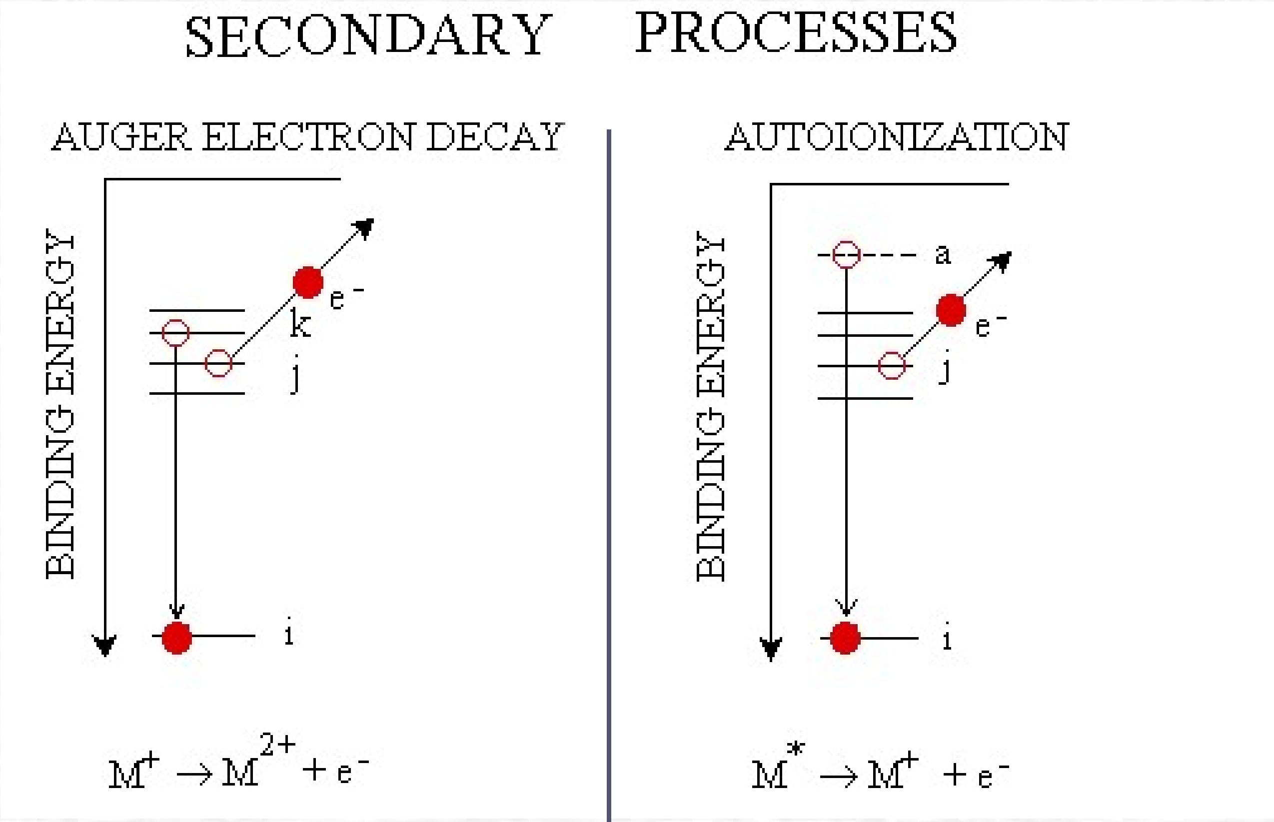


F. Heiser et al. VOLUME 79, NUMBER 13 PHYSICAL REVIEW LETTERS

# Application to surfaces



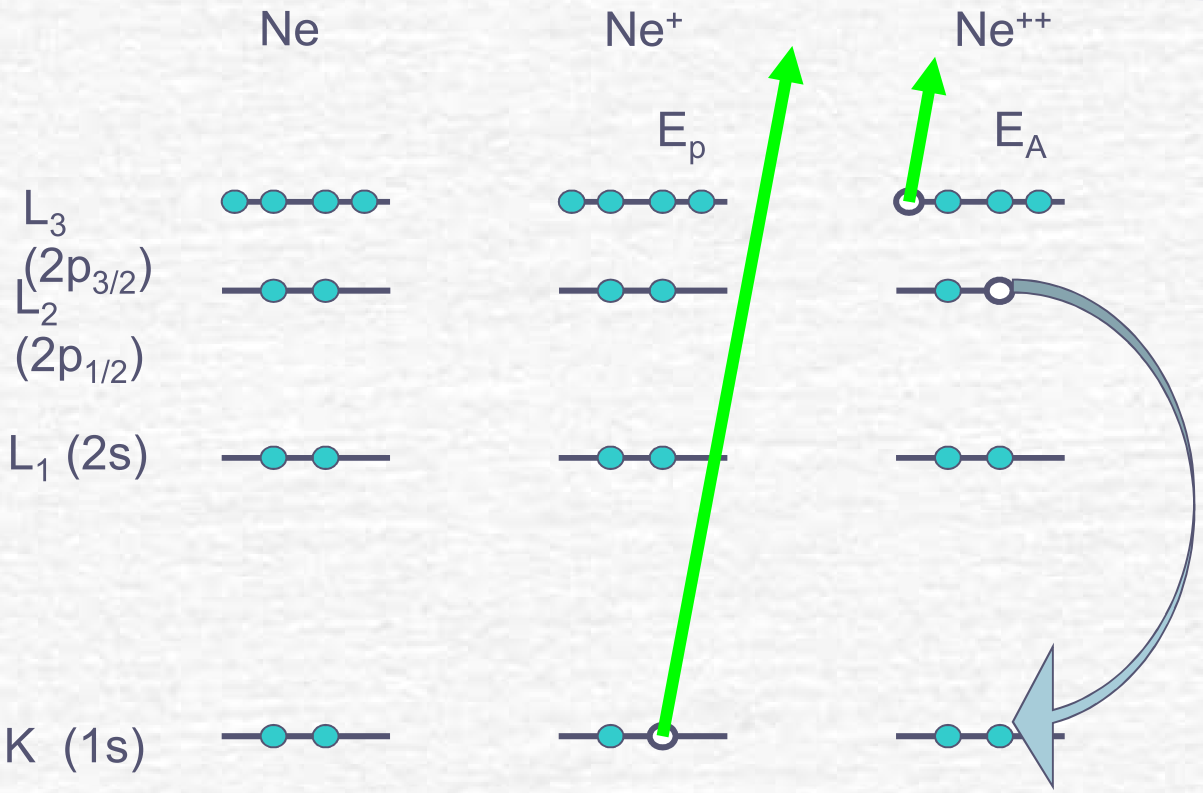
# Core hole relaxation



Global energy, angular
Momentum and parity

Energy, angular momentum,
Dipole selections at each step

# Auger decay

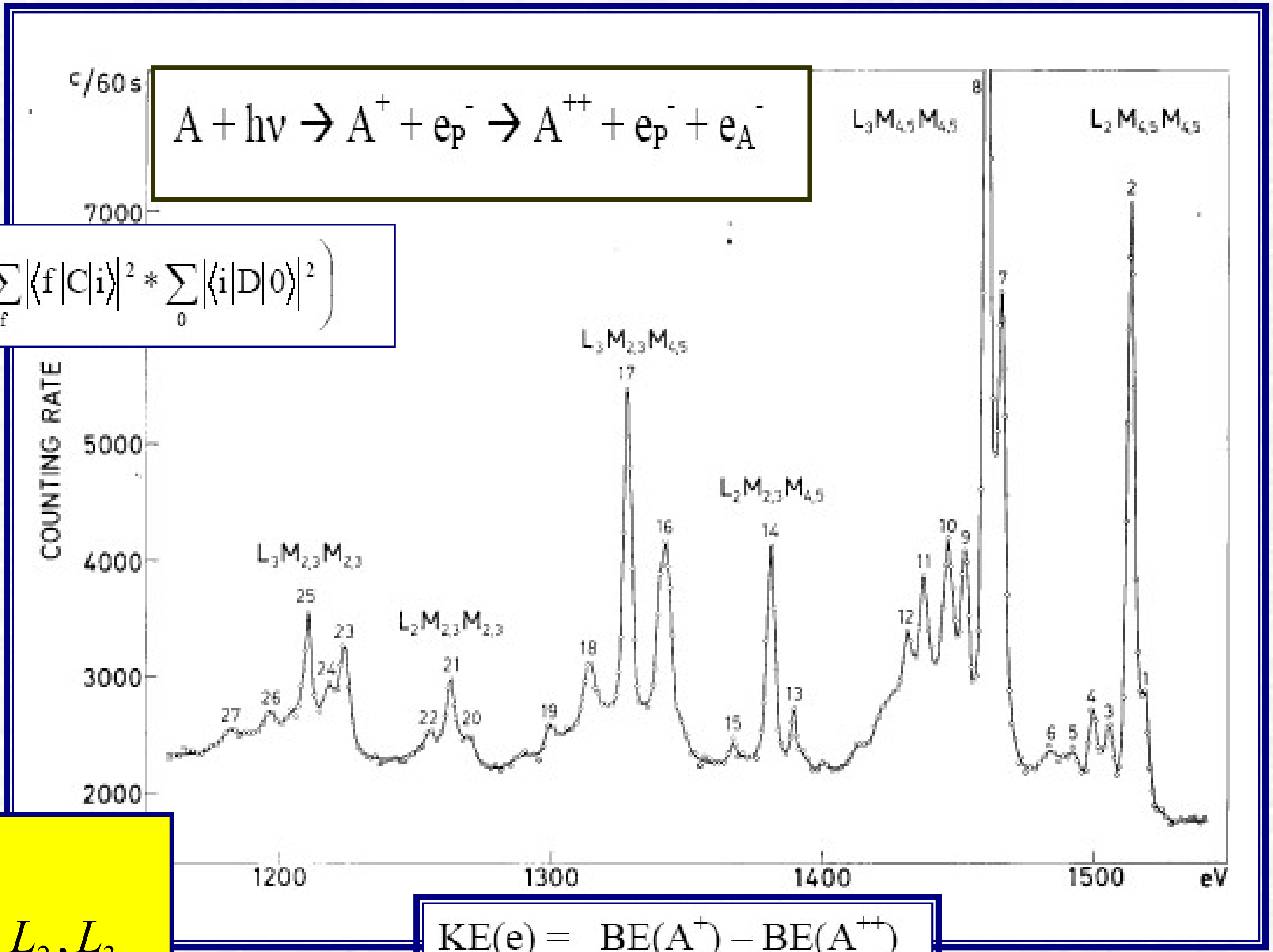


| Auger Transition | Double ion valence configuration | Multiplet Terms |
|---|---|---|
| $KL_1L_1$ | $2s^0\ 2p^6$ | $^1S_0$ |
| $KL_1L_{2,3}$ | $2s^1\ 2p^5$ | $^1P_1,\ ^3P_0,\ ^3P_2,\ ^3P_1$ |
| $KL_{2,3}L_{2,3}$ | $2s^2\ 2p^4$ | $^1S_0,\ ^3P_0,\ ^3P_2,\ ^1D_2$ |

$$\mathbf{EA(KL_1L_2) = E(K) - E(L_1) - E(L_2, L_1)}$$

# Kr Auger spectrum

K. Siegbahn et al
“ESCA Applied
to free molecules”



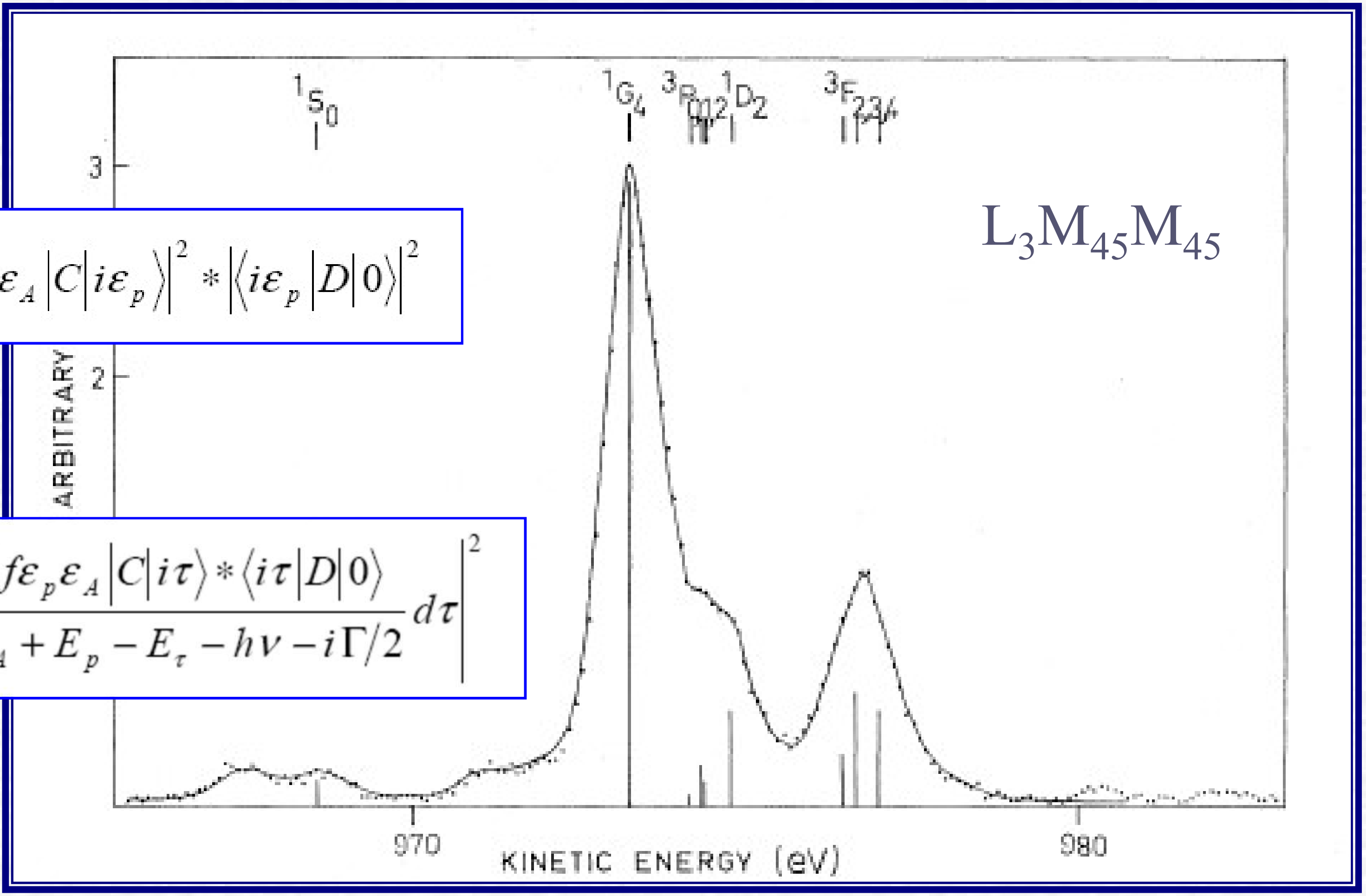
$$A + h\nu \rightarrow A^{+} + e_P^{-} \rightarrow A^{++} + e_P^{-} + e_A^{-}$$

$$P \propto \sum_i \left( \sum_f \left|\langle f|C|i\rangle\right|^2 * \sum_0 \left|\langle i|D|0\rangle\right|^2 \right)$$

$$KE(e) = BE(A^{+}) - BE(A^{++})$$

$$|0\rangle \rightarrow Kr^{I}$$
$$|i\rangle \rightarrow Kr^{II} \rightarrow L_2, L_3$$
$$|f\rangle \rightarrow Kr^{III} \rightarrow M_i M_j$$

# Zn Auger multiplet splitting

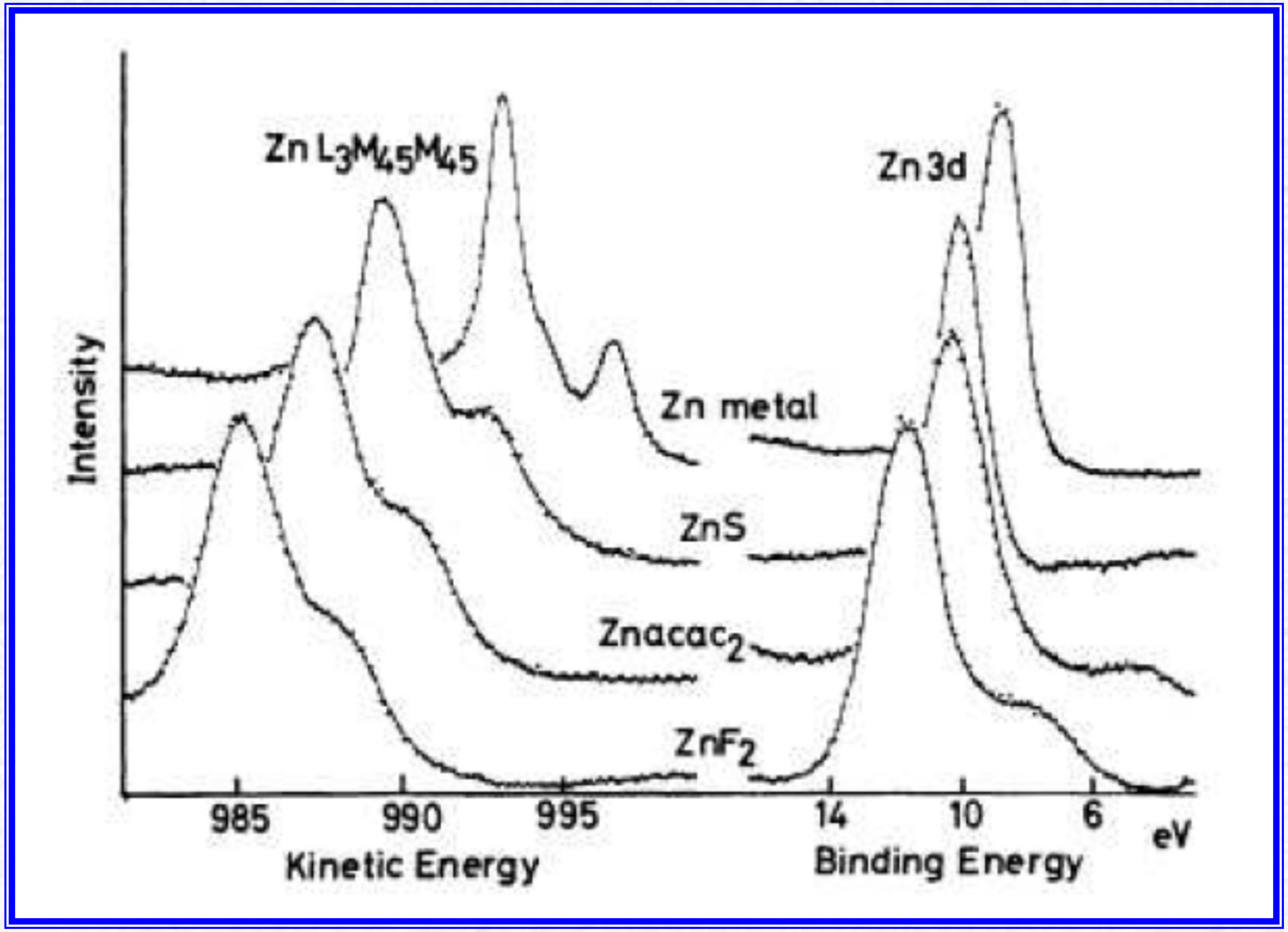


$$P(0,i,f) \propto \left|\langle f\varepsilon_p\varepsilon_A|C|i\varepsilon_p\rangle\right|^2 * \left|\langle i\varepsilon_p|D|0\rangle\right|^2$$

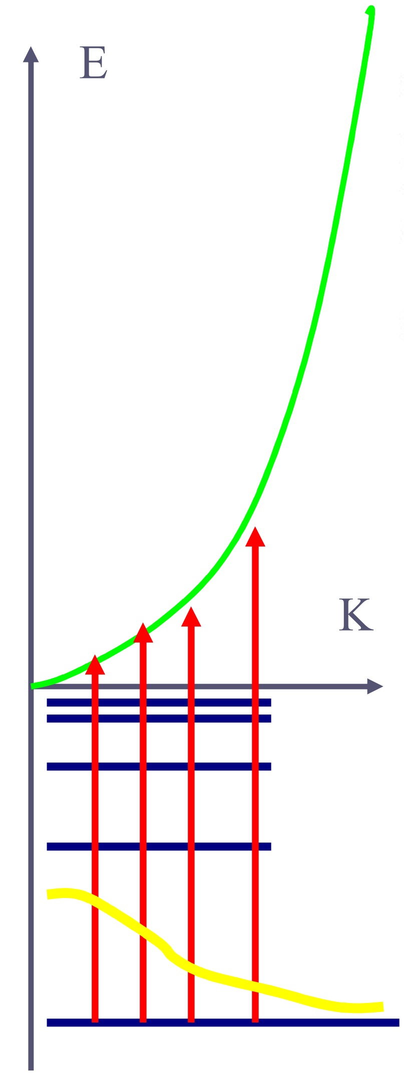
$$P(0,i,f) \propto \left|\int \frac{\langle f\varepsilon_p\varepsilon_A|C|i\tau\rangle * \langle i\tau|D|0\rangle}{E_A+E_p-E_\tau-h\nu-i\Gamma/2}\,d\tau\right|^2$$

