Introduction of X-ray (XPS, XES, and XAS) analysis method

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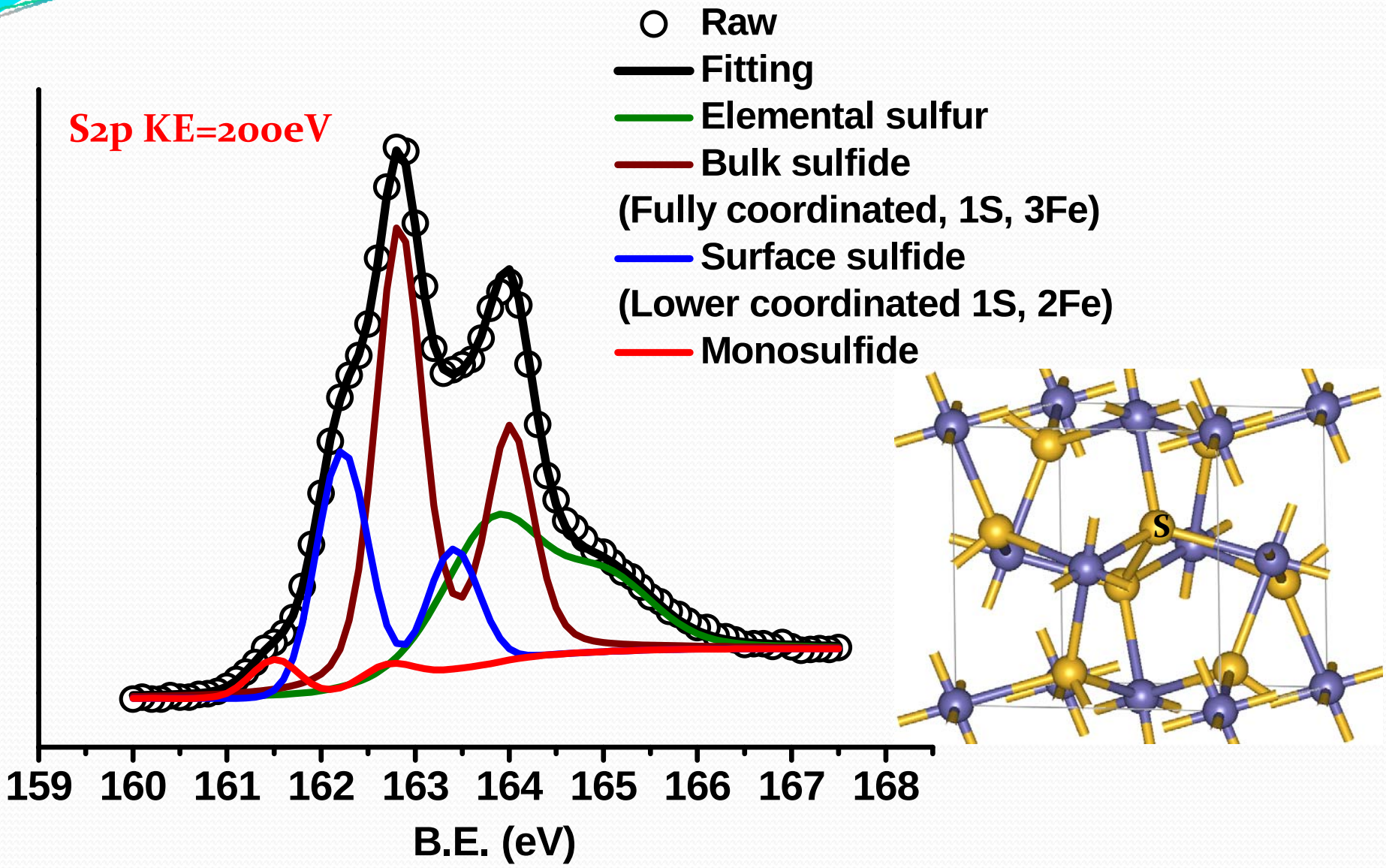
Surface structure of Pyrite thin films on Si