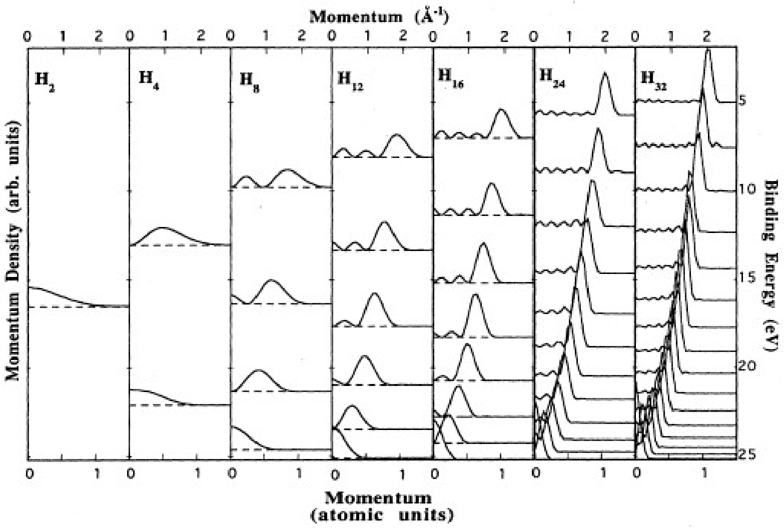
Aksela et al. PRL 33,999 (1974)

# Auger chemical shift



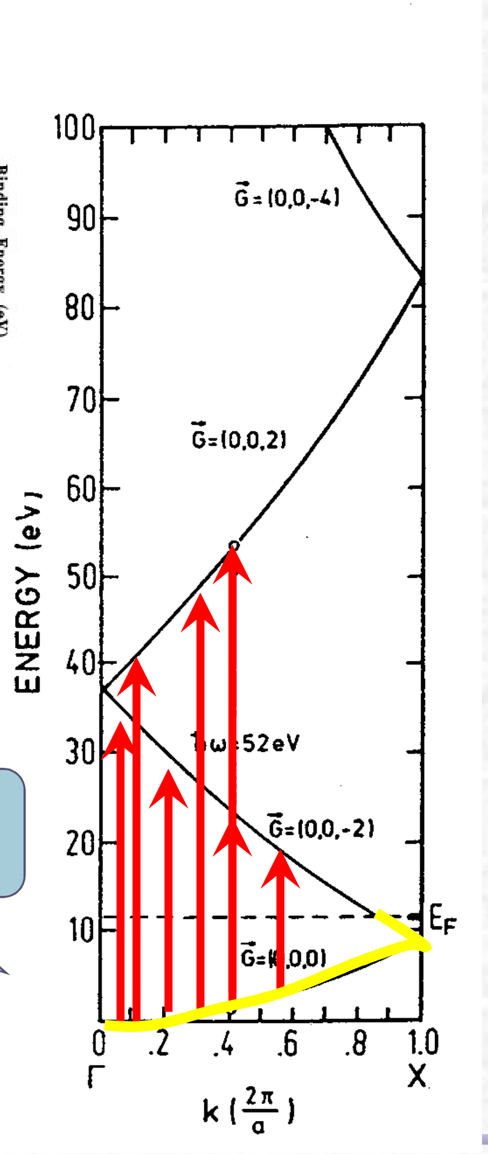
# From central to periodic potential



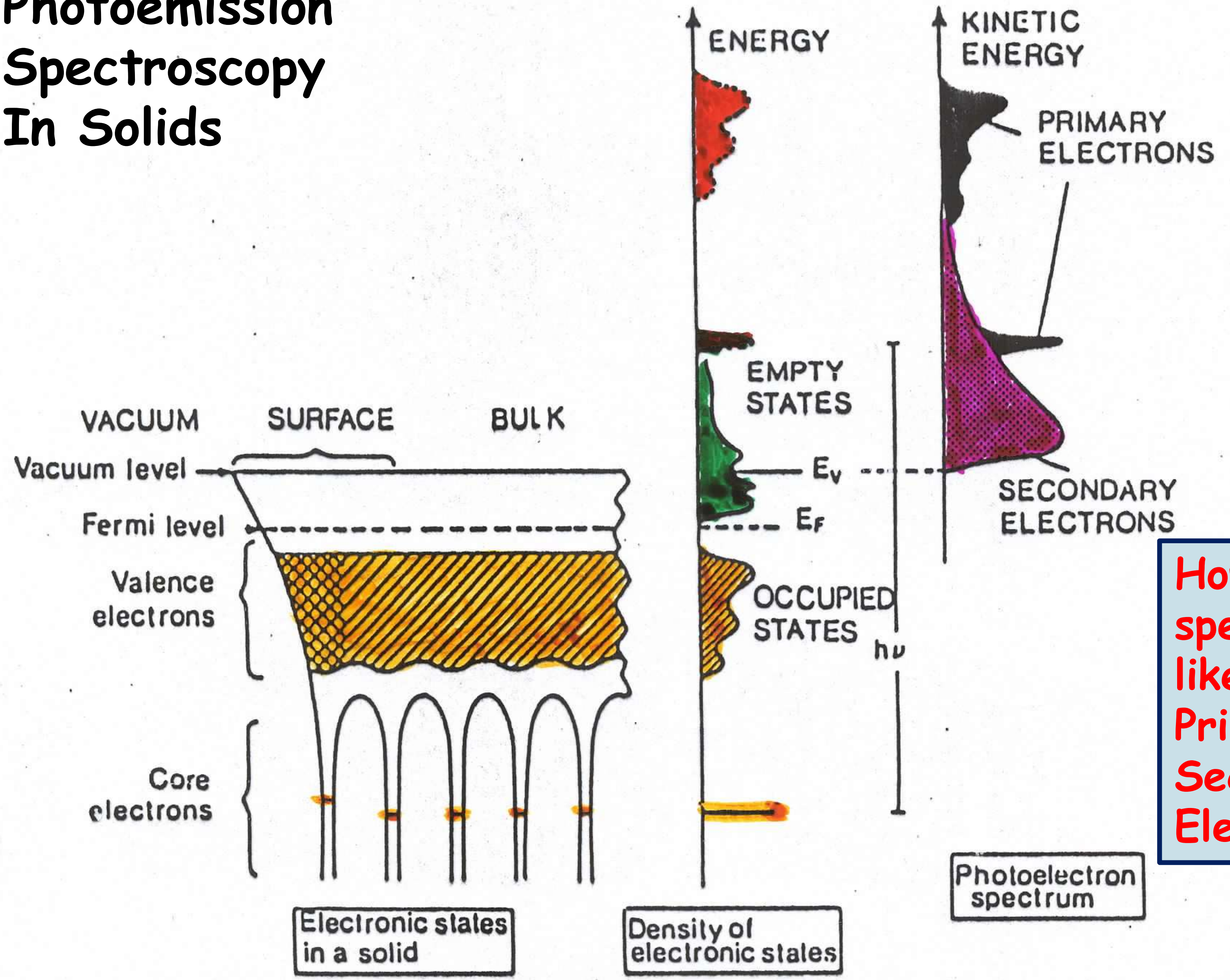


$$\langle \varepsilon_l | \vec{r}_j | \phi_j(\vec{r}_j,\sigma_j) \rangle \langle \Psi_B^{(N-1)} | \Psi_R^{(N-1)} \rangle$$

$$\langle \varepsilon_l | \vec{r}_j | \phi_j(\vec{r}_j,\sigma_j) \rangle A(\vec{k},E)$$



# Photoemission Spectroscopy In Solids



How real spectra look like:
Primary and Secondary Electrons

# Spectral Function in Interacting Solids

$$\boxed{\Psi_{Nf} = A\, \Psi^{N-1}{}_{f}\, \Phi_{kf}}$$

$$Je \propto \Sigma_{if}|M^{2}{}_{if}|\ \Sigma_{m}|m_{im}|^{2} \times \delta(E^{N}{}_{i} + h\nu - E^{N-1}{}_{m} - E_{kin})$$

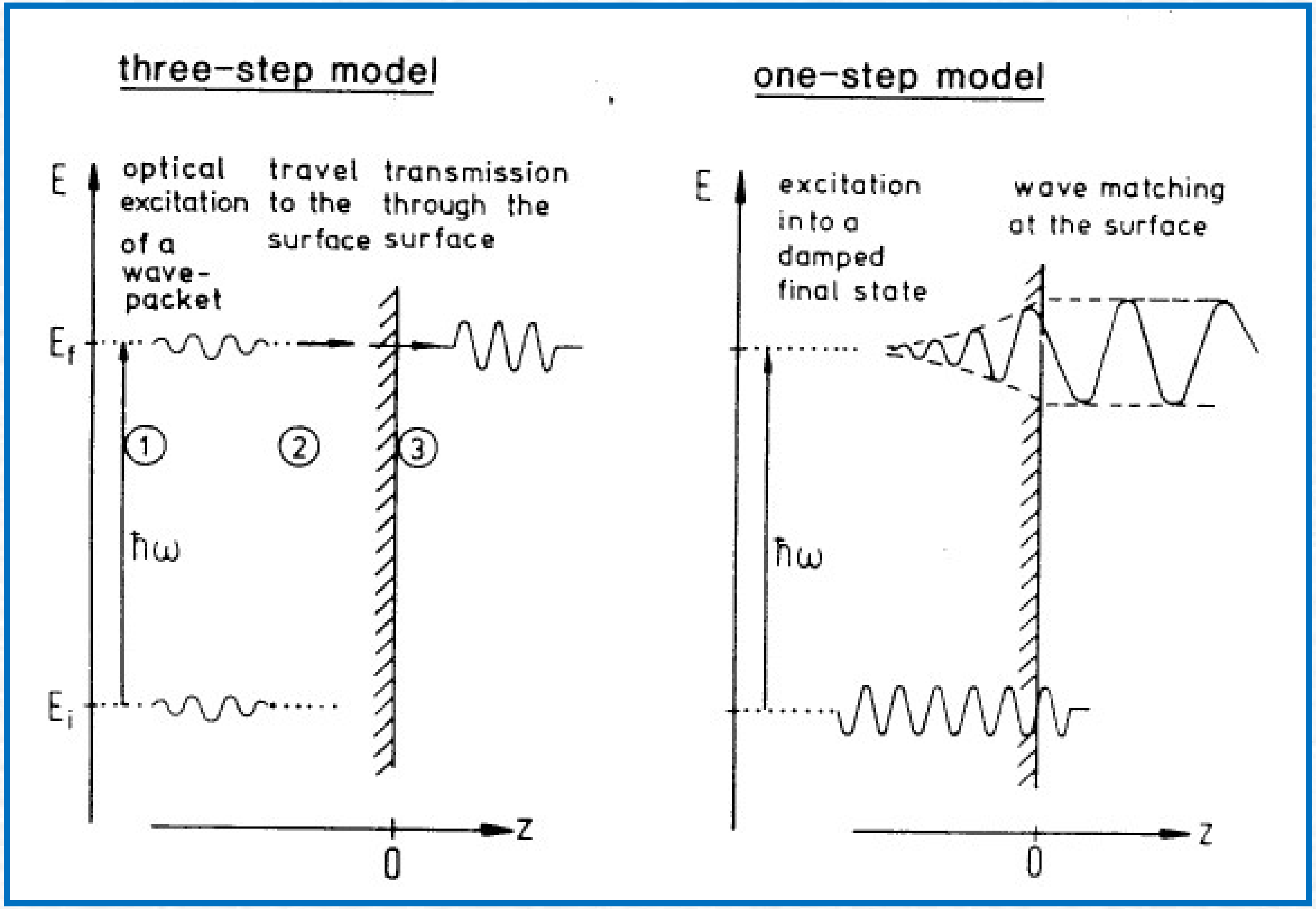
$$A(k, \varepsilon) = \Sigma_{m}\ (|<\Psi^{N-1}{}_{m}|c_{k}|\Psi^{N}{}_{i}>)|^{2} \times \delta(\varepsilon + E^{N-1}{}_{m} - E^{N}{}_{i})$$

$$\boxed{Je(k, \omega) \propto \Sigma_{if}|M_{if}|^{2}\, A(k, E_{kin} - h\nu)\, f(E_{kin} - h\nu)}$$

For non interacting particles $\boxed{A(\varepsilon, k) = \delta(\varepsilon - E_{k})}$ where $\boxed{E_{k} = E_{i}{}^{N-1} - E_{i}{}^{N}}$

$$\boxed{A(\varepsilon, k) = 1/\pi\ |\Sigma''(k, \varepsilon)|\ /\ [|\varepsilon - E_{k} - \Sigma'(k, \varepsilon)|^{2} + |\Sigma''(k, \varepsilon)|^{2}]}$$

# The Three-Step model 1



# The three-step model 2

1. **Dipole transition**

$$Je = \Sigma_{if}\, f(E_i)\, [1-f(E_f)]\, M^2_{if} \times \delta[E_{kin}-(E_f-\Phi)]\, \delta(E_f-E_i-h\nu)\, \delta(k_i+G-k_f)$$

2. **Elastic transport**

$$d(E_f, k) = \alpha\lambda/(1+\alpha\lambda)$$

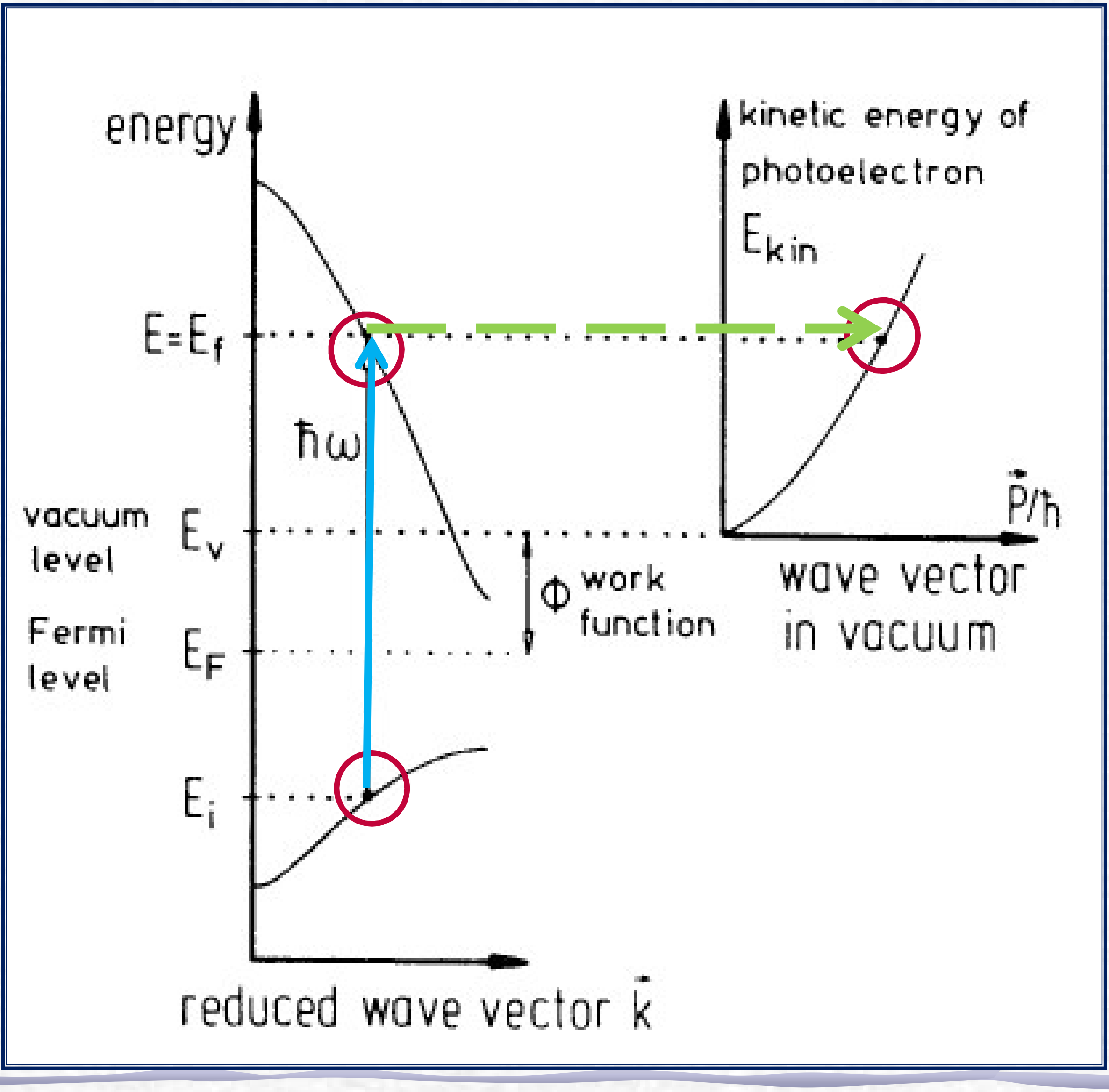
3. **Exit to vacuum**

$$T(E_f, k_{ext}) = \begin{cases} 0 \text{ if } E_f < E_F + \Phi \\ 1/2\ \sqrt{[1-(E_F+\Phi)/Ef]} \text{ if } E_f > E_F + \Phi \end{cases}$$

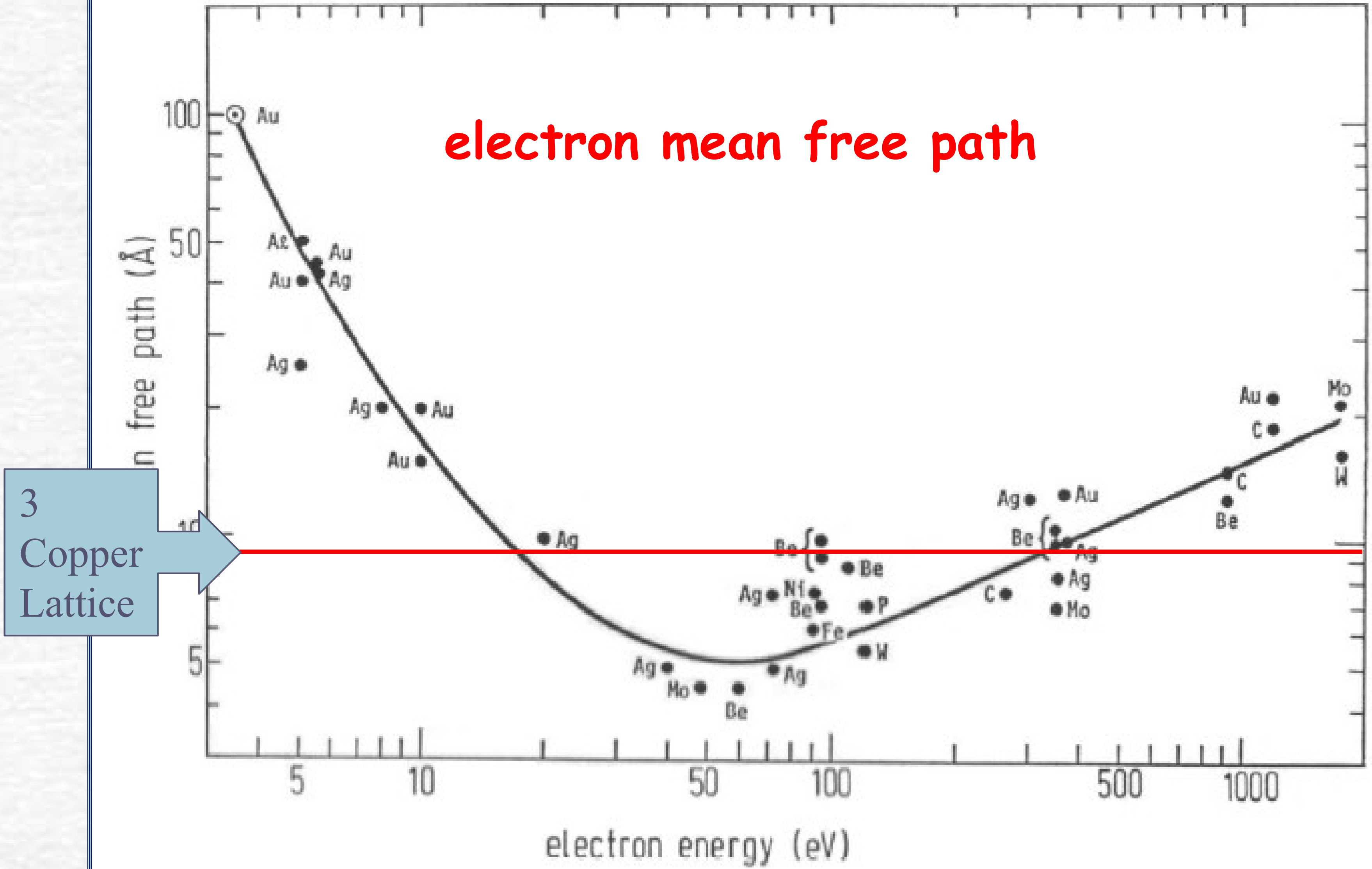
**Total current**

$$Je \propto \Sigma_{if}\, f(E_i)\, [1-f(E_f)]\, M^2_{if} \times T(E_f, k_{ext}) \times d(E_f, k) \times \delta[E_{kin}-(E_f-\Phi)]\, \delta(E_f-E_i-h\nu) \times \delta\, (k_i+G-k_f) \times \delta\, (k^{//}_i+G^{//}-k^{//}_{ext})$$

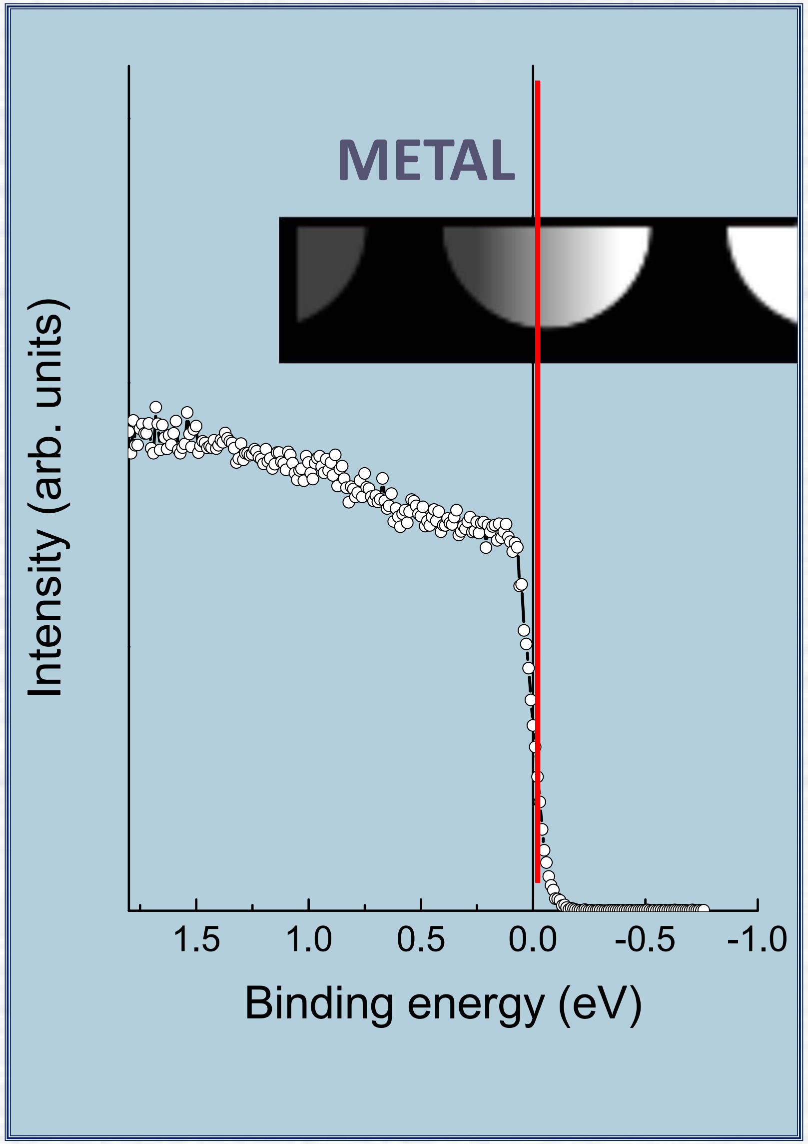
# How to reconstruct the initial state in 3 step model

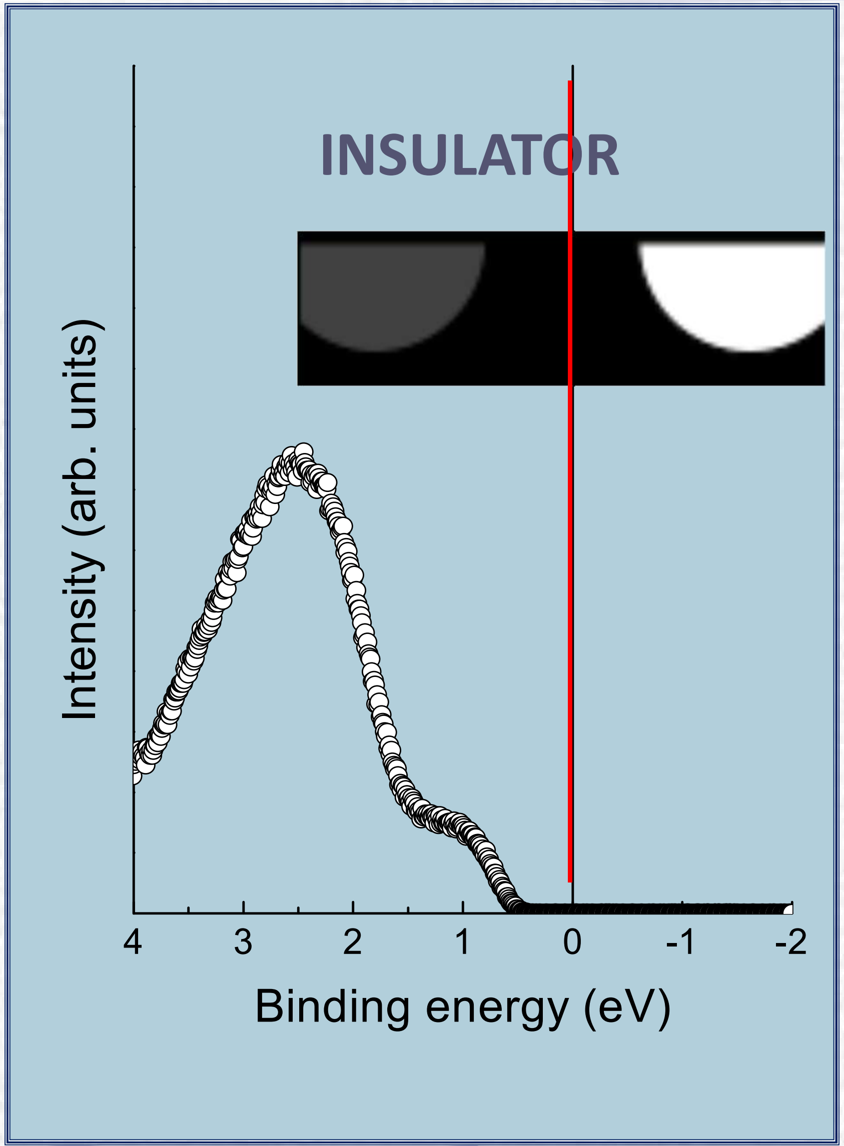


# Surface vs. Bulk Sensitivity in Photoemission

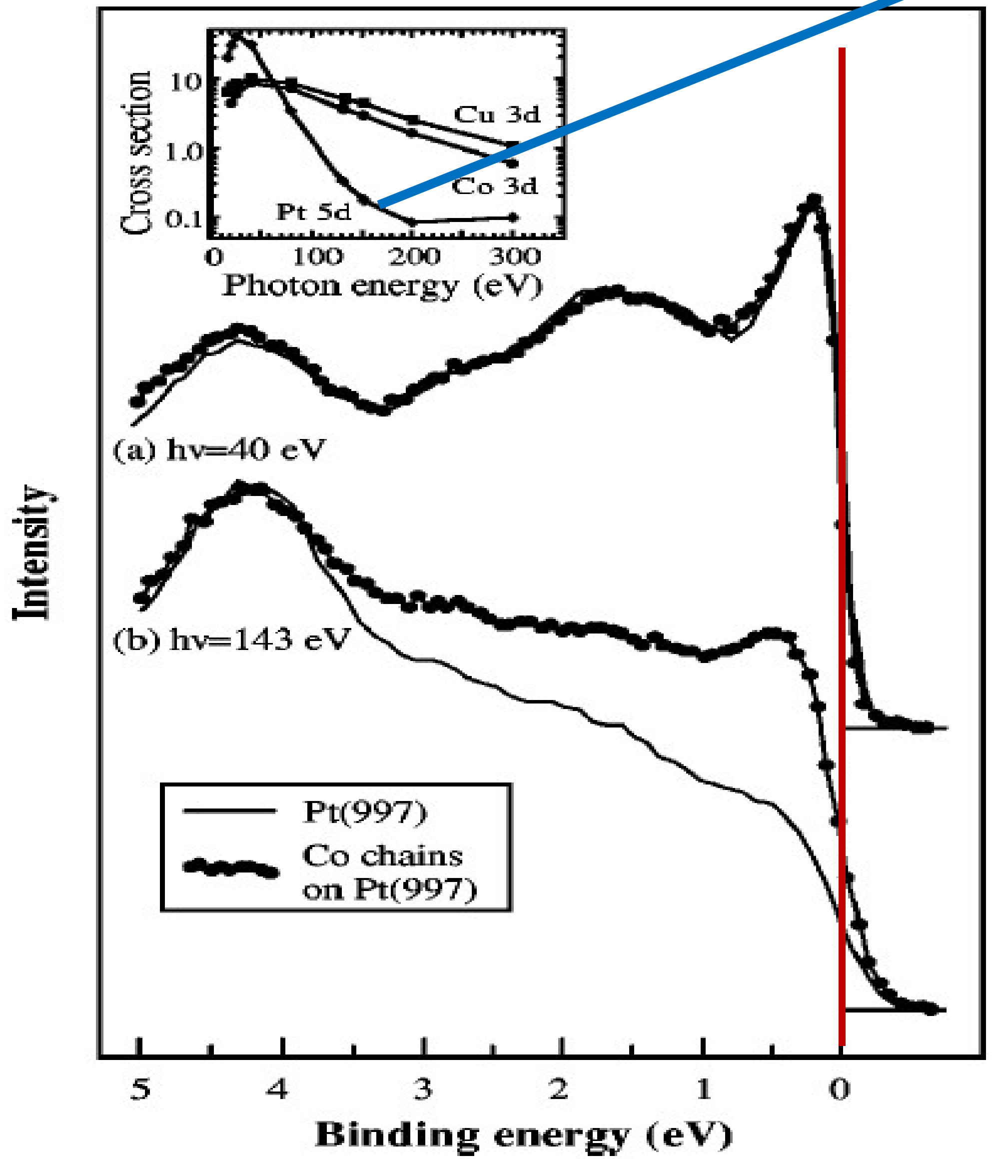


# Photoemission spectrum at Fermi Edge



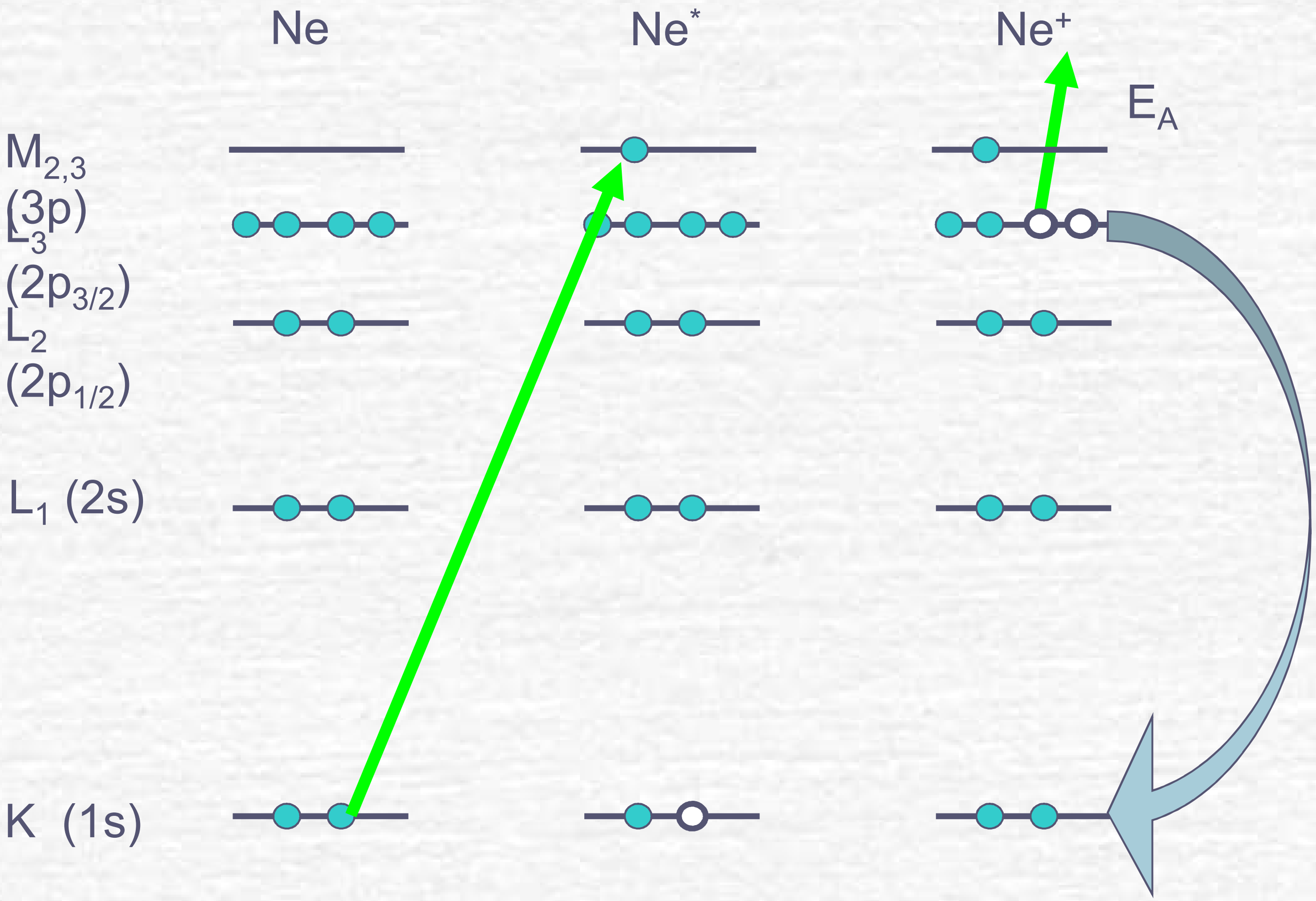


# Valence band Energy Distribution Curves and Cooper minimum

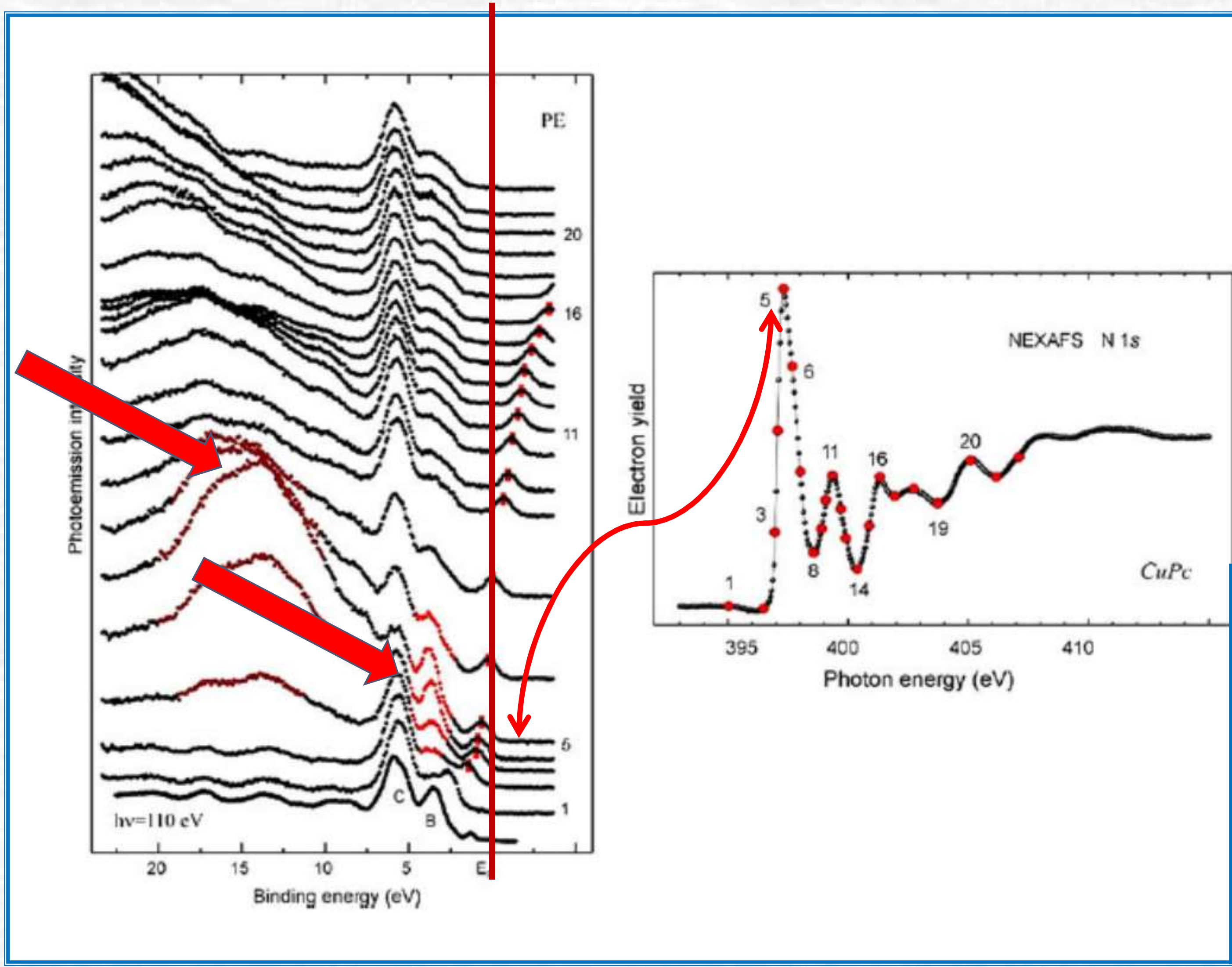


Valence Band EDCs of the clean Pt(997) surface (thin lines) and of Co-nanowires grown on Pt(997) (dots and thick lines), taken at different photon energies