Advanced X-Ray Analysis Methods

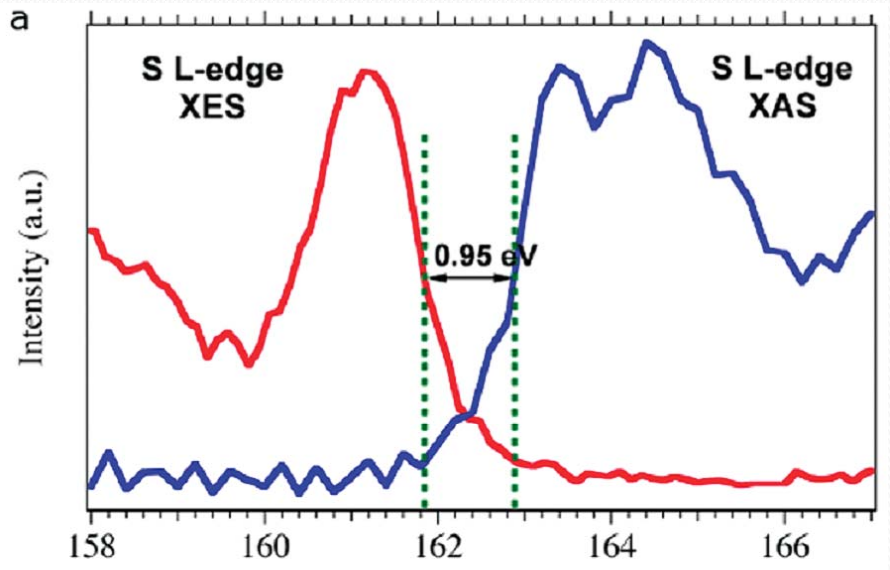
XPS (Photoemission) → Binding Energy
(beamiline 11.0.2, beamline 9.3.2)
XAS (Absorption) → Unoccupied Density of state (HOMO)
(beamiline 11.0.1, beamiline 10.3.2)
XES (Emission) → Occupied Density of state (LOMO)
(beamiline 8.0.1)

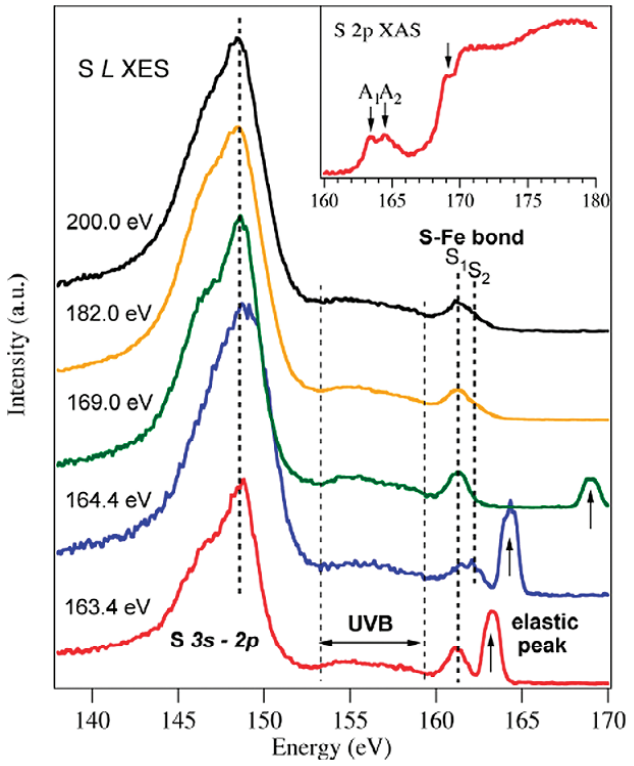
All in one?

XPS, XAS, XES all in Beamline 11.0.2?

Purpose

- **XPS & Electron Yield XAS**
  - Binding Energy, Density of State of Conduction Band
  - Fermi Surface Determination: Valence Band Spectrum, or know BE element
  - Band Gap
  - Testing experiment on Si
- **Electron Yield XES & XAS**
  - Density of State of Valence and Conduction Band
  - Band Gap and Core Hole Effect