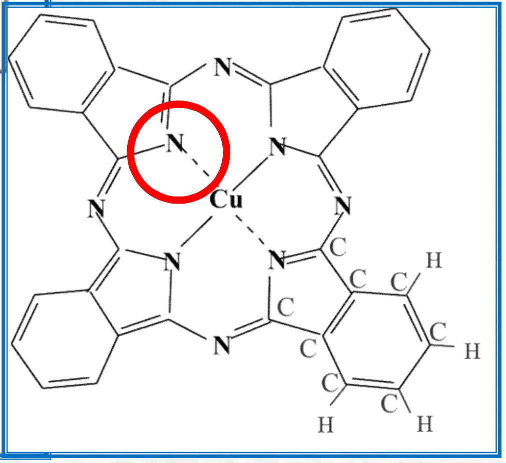
# Autoionizing decay



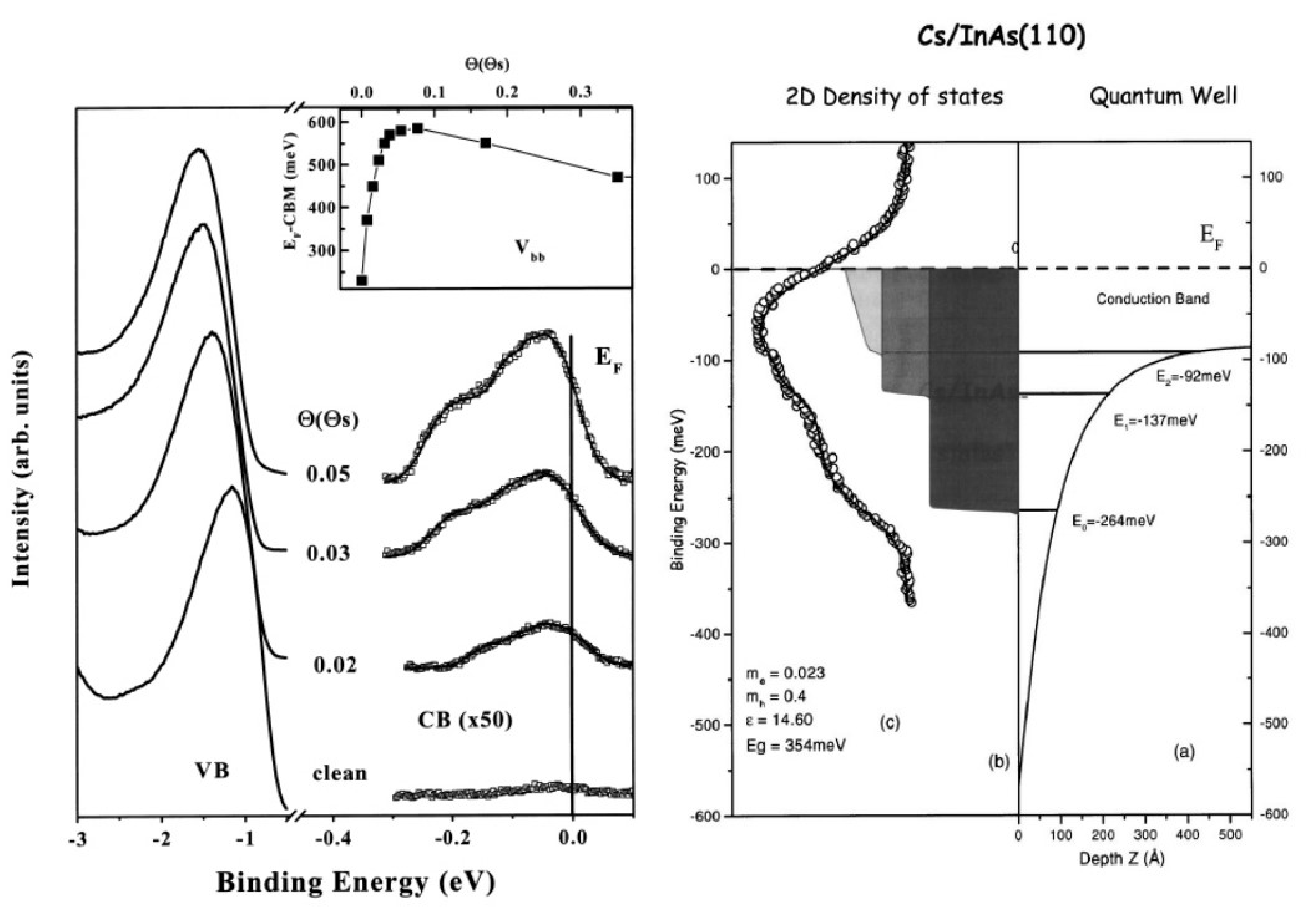
# Resonant photoemission EDC



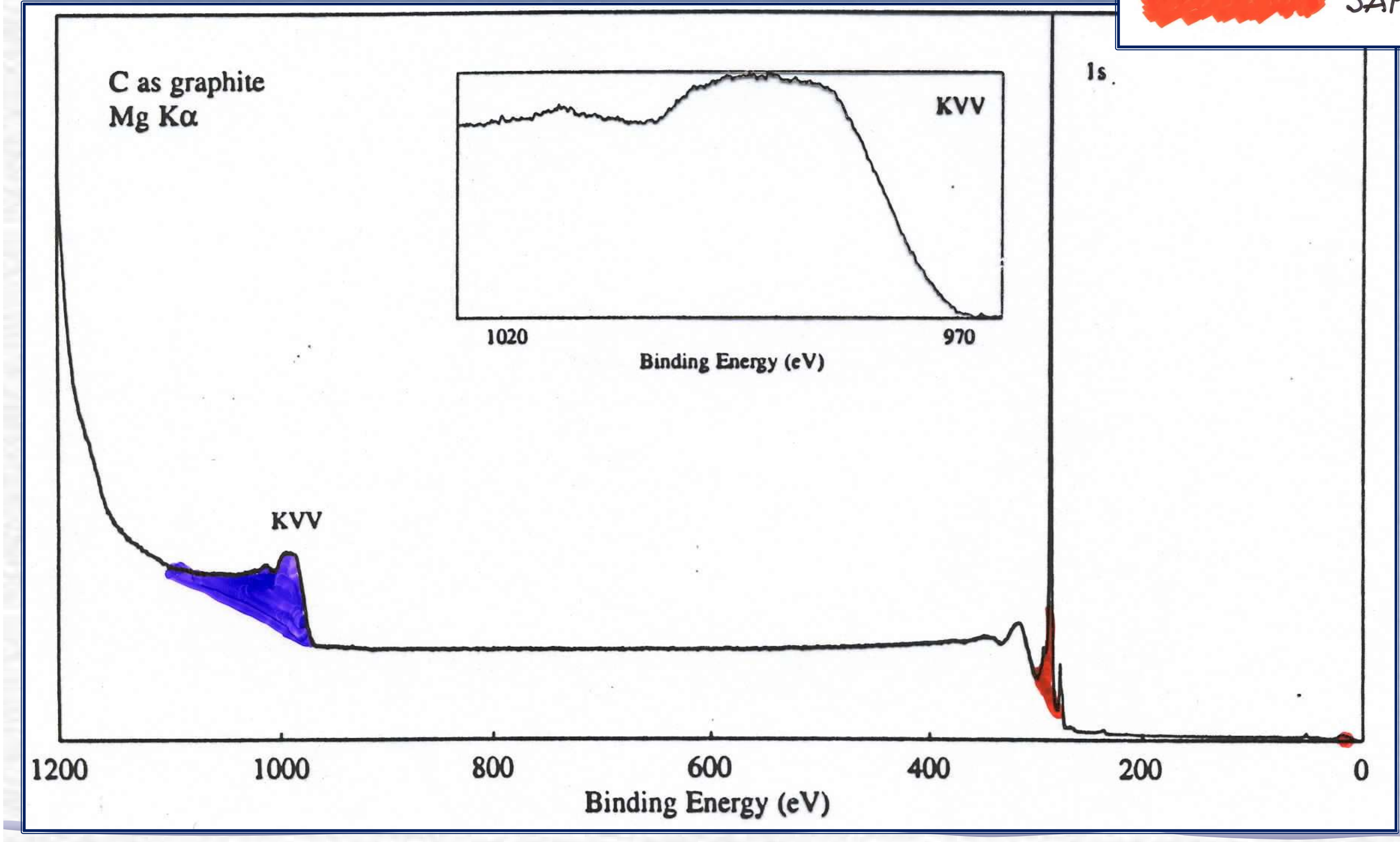
Valence Band EDCs of a CuPc thin-film taken at different photon energies (left panel) and X-ray Absorption Spectroscopy (XAS) from the same CuPc across the N K-edge (right panel).



# 2D electron gas spatially confined Cs/InAs(110)

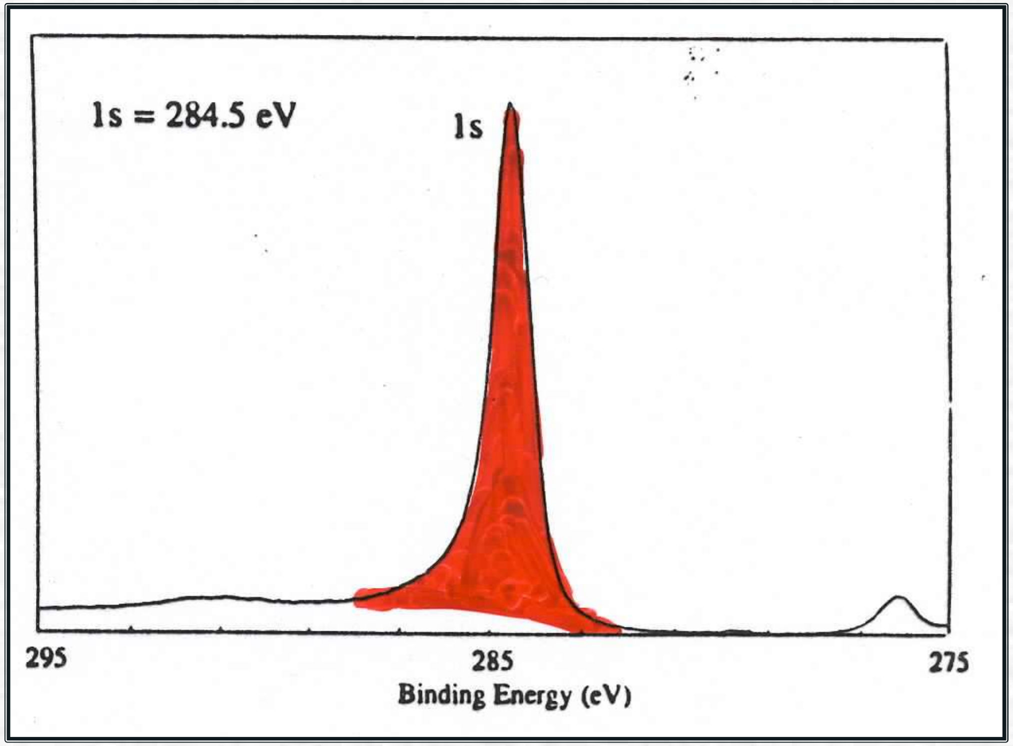


# Wide XPS spectrum of graphite (C)



# Photoemission Spectroscopy

Core level XPS spectrum of graphite (C)



The singlet C 1s line is characterized by:

1) A specific binding energy which reflects the specific atomic species (C) in a specific chemical environment

2) A finite width reflecting the instrumental resolution, lifetime broadening and other many-body effects

# Core Levels, chemical shift

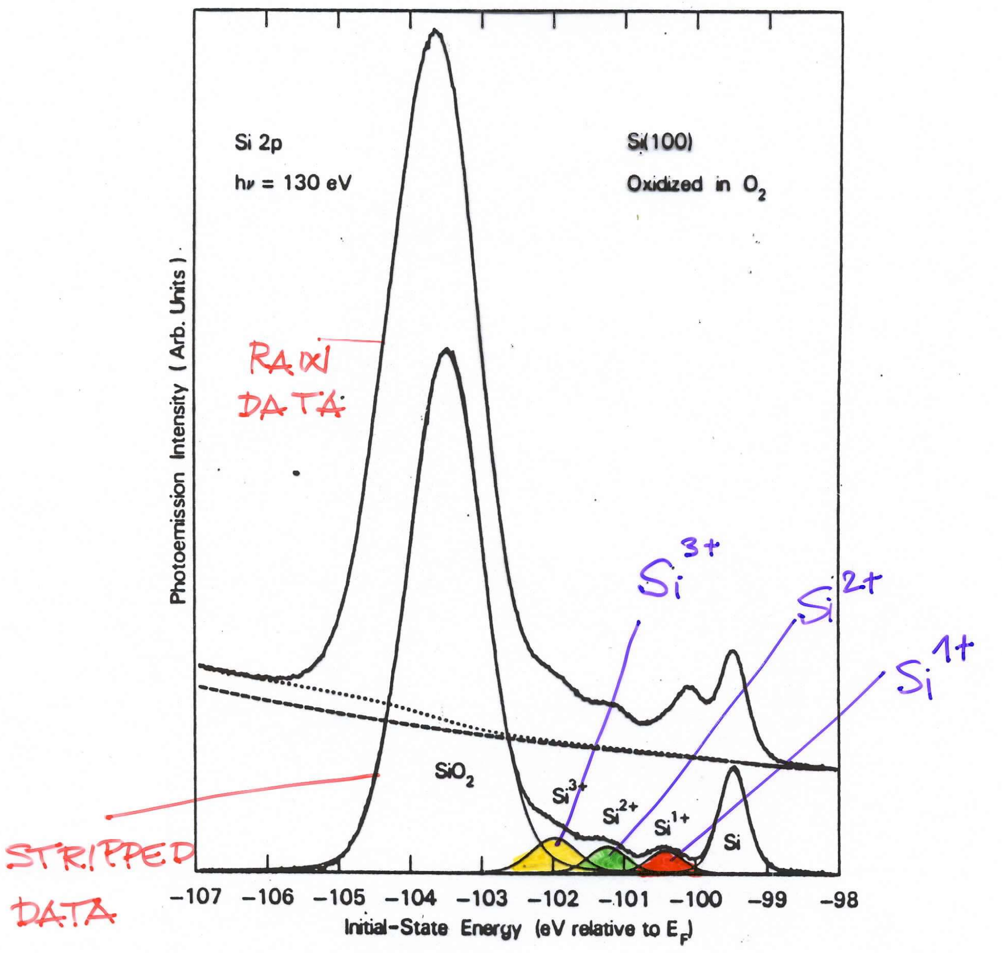
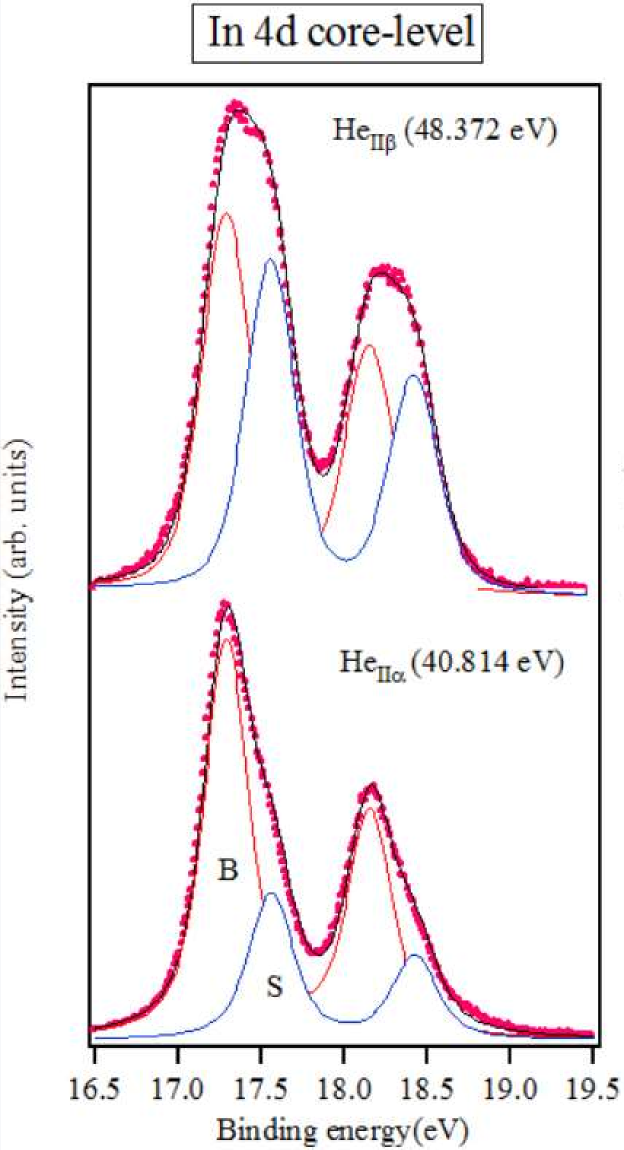
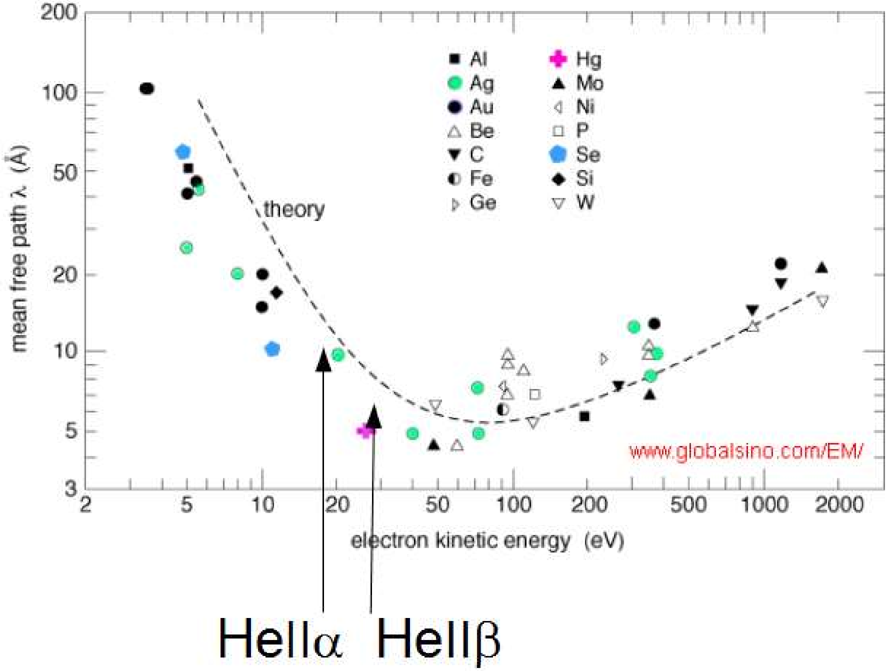


FIG. 1. Intermediate-oxidation states at the $SiO_2$/Si(100) interface, identified by their Si 2*p* core-level shifts. The top curve represents the raw photoemission data for the Si $2p_{1/2,3/2}$ core levels. The bottom curve has the Si $2p_{1/2}$ line and the secondary electron background subtracted. All three intermediate-oxidation states are seen. For a truncated bulk structure only $Si^{2+}$ would be present since the Si(100) surface has two broken bonds per atom.

**The Si 2*p* line is characterized by the occurrence of 5 chemically distinct components which reflect different chemical states of the Si atoms at the interface**

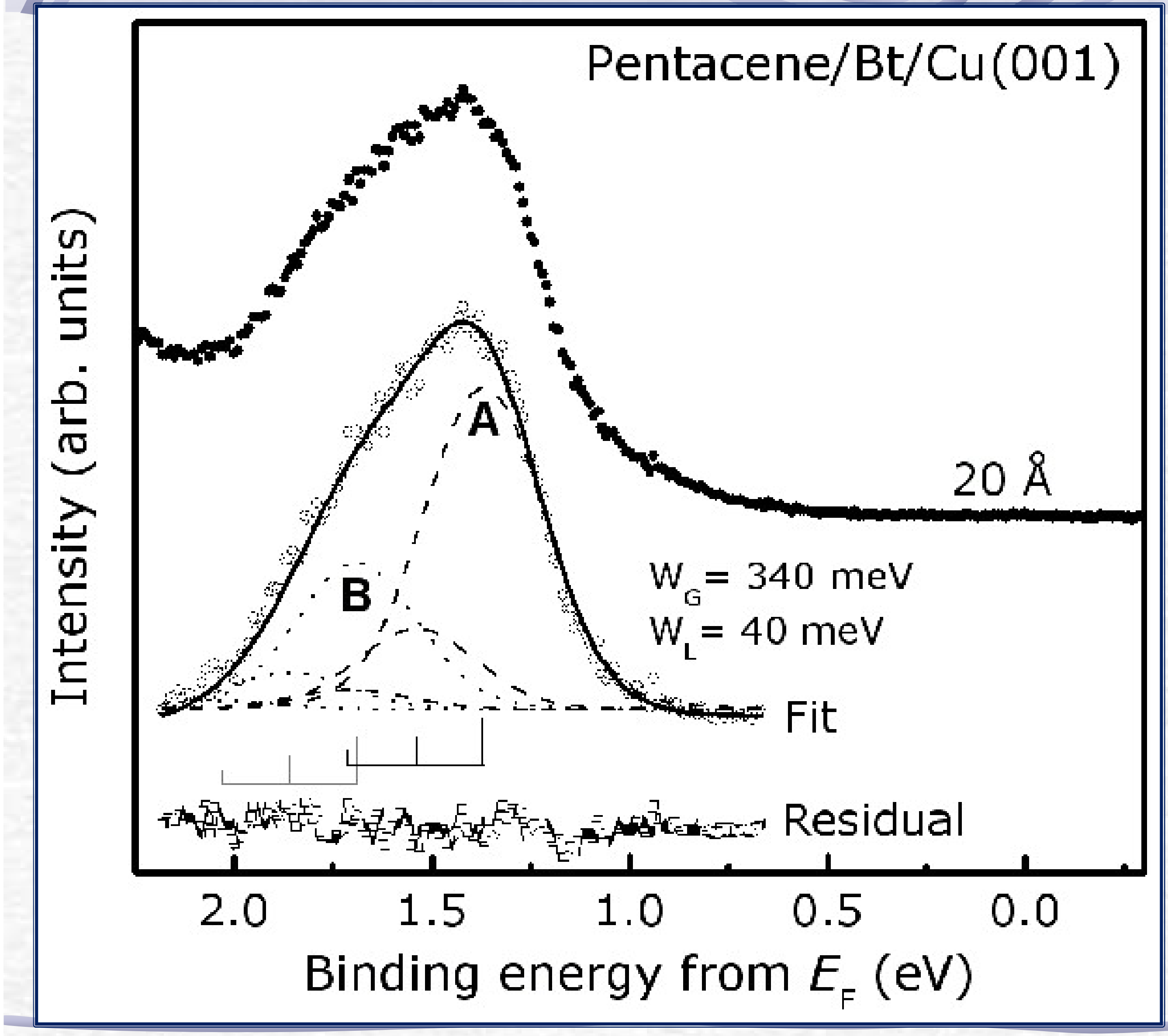
# Surface core level shift vs. mean free path In 4d

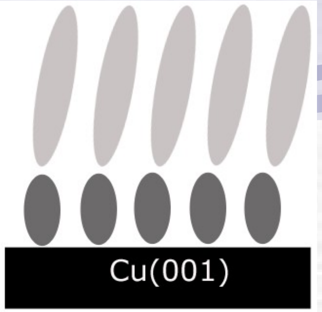


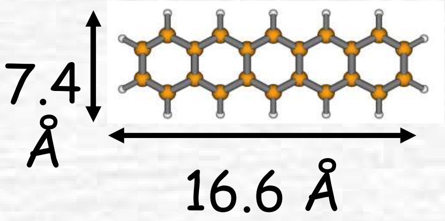


High-resolution In-4d core-levels at freshly cleaved InAs(110), taken with $He_{IIa}$ and $He_{IIb}$ radiation; Voigt-profiled fit with surface (S, blu lines) and bulk (B, red lines) doublet components (left panel)

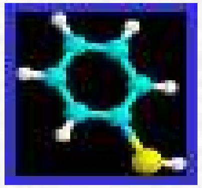
# Valence PE vibrational spectrum







pentacene: $C_{22}H_{14}$

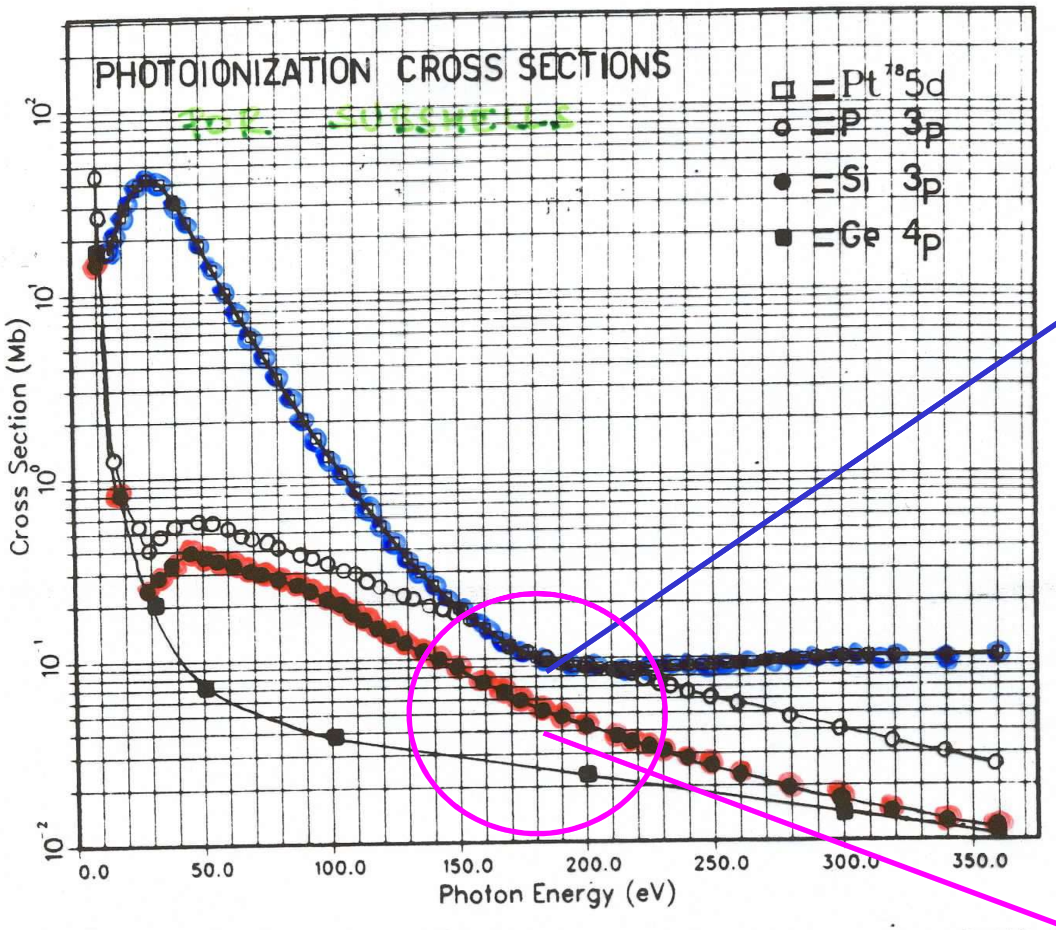


benzene-thiol:
$C_6H_5$-SH

Betti, Kanjilal and Mariani, J. Phys. Chem. A **111**, 12454 (2007)

# Cooper Minimum Photoemission

**It is possible when one of the valence band orbital shows a Cooper minimum in the photoionization cross section**



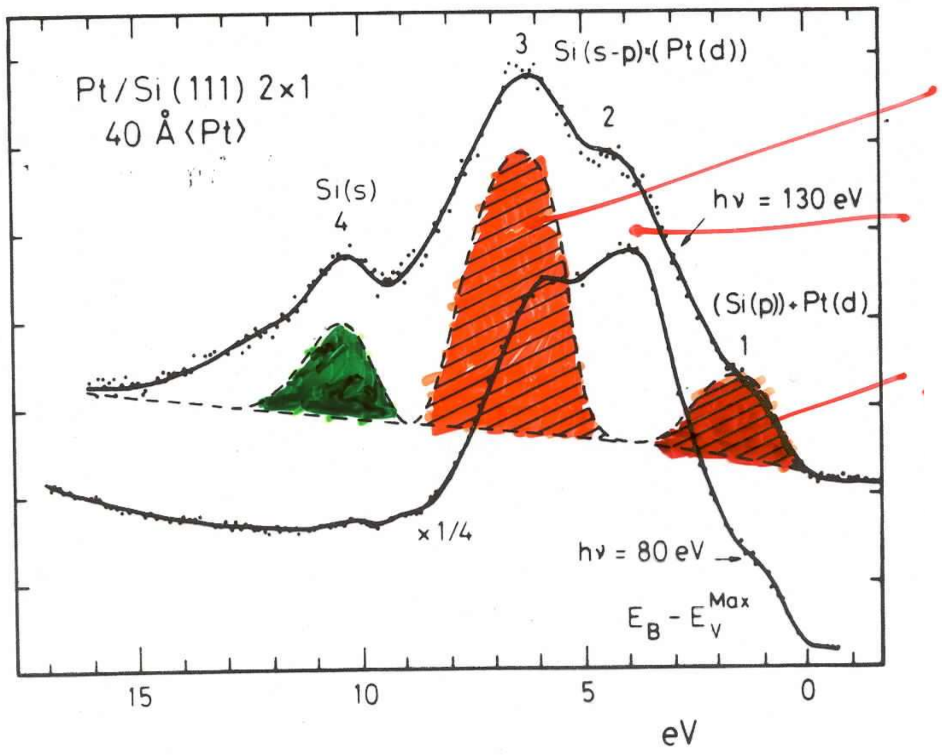
. Photoionization cross section for 4d and 5d subshells in the energy range 0–200 eV compared to the cross sections for the 3ps and 4sp valence states of the semiconductors [21].

Cooper minimum in the Pt 5*d* cross section

A Cooper minimum exists when the radial part of the orbital wave function exhibits a node

The Pt 5*d* and Si 3*p* cross sections are comparable

# Cooper Minimum Photoemission



Pt 5*d* anti-bonding

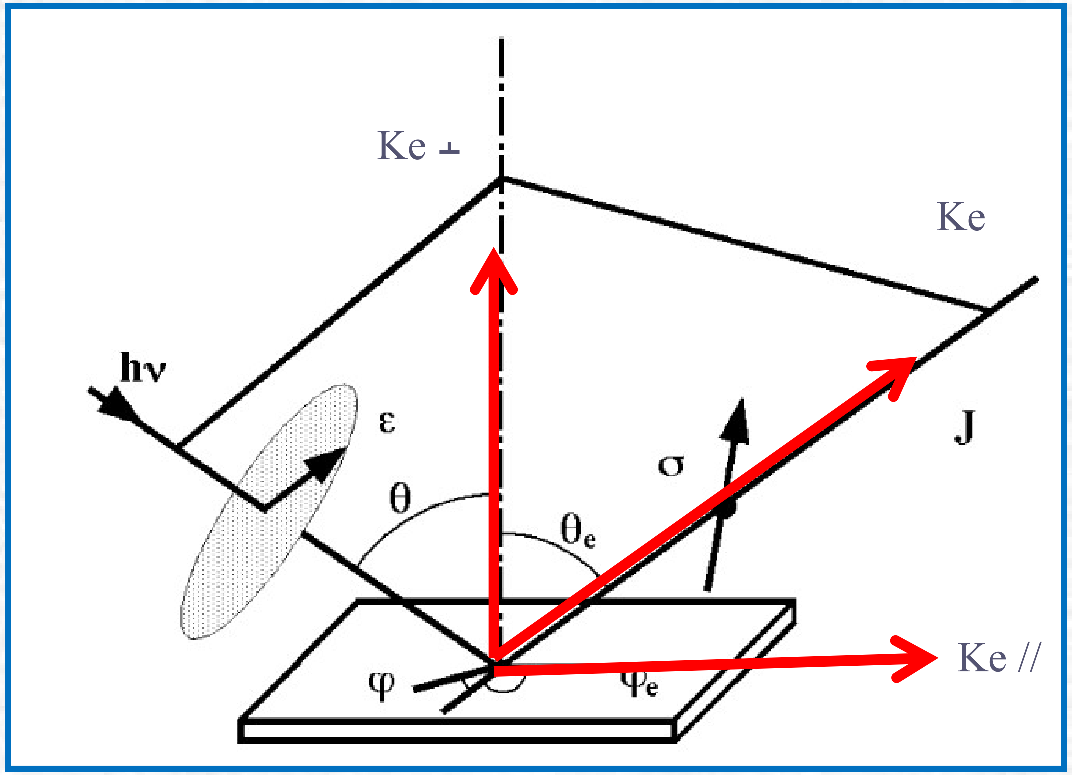
Pt 5*d* non-bonding

Pt 5*d* bonding

. Analysis of the Si sp partial DOS at the Pt–Si(111) reacted interface (40 Å Pt–Si(111) at room temperature). The top panel displays the CM and the $h\nu = 80$ eV photoemission data, and a three-peak partial DOS that accounts for the Si hybridized 3sp charge at the interface; a gap is present in correspondence to the localized Pt 5d states. The same three-peak partial DOS is then self-convoluted and compared to the integrated Si $L_{2,3}$VV lineshape. The correspondence of all peaks and relative intensities (a part of the known reduction of the Si 3s contribution) confirms the CM derivation of the Si sp partial DOS [159].

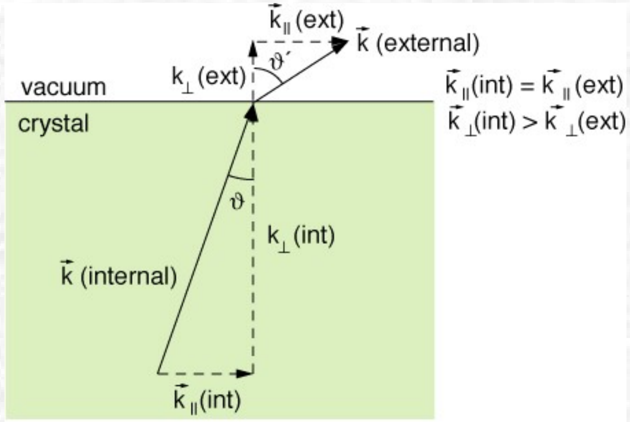
**A joint analysis of VB photoemission spectra taken at and off the Cooper minimum enables one to disentangle the differing site- and orbital-specific contributions**

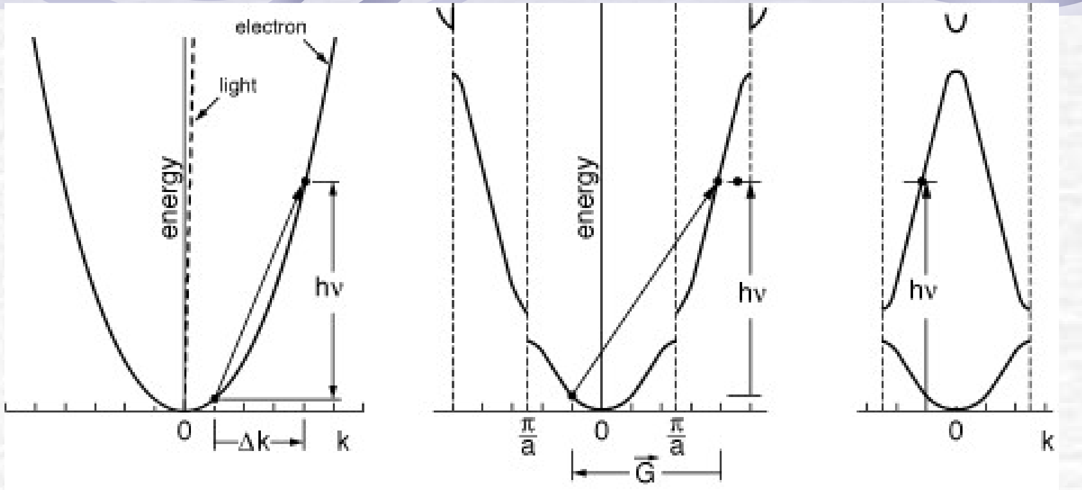
# Angular resolved photoemission



# angular resolved photoemission

How to photo-excite electrons from a crystal in a periodic potential, by photoemission

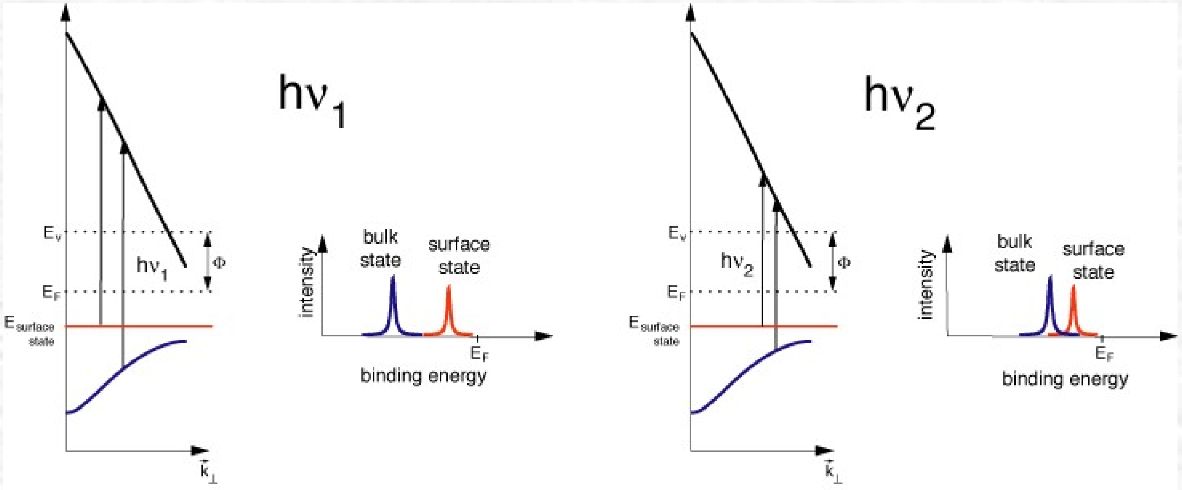




free electron/ constant potential

extended zone periodic potential

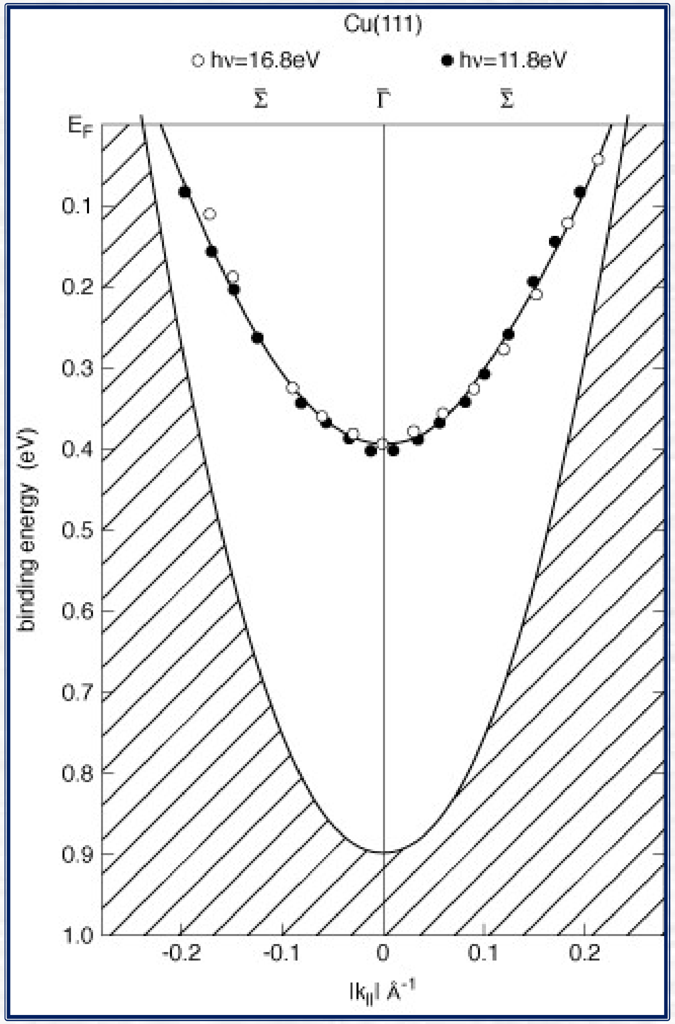
reduced zone periodic potential



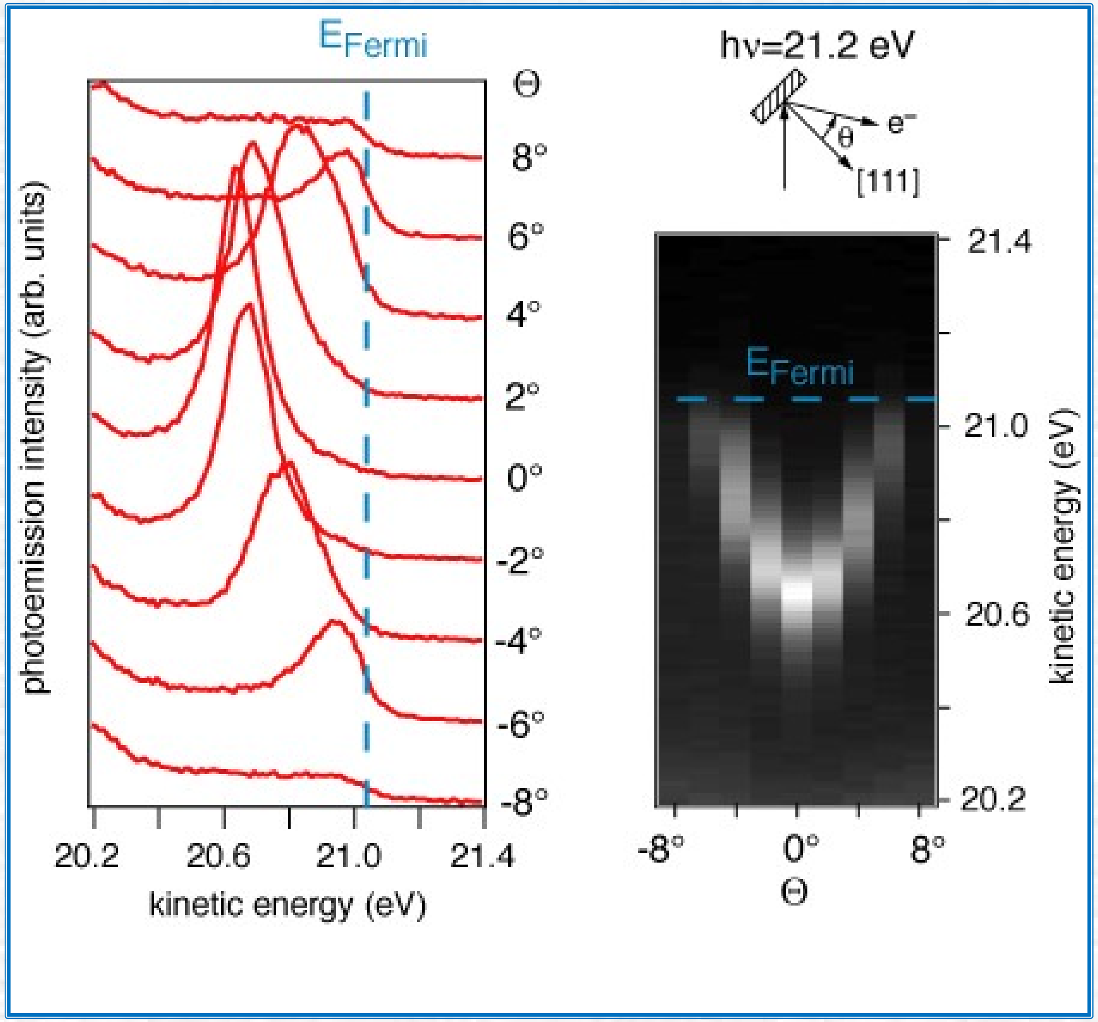
graphs from Ph. Hoffmann

$$\vec{k}_{||i} = \vec{k}_{||f} = \sin(\Theta)\sqrt{\frac{2m}{\hbar^2}}\sqrt{E_{kin}} = \sin(\Theta)\sqrt{\frac{2m}{\hbar^2}}\sqrt{h\nu - E_{bin} - e\Phi}$$

# electronic surface states at Cu(111)

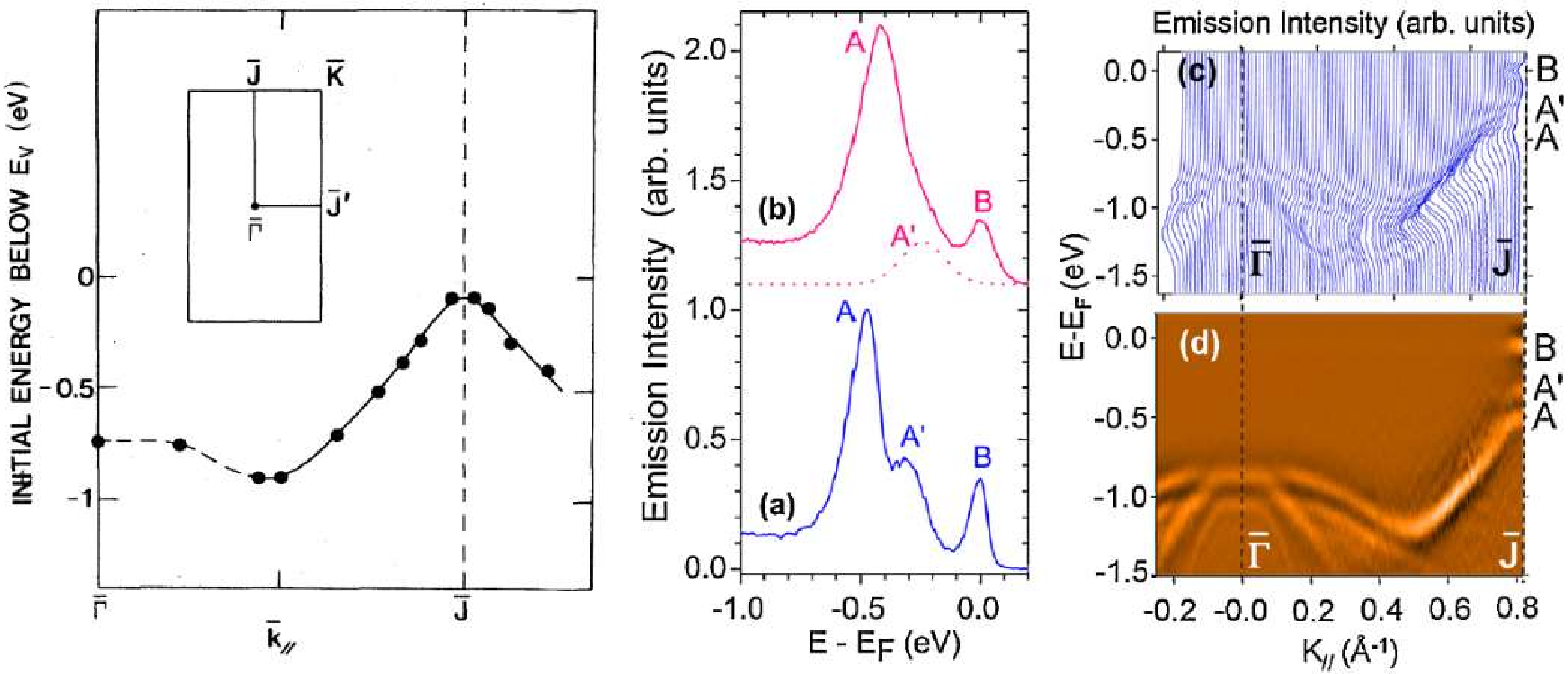


S.D. Kevan, Phys. Rev. Lett. 50,526 (1983).