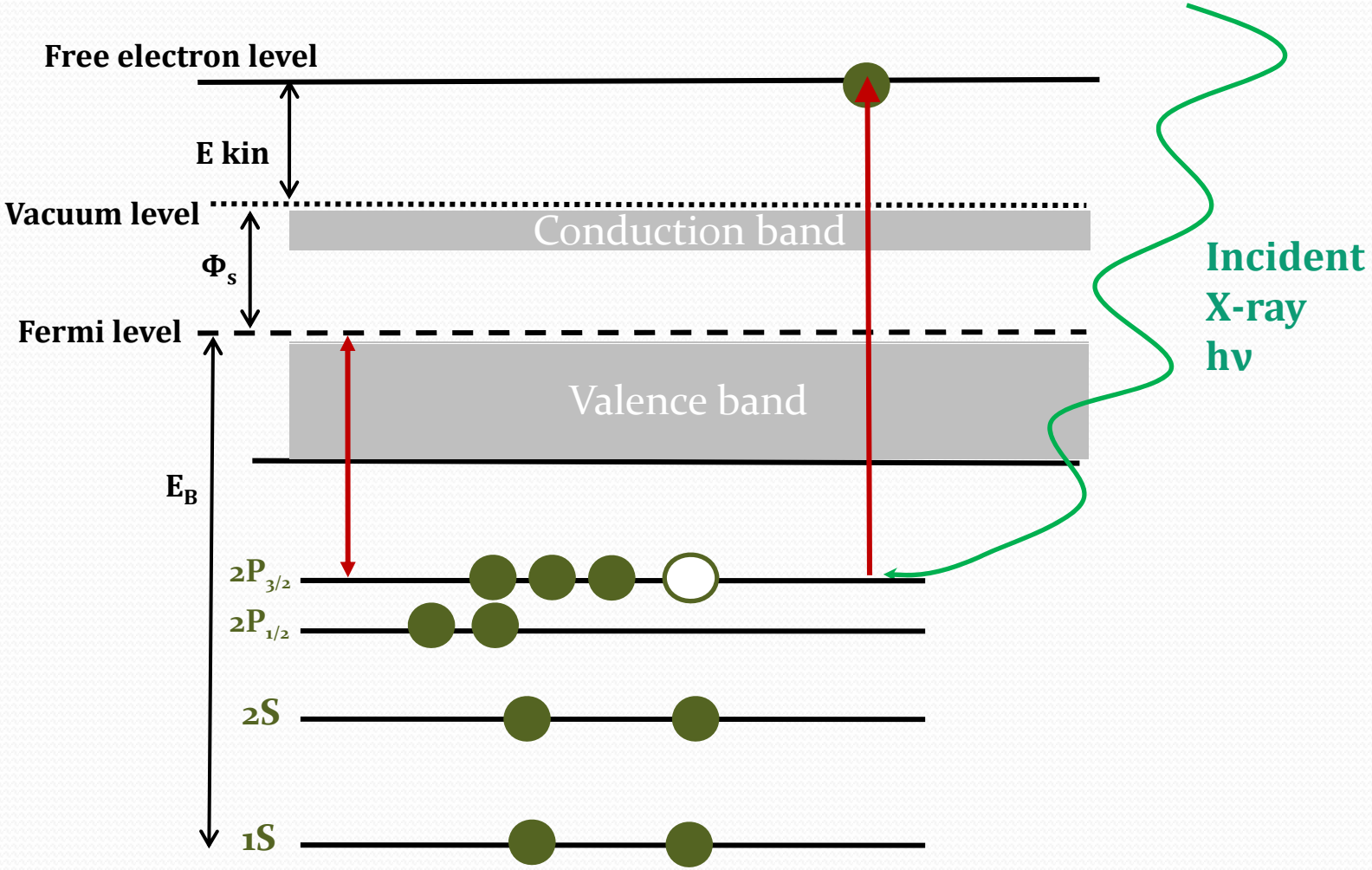


Chem. Mater. 2009, 21, 2568–2570

XPS

One Photon process: Photon in Electron out

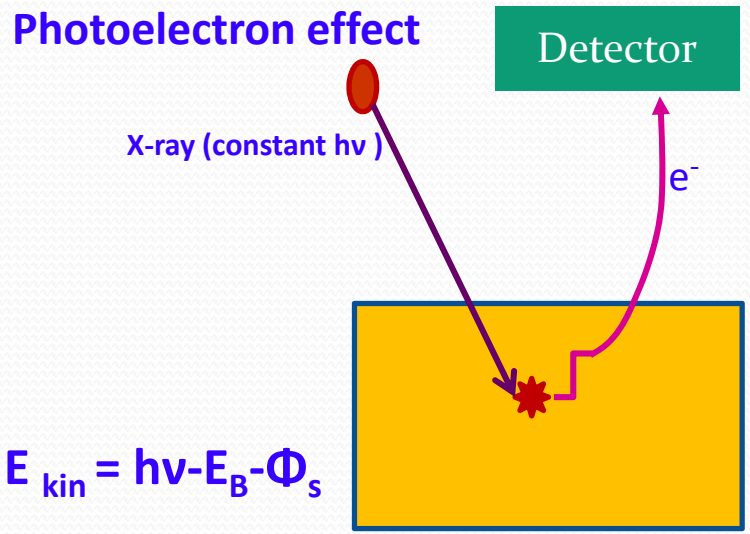
XPS Cartoon Mechanism

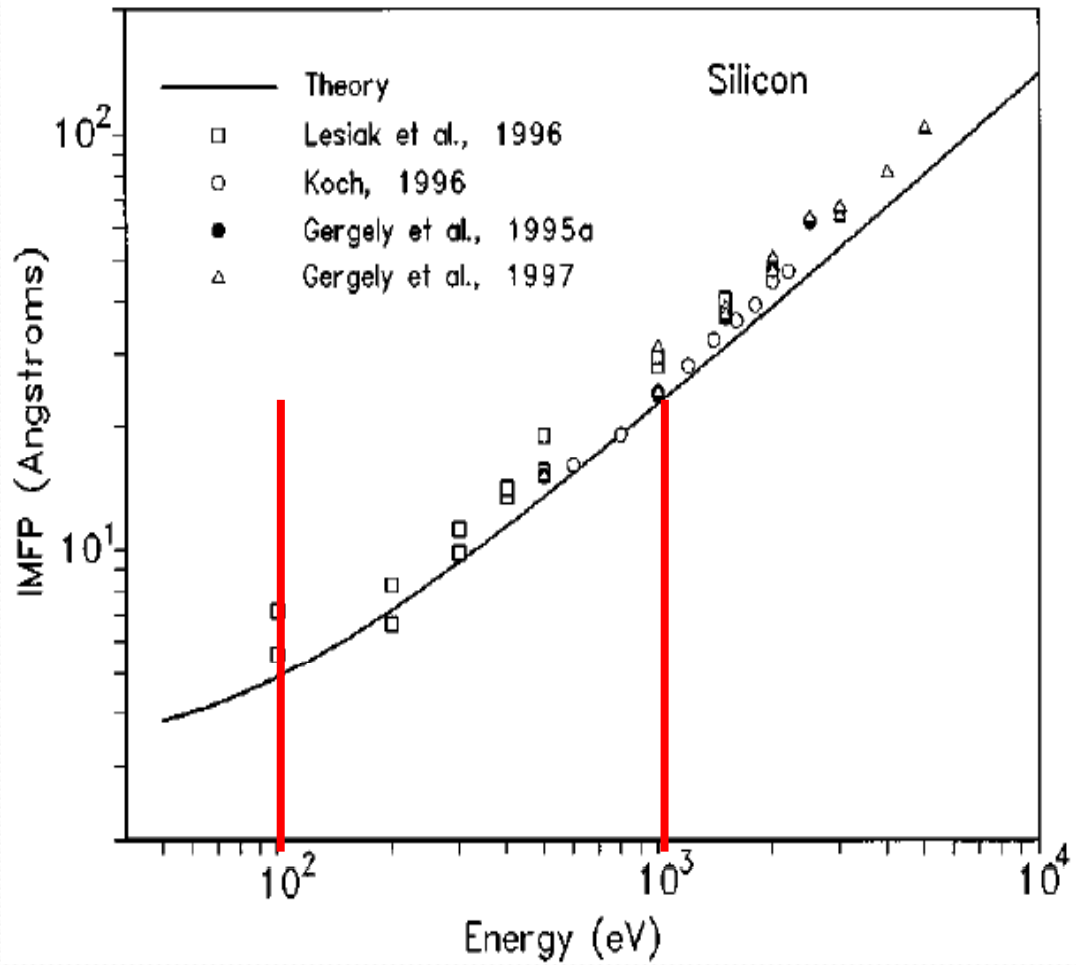