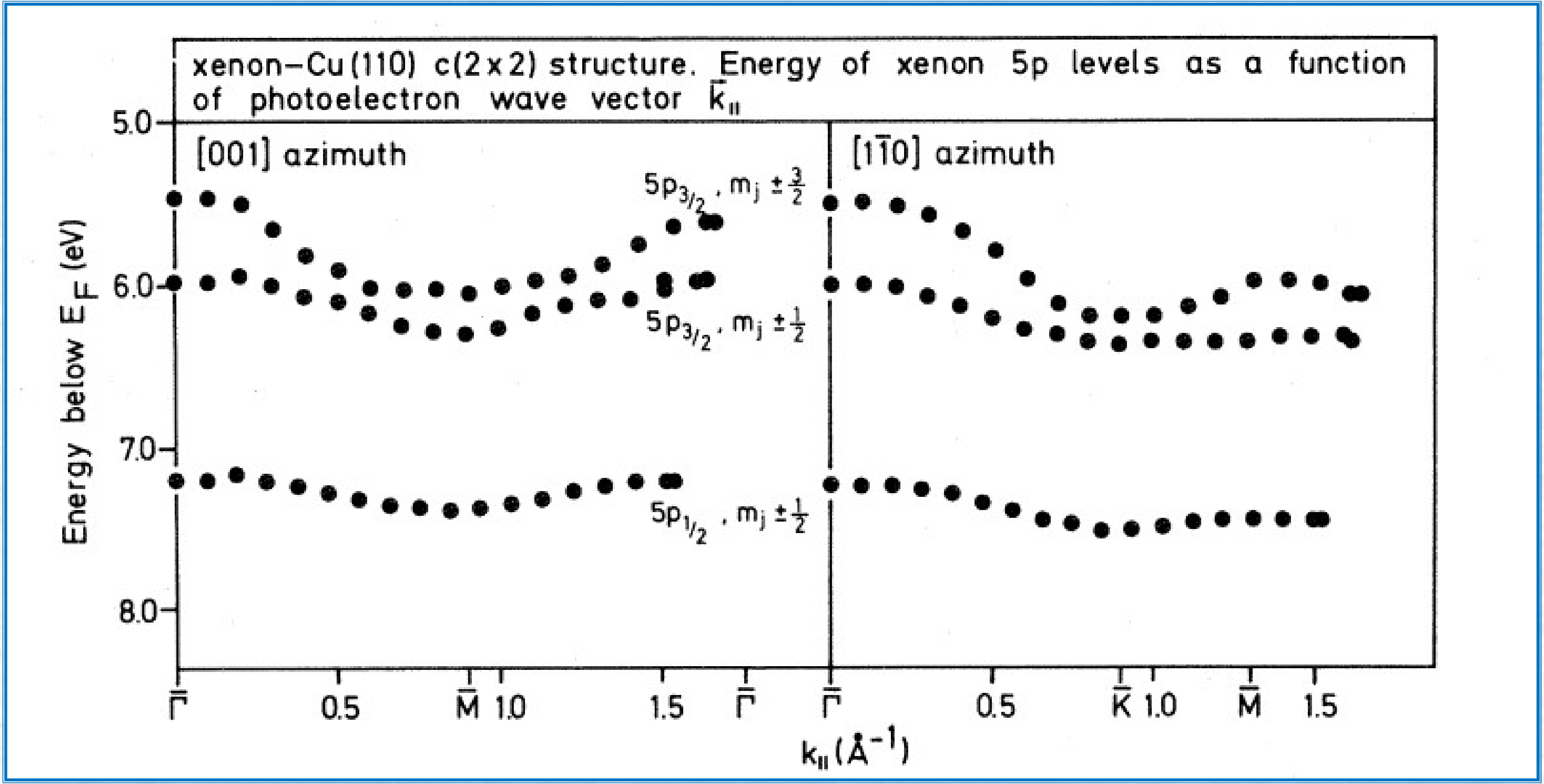
**quasi-free electron surface state** on Cu(111),
Schockley state, *s-like*

# Dangling bonds Si(111)-(2x1)



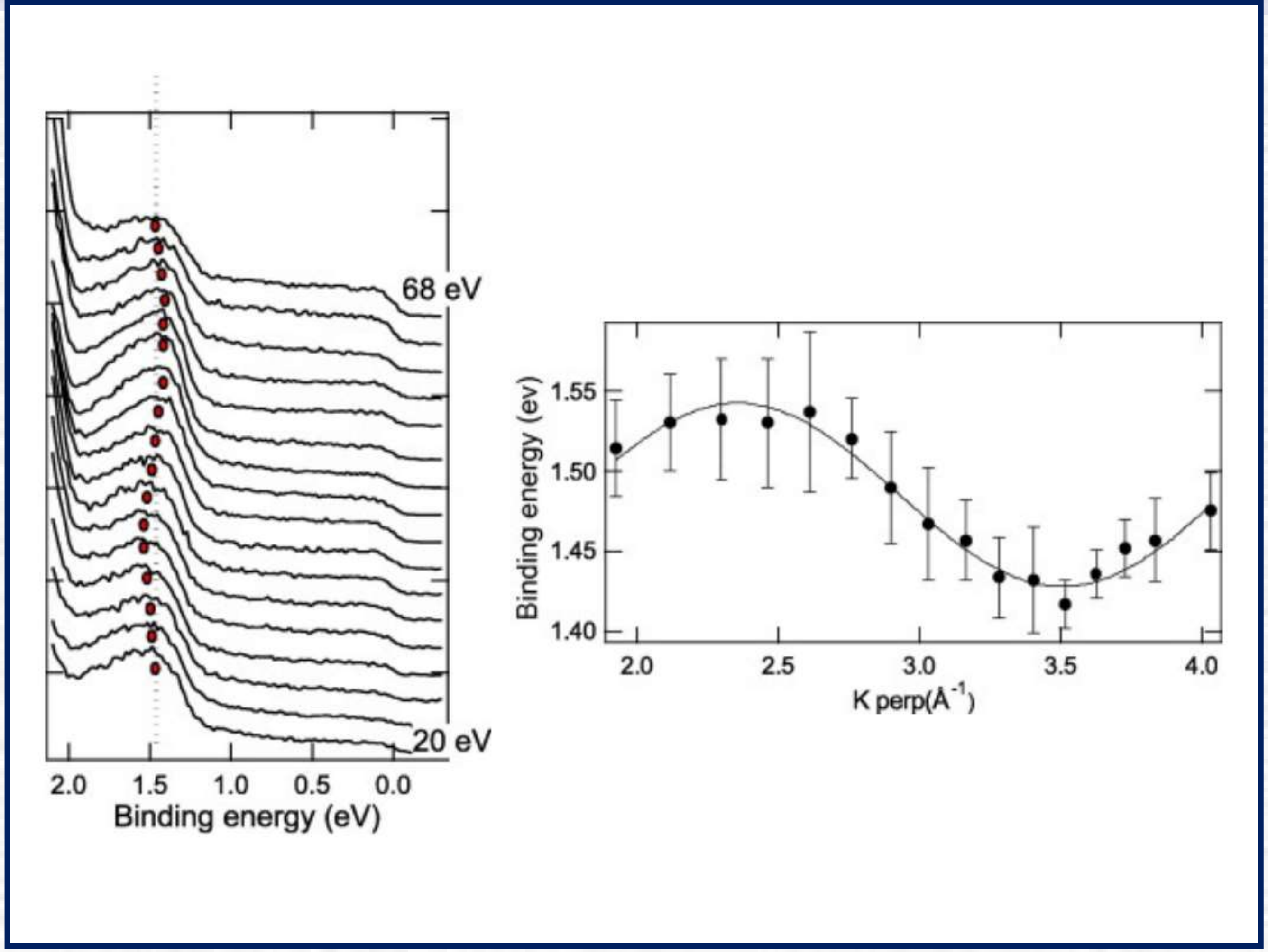
Dangling-bond surface state dispersion at the Si(111)-(2x1) reconstructed surface along the ΓJ direction of the Surface Brillouin Zone (SBZ). One of the first experimental ARPES dangling-bond dispersion (left panel); recent high-resolution ARPES dangling-bond dispersion.

# Physisorbed Xe c(2x2)/Cu(110)



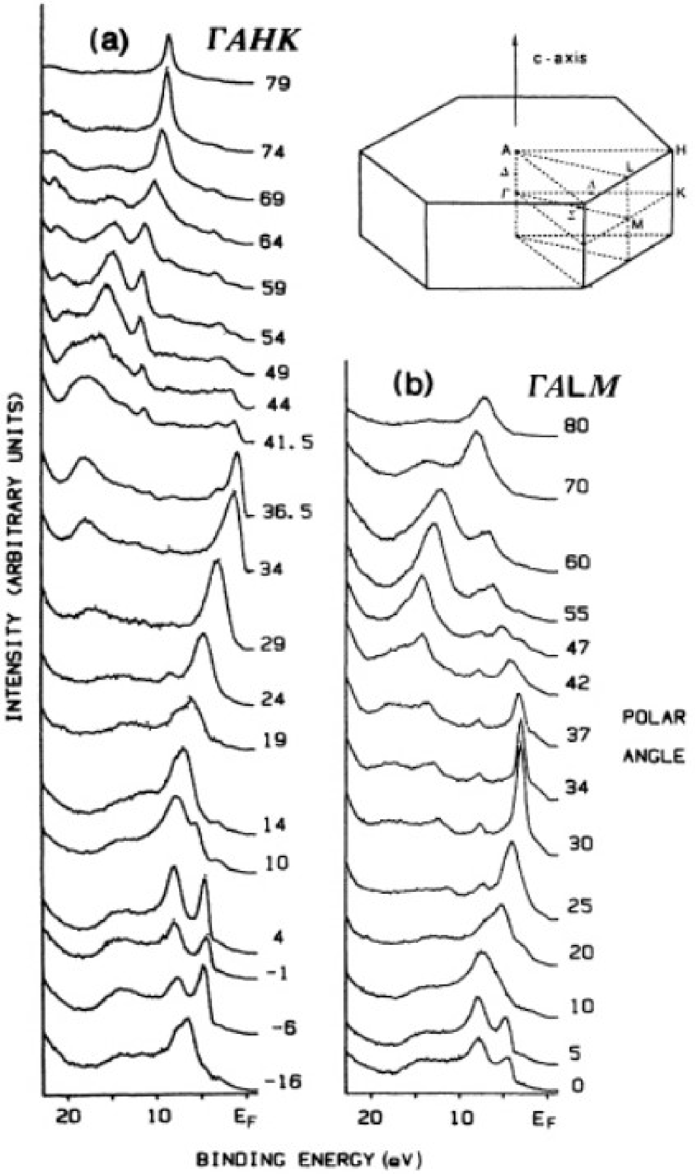
Experimental band structure of the 5p levels of Xe physisorbed in an ordered c(2×2) structure onto the Cu(110) surface. ARPES bands

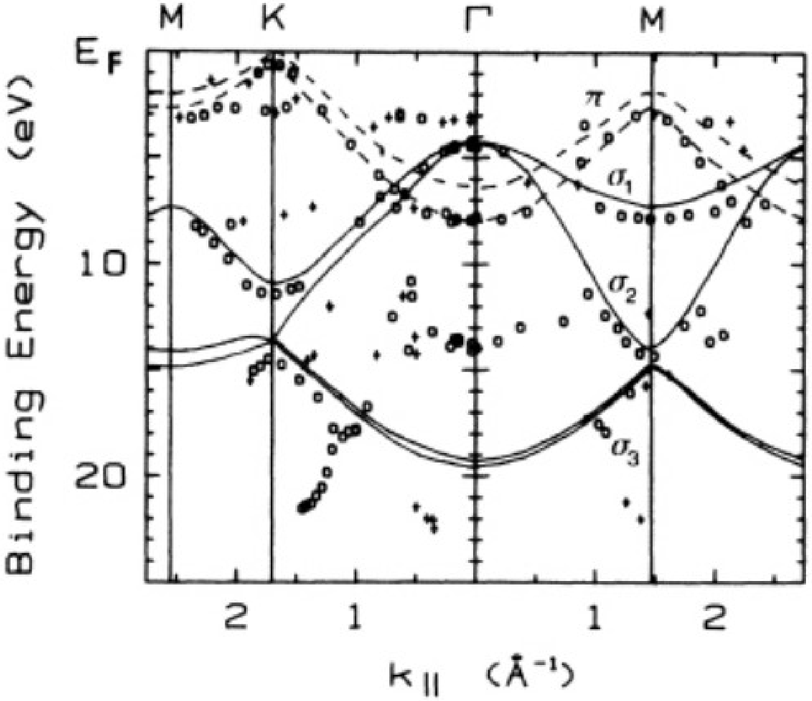
# Pentacene HOMO on Cu(119)



2-nm thick pentacene film grown on Cu(119). ARPES selection of spectra taken at normal emission and varying the photon energy (left); highest-occupied molecular-orbital (HOMO) band dispersion along $k_{\perp}$ (right).

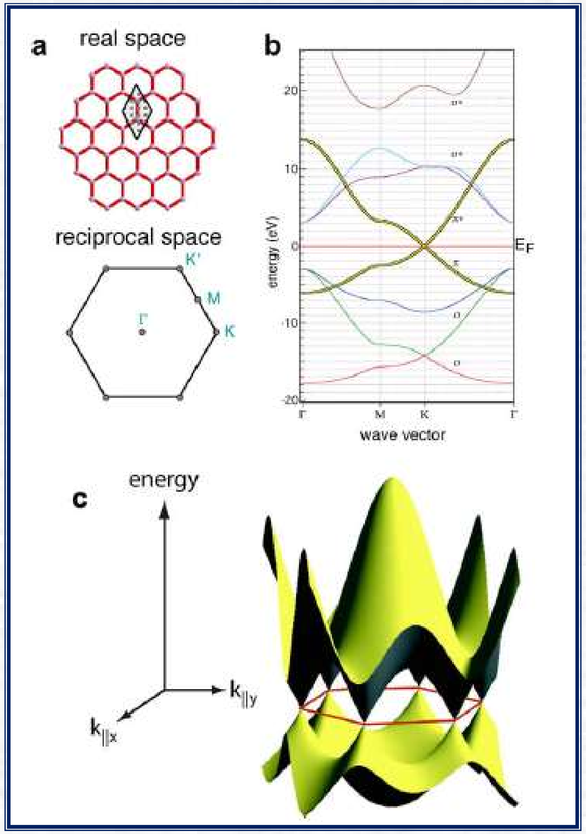
# ARPES graphite (HOPG)

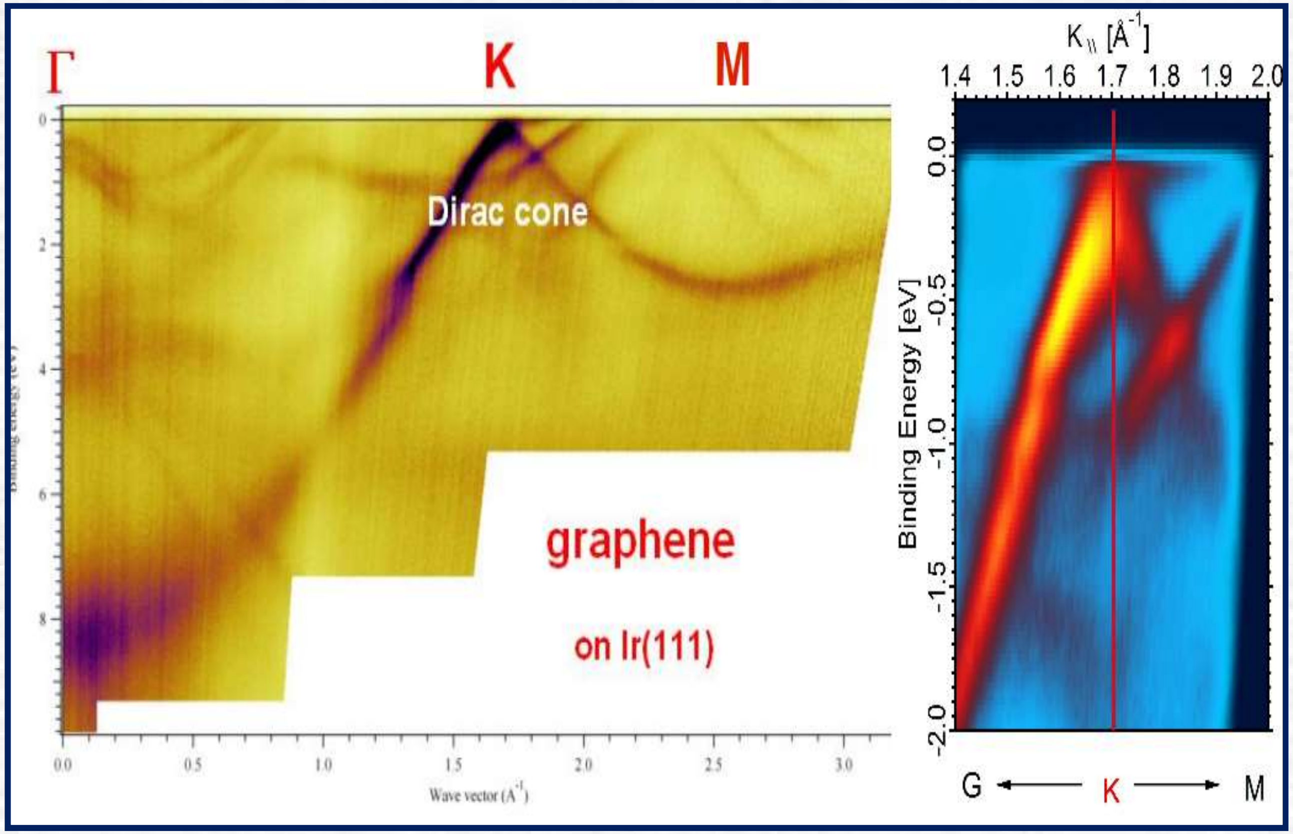




Valence band of graphite (HOPG), stacking of the ARPES spectra as a function of polar angle (left) and experimental band structure (right).

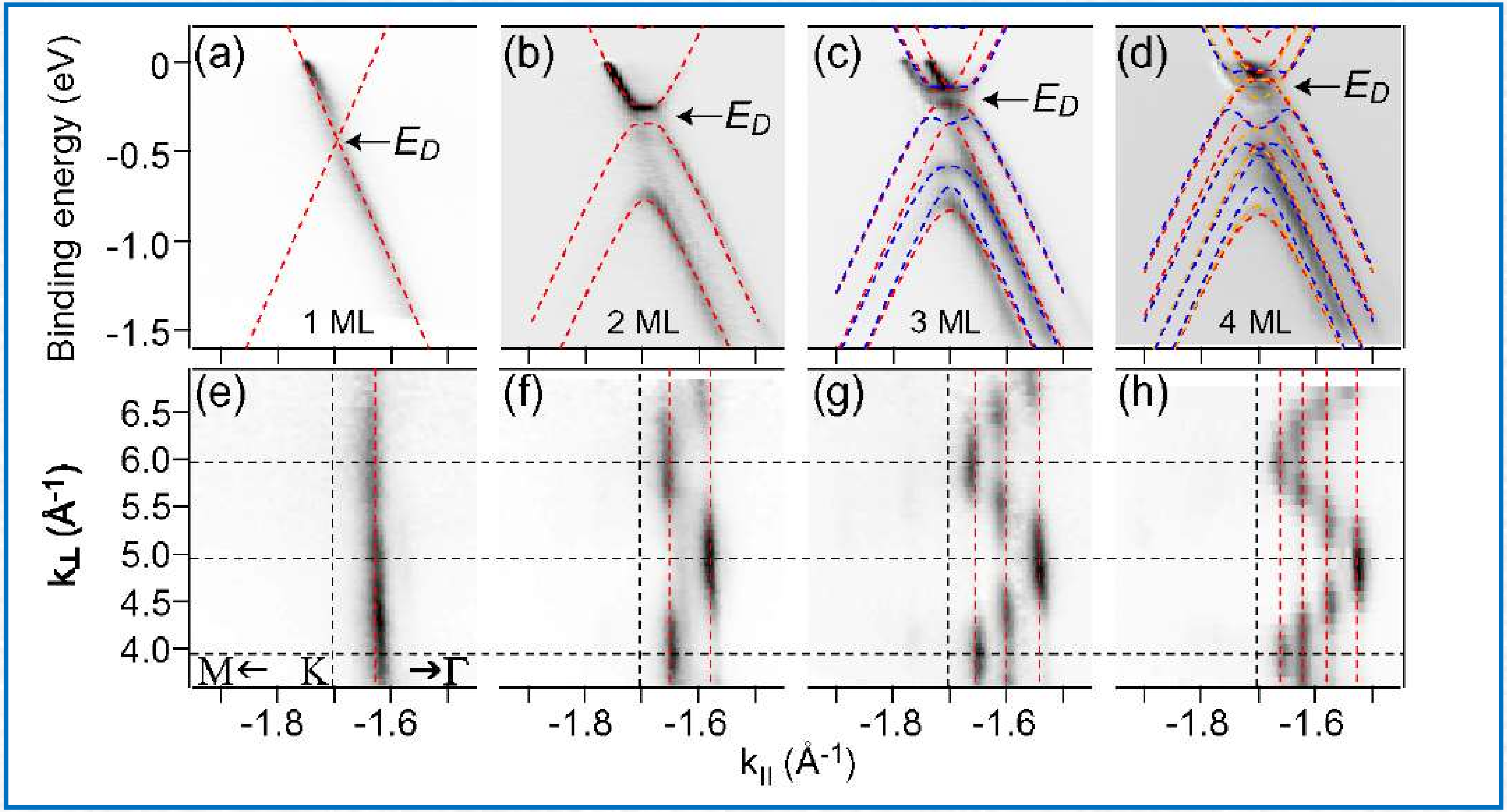
# Graphene band structure





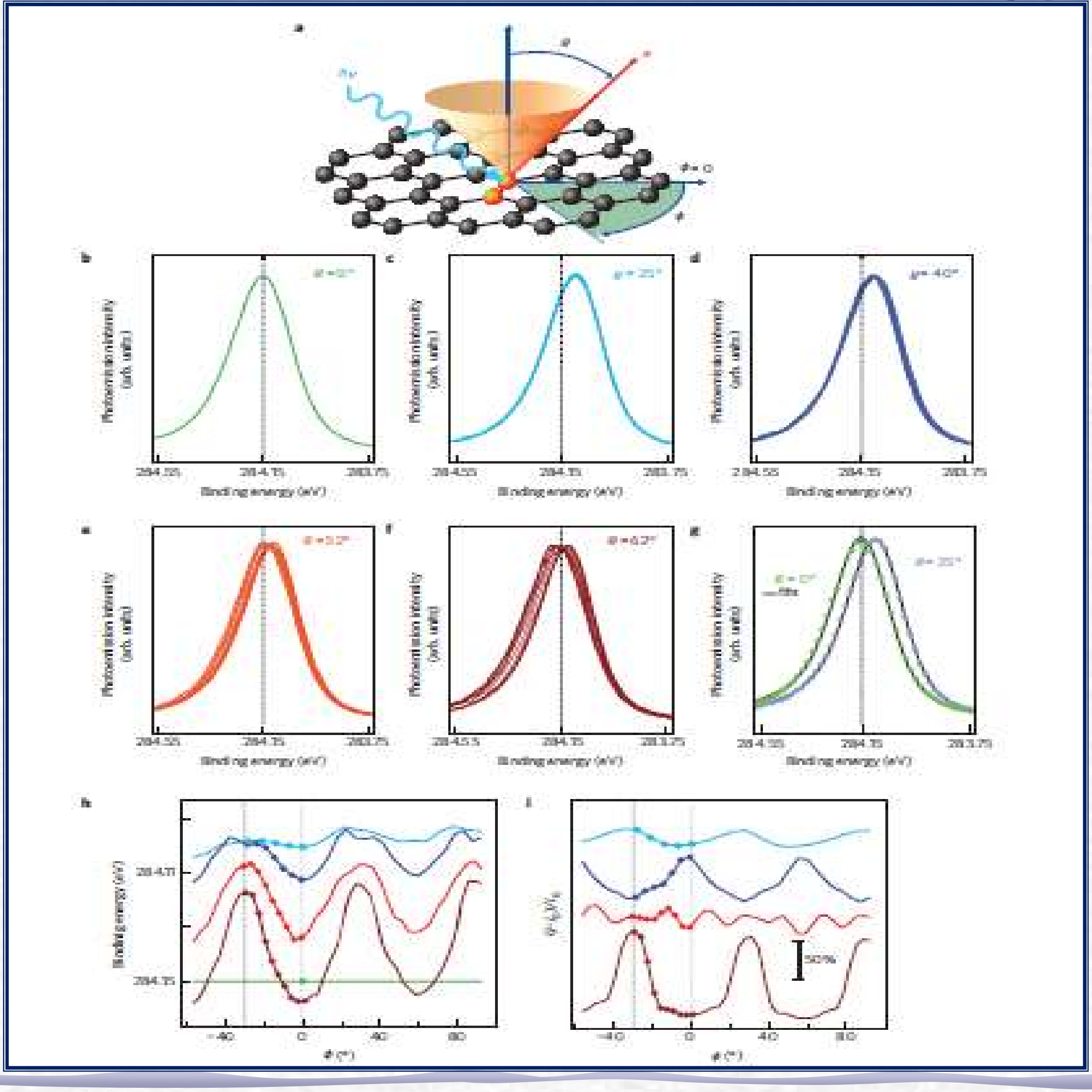
Graphene band structure along ΓKM and zoom of the Dirac cone around the K point of the SBZ. ARPES data taken with high-resolution ARPES and a He discharge source

# Band formation in graphene multilayers



Formation of an electronic band, stepwise: from 1-layer (extreme left) to 4-layer (extreme right) graphene band structure along across the Dirac point.

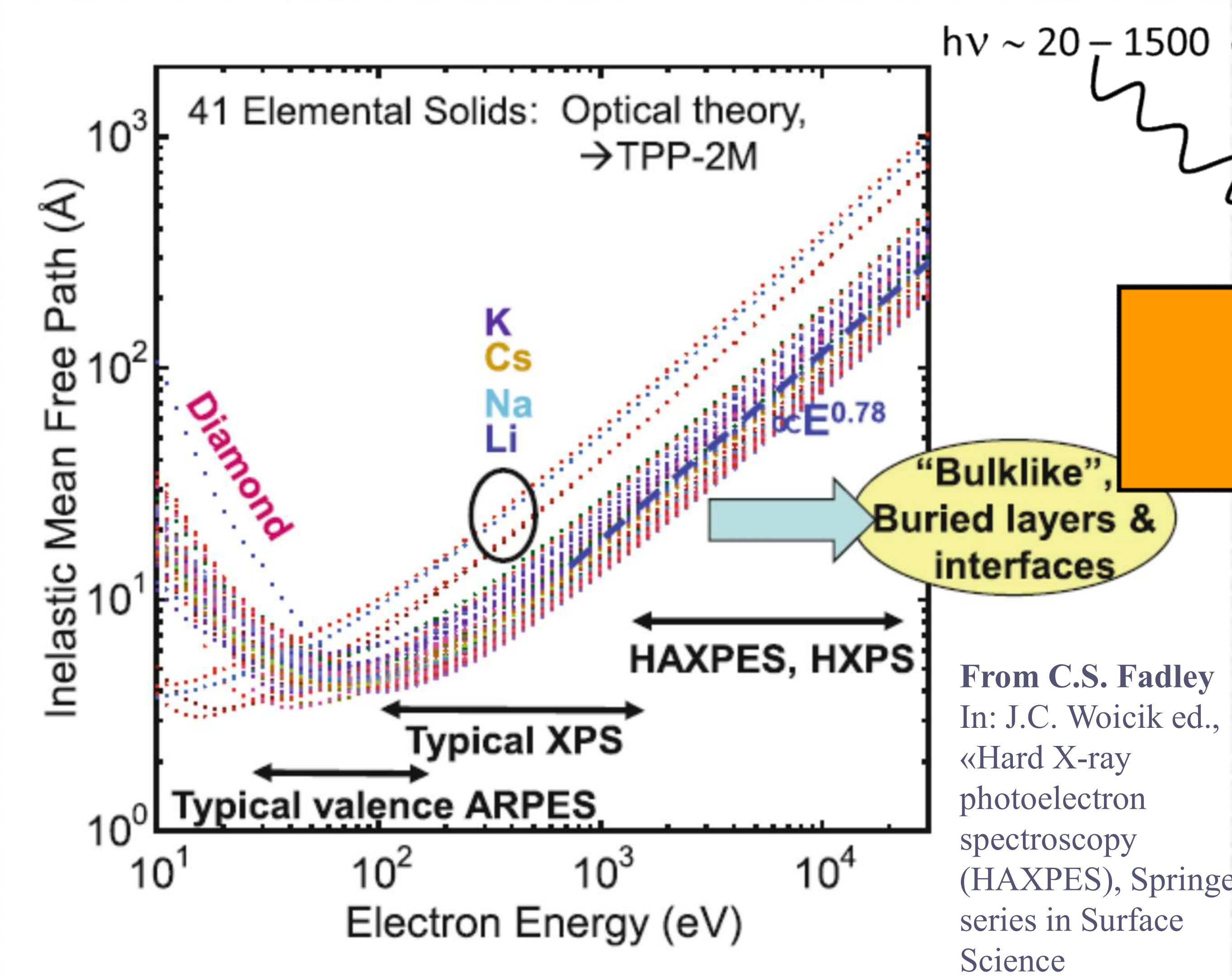
# K shell dispersion in graphene



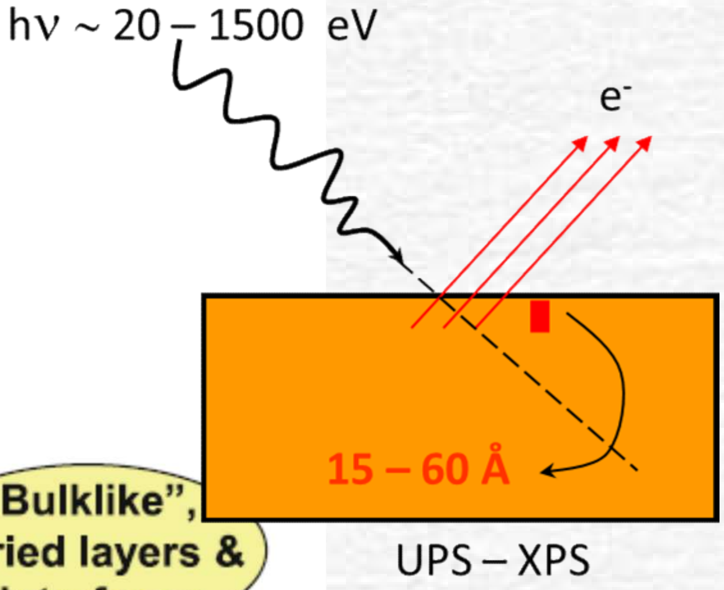
Spectral function of the C 1s core-level in graphene as a function of the emission polar angle

Silvano Lizzit, et al.: Nature Physics **6**, 345-349 (2010)

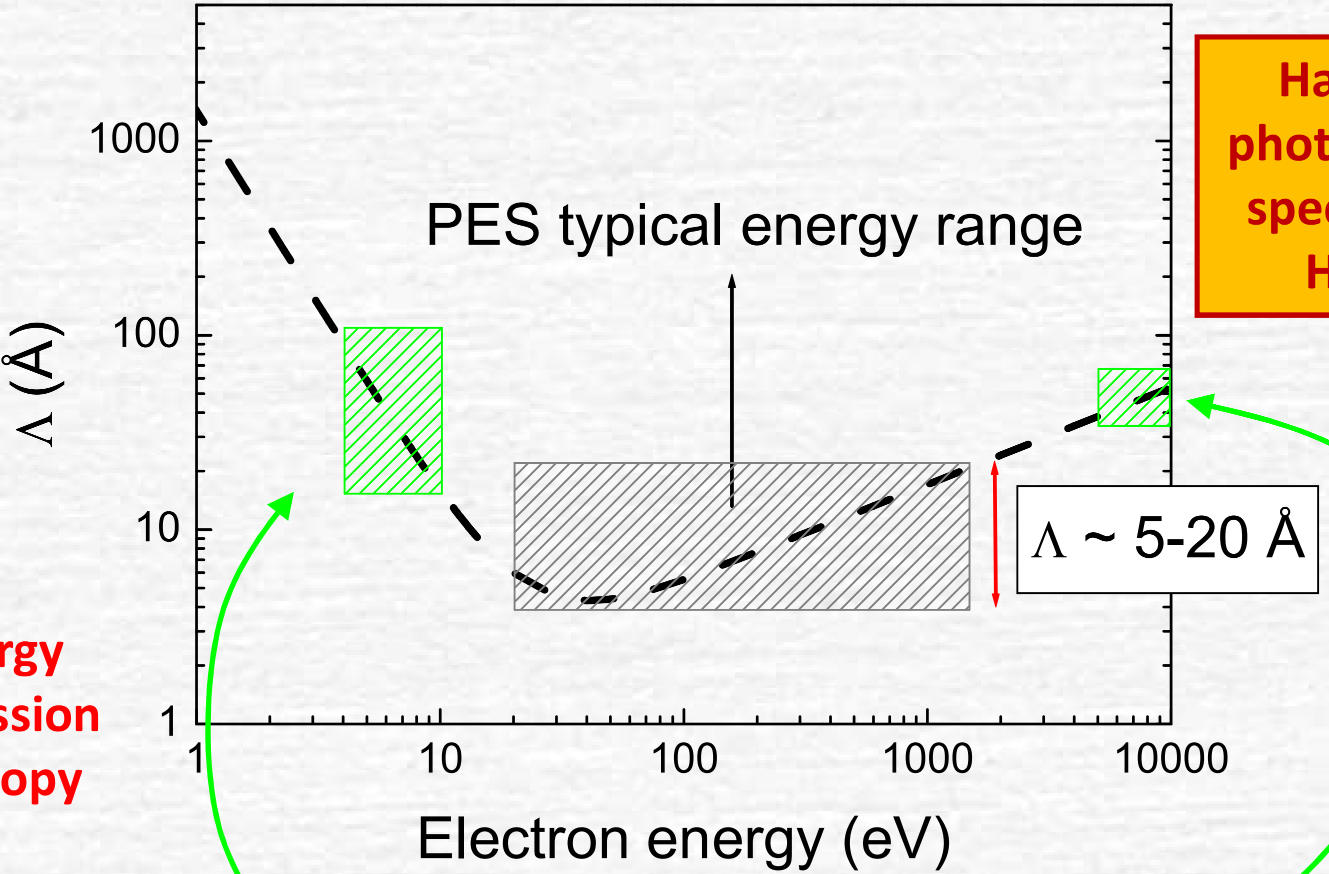
# Why Hard X-ray PES (HAXPES) ?



**From C.S. Fadley**
In: J.C. Woicik ed., «Hard X-ray photoelectron spectroscopy (HAXPES), Springer series in Surface Science



PES is extremely **surface sensitive**: typically information is retrieved from the topmost ~ 10 – 50 Å.



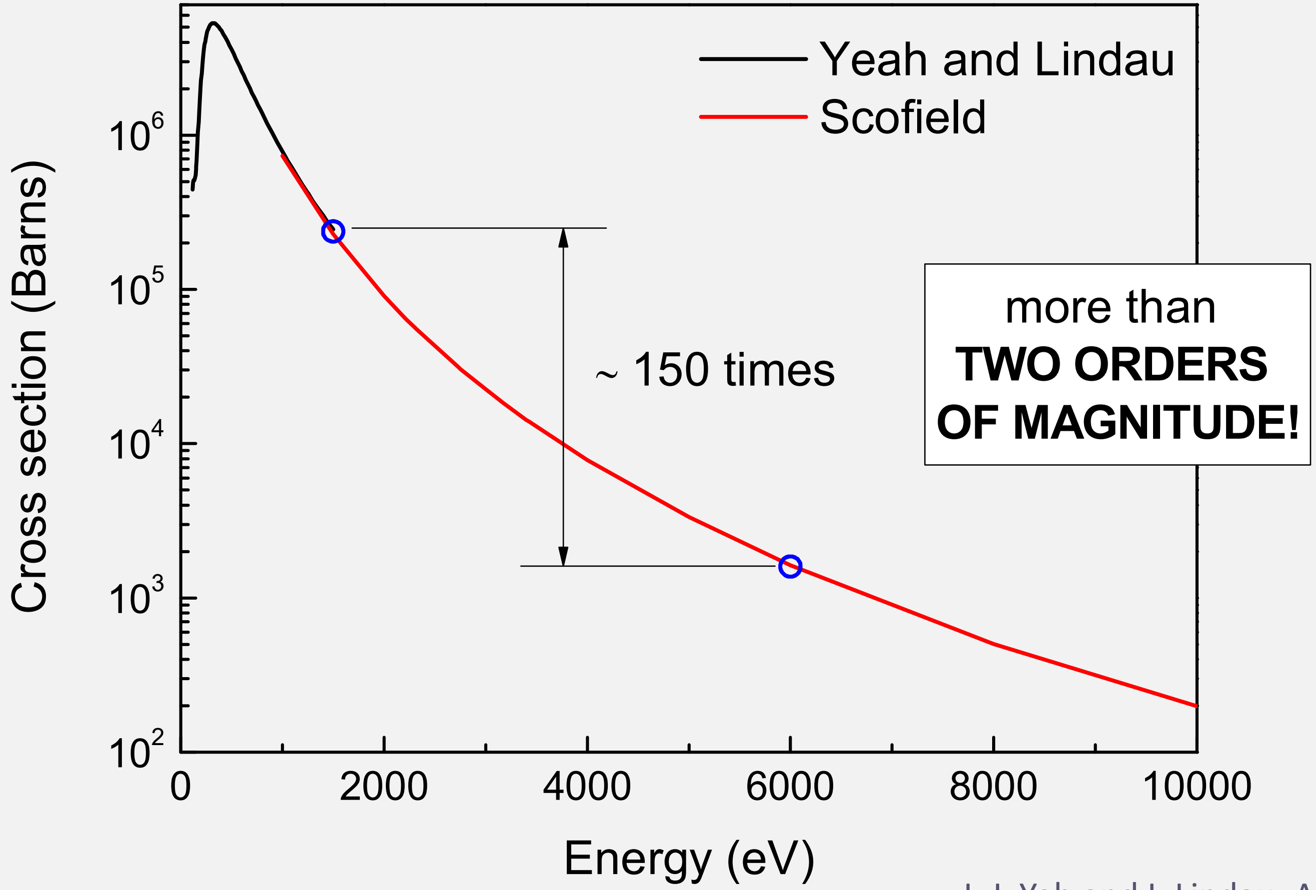
**Hard x-ray photoemission spectroscopy HAXPES**

**Low energy photoemission spectroscopy LEPES**

IMFP enhanced at both low (< 10 eV) and high energy (> 5 keV)

Courtesy of F. Offi

# Main difficulty with HAXPES



more than
**TWO ORDERS**
**OF MAGNITUDE!**

J. J. Yeh and I. Lindau, At. Data Nucl. Data Tables **32**, 1 (1985)
J. H. Scofield, LLNL Report, UCRL-51326 (1973)

Courtesy of F. Offi

# Early attempts

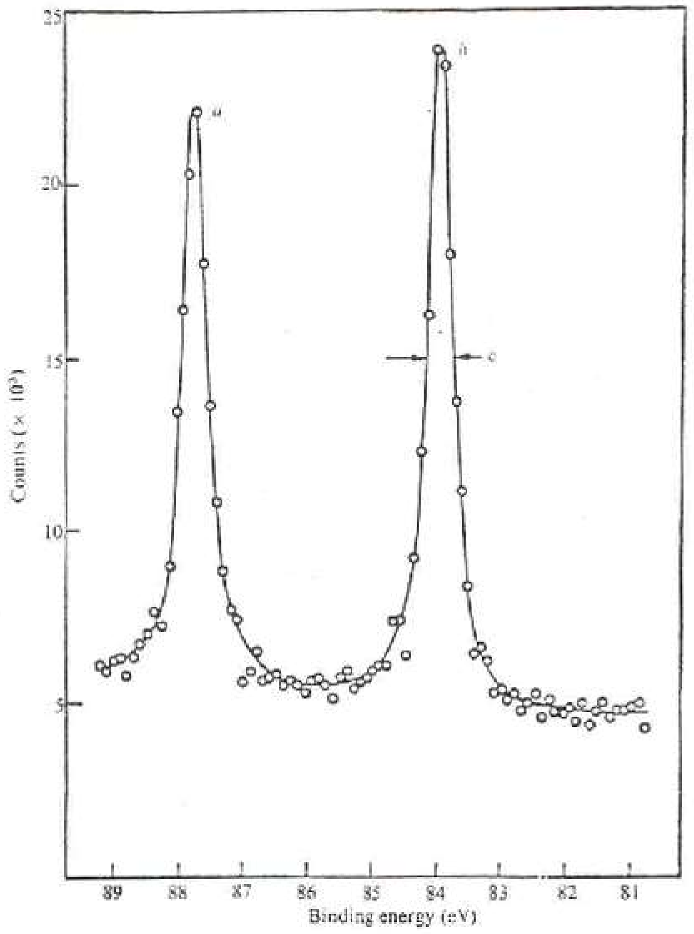


Fig. 2 Electron distribution curve for the 4f doublet of gold. The Fermi level is chosen as the reference level for the binding energy. a, $4f_{5/2}$ peak; b, $4f_{7/2}$ peak; c, 0.42 eV (FWHM).