XPS: $E_B = h\nu - E_{kin} - \Phi_s$ For example, E_B for $S2p_{3/2}$

Surface Sensitivity

- **Electron Inelastic Mean Free Path**



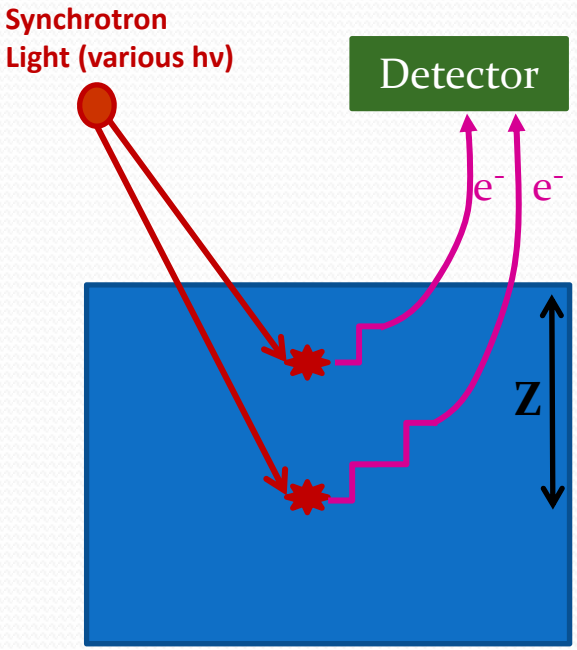


J. Phys. Chem. Ref. Data, Vol. 28, No. 1, 1999

Depth profile experiment and inelastic mean free path (IMFP)