Courtesy of F. Offi

Au 4*f* core level

**25 counts/s**

~8 keV Kinetic Energy

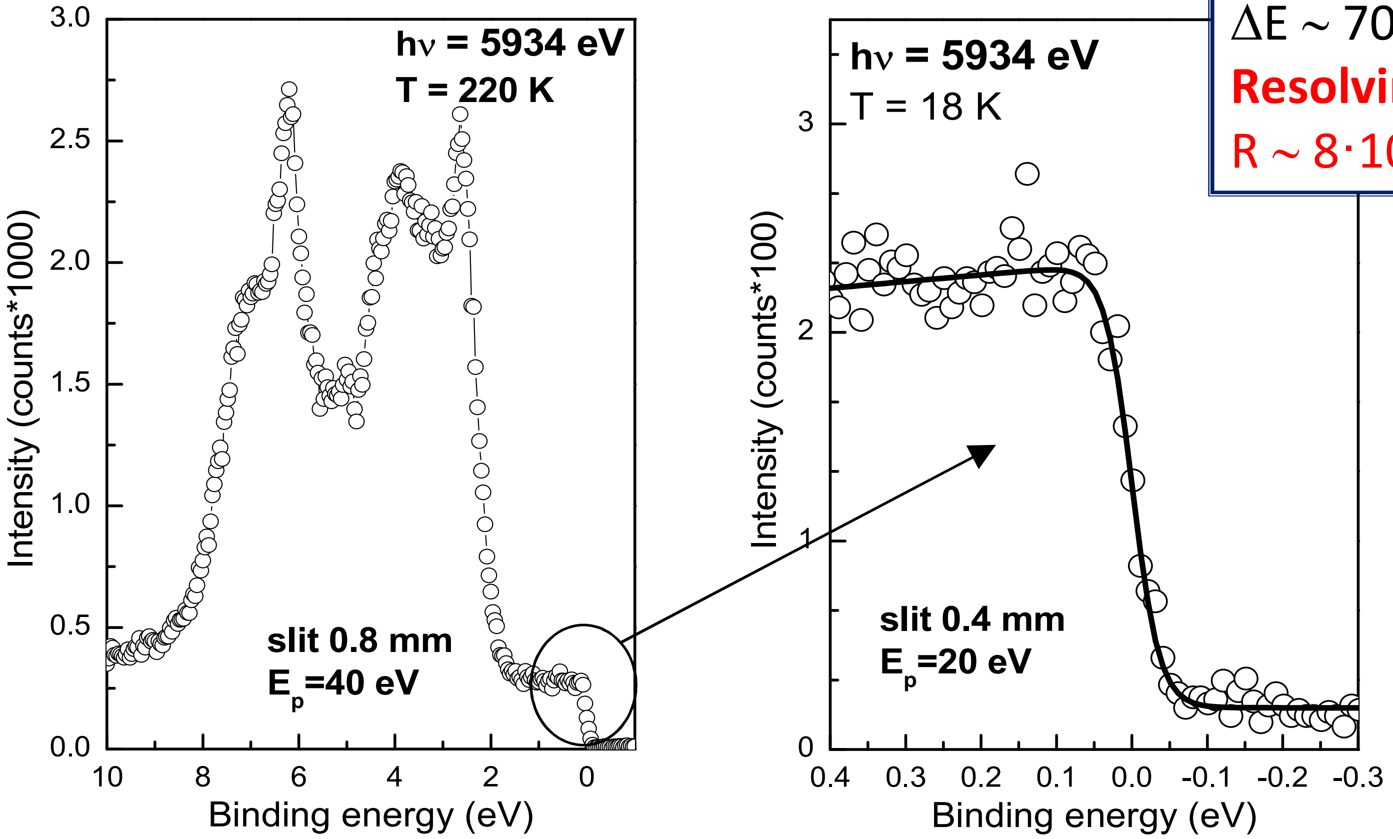
Total Energy Res. 420 meV

**NOT POSSIBILE TO MEASURE VALENCE BAND**

I. Lindau, P.Pianetta, S. Doniach, W.E. Spicer
Nature **250**, 214 (1974)

# RECENT RESULTS ON VALENCE BAND

**Au polycrystalline**



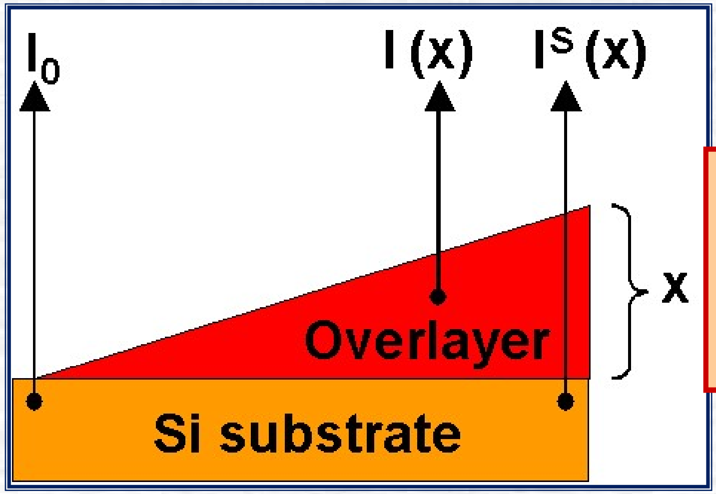
**Energy resolution**
ΔE ~ 70 meV
**Resolving power**
R ~ $8\cdot10^4$

G. Paolicelli *et al.,* Journal of Electron Spectroscopy and Related Phenomena **144-147**, 963 (2005)

# Estimation of the bulk sensitivity

Bulk sensitivity in PES is typically estimated via measurements of electron effective attenuation lenght (λ), the thickness of the overlayer that reduces to 1/e the intensity $I^S$ of a core level emission from the substrate.

The “overlayer” experiment:



$I^0$ = intensity from the bare substrate

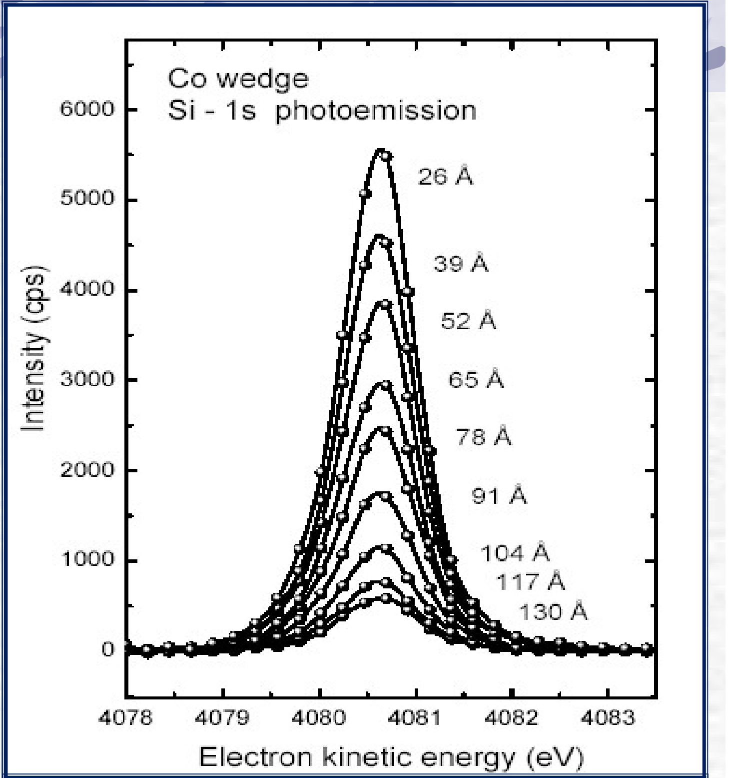
$$I^S(x) = I^0 e^{-\frac{x}{\lambda}}$$

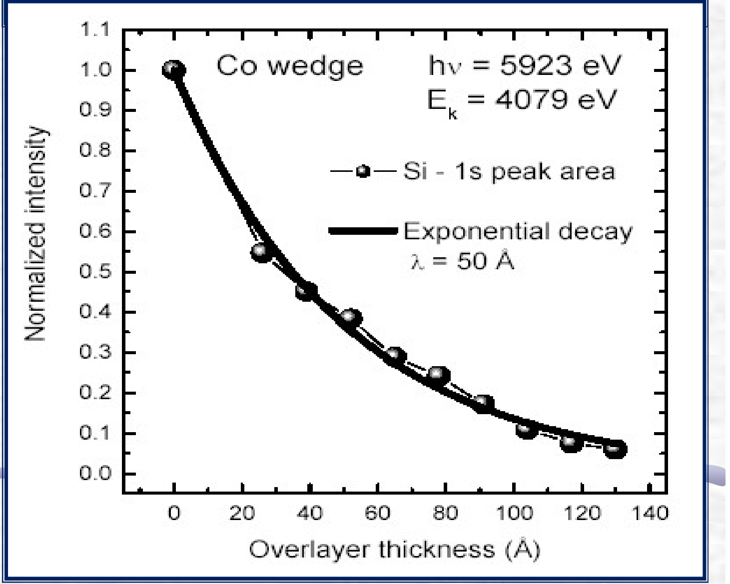
$$I(x) = I^T(1 - e^{-\frac{x}{\lambda}})$$

$I^T$ = intensity for an infinite overlayer

**Overlayer:**
**Co, Cu, Ge, and $Gd_2O_3$**

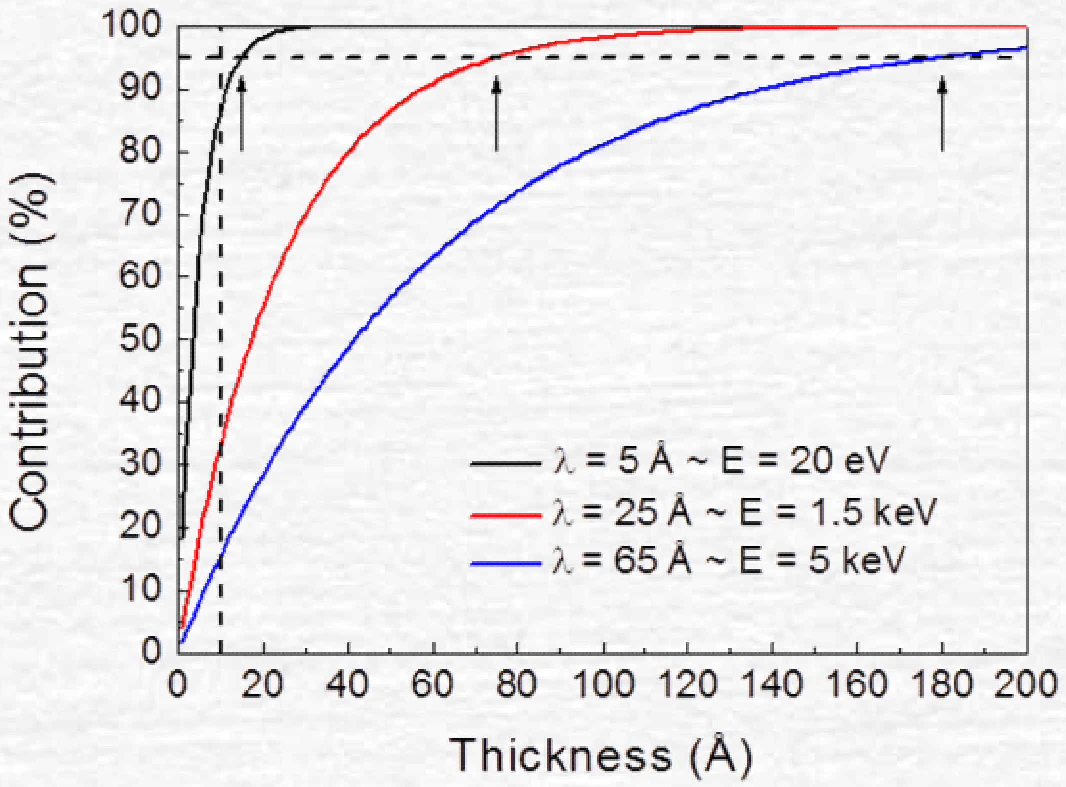
M. Sacchi *et al.*, Phys. Rev. B **71**, 155177 (2005)





Courtesy of F. Offi

# Contribution of the surface layer



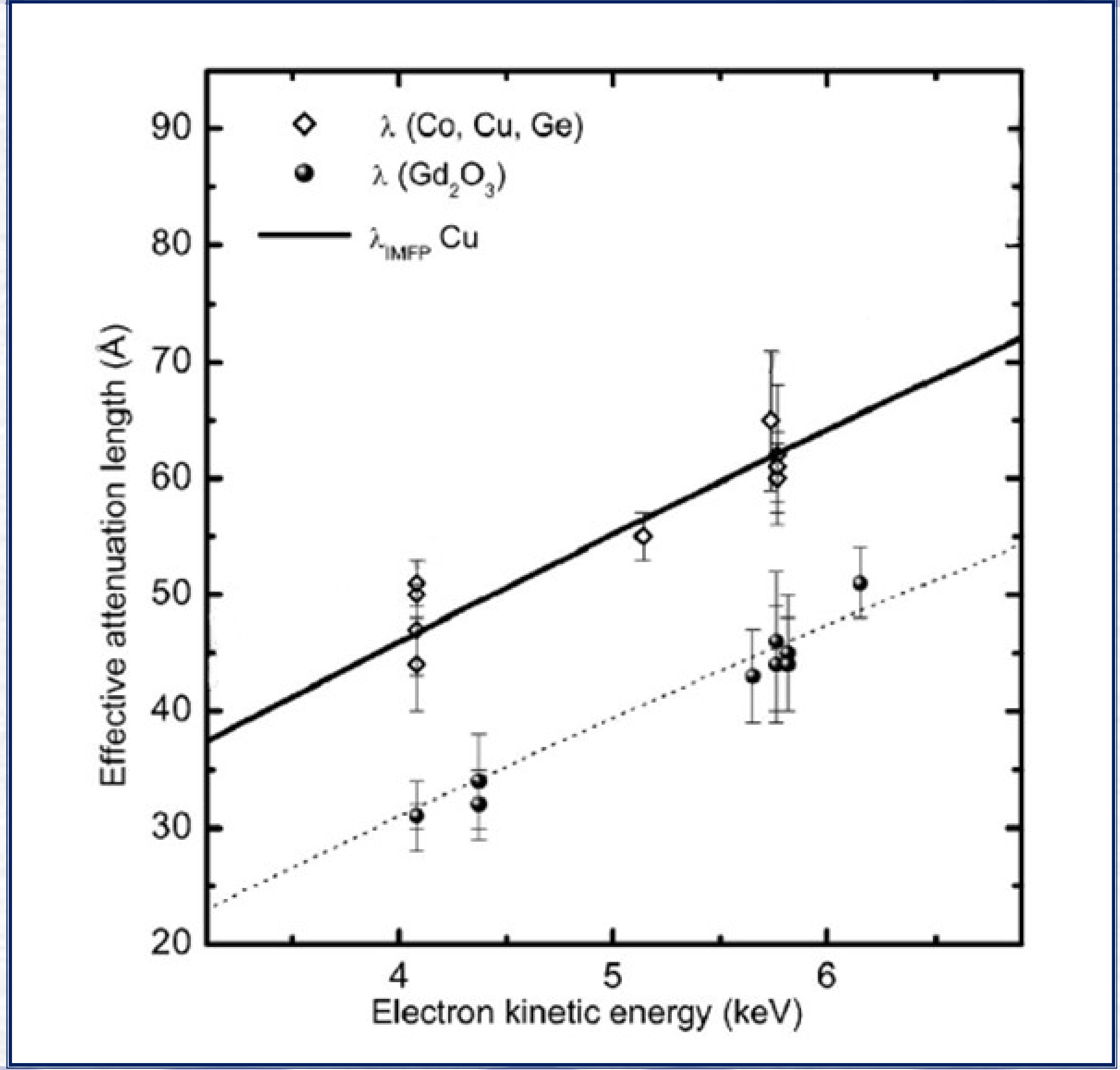
Courtesy of F. Offi

$$I(x) = e^{-\frac{x}{\lambda}}$$

**Information depth**
layer thickness from which 95% of the total signal is produced

| E (eV) | EAL (Å) | Inf. Depth (Å) |
|---|---|---|
| 20 | 5 Å | 15 Å |
| 1500 | 25 Å | 75 Å |
| 6000 | 65 Å | 195 Å |

# EAL in different materials

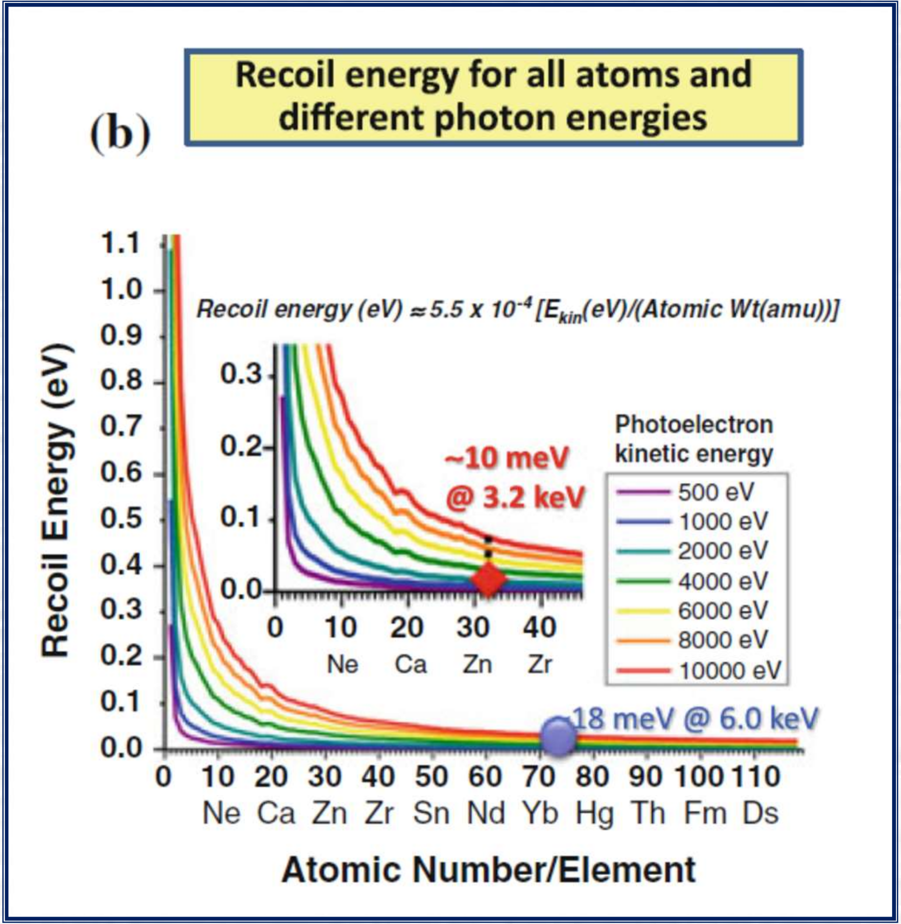


Courtesy of F. Offi

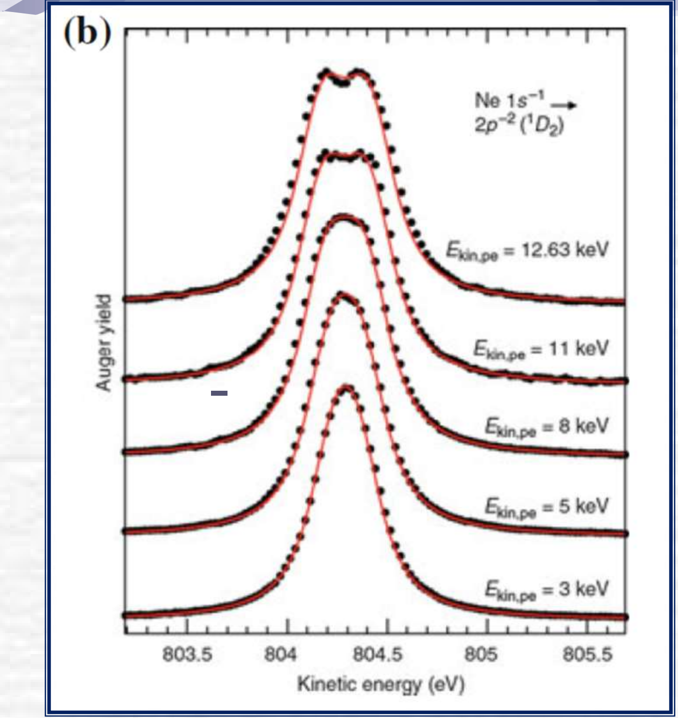
For most materials the experimental values of EAL are quite **higher than what obtained at lower photon** energies and quite in **agreement with theoretical models**

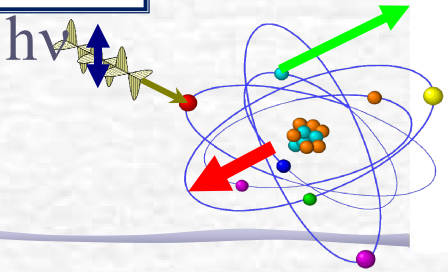
M. Sacchi *et al.,* Phys. Rev. B **71**, 155177 (2005)

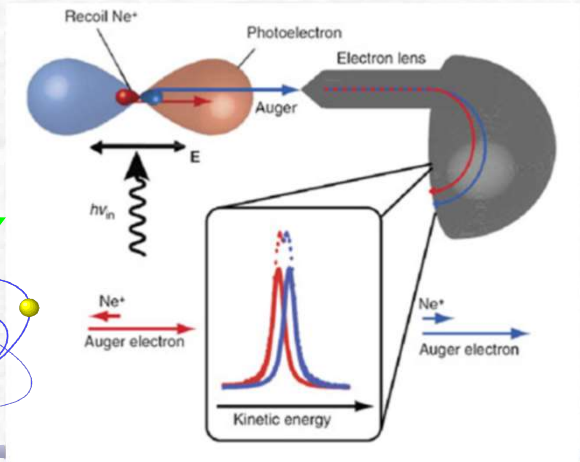
# The non negligible recoiling nucleus



From C.S. Fadley
In: J.C. Woicik ed., «Hard X-ray photoelectron spectroscopy (HAXPES), Springer series in Surface Science







# The End

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