- Continuous
- Changeable

Depth profile experiment

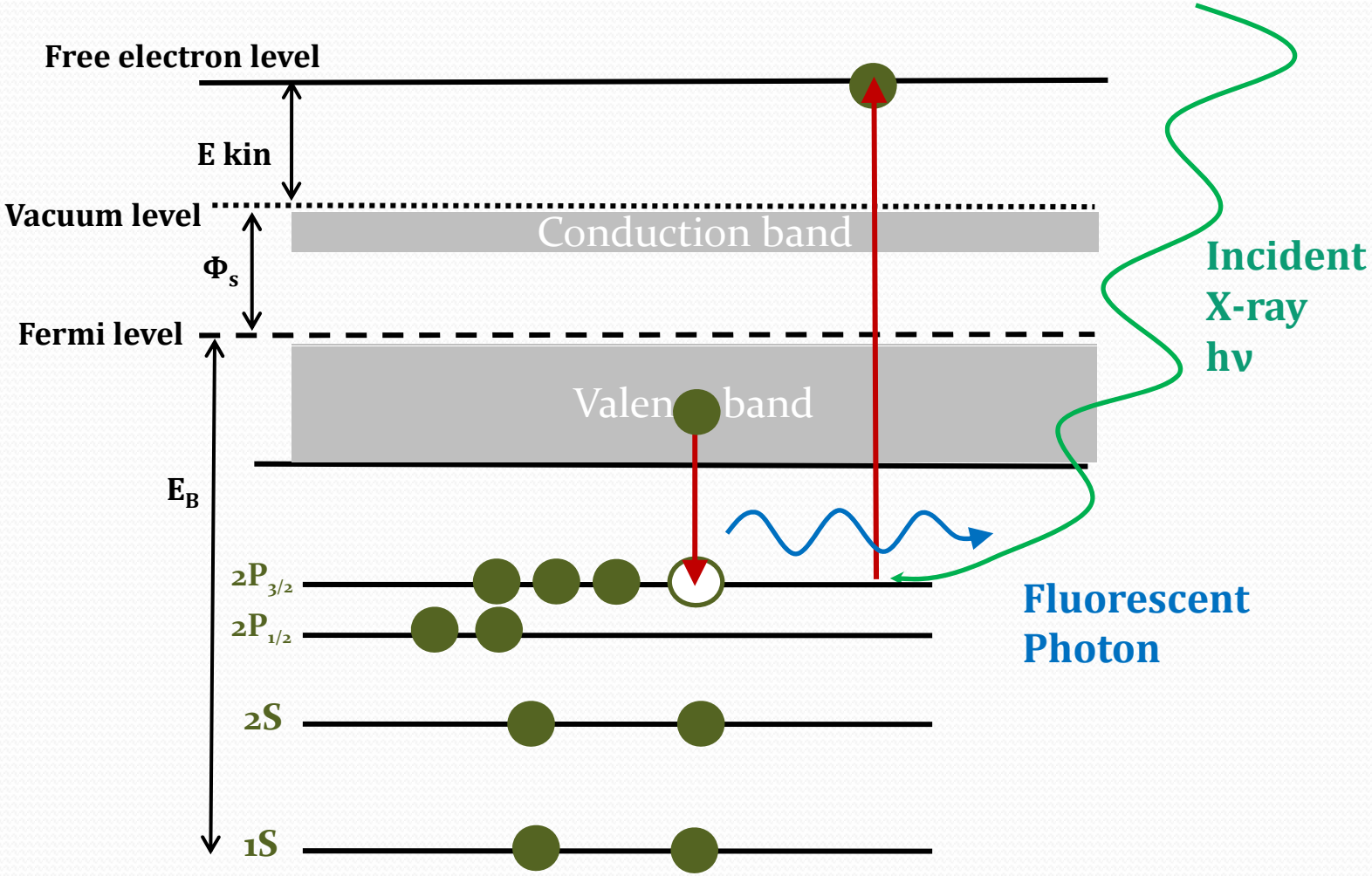


Photoelectrons with different kinetic energies come from different depth of the sample.

XES and XAS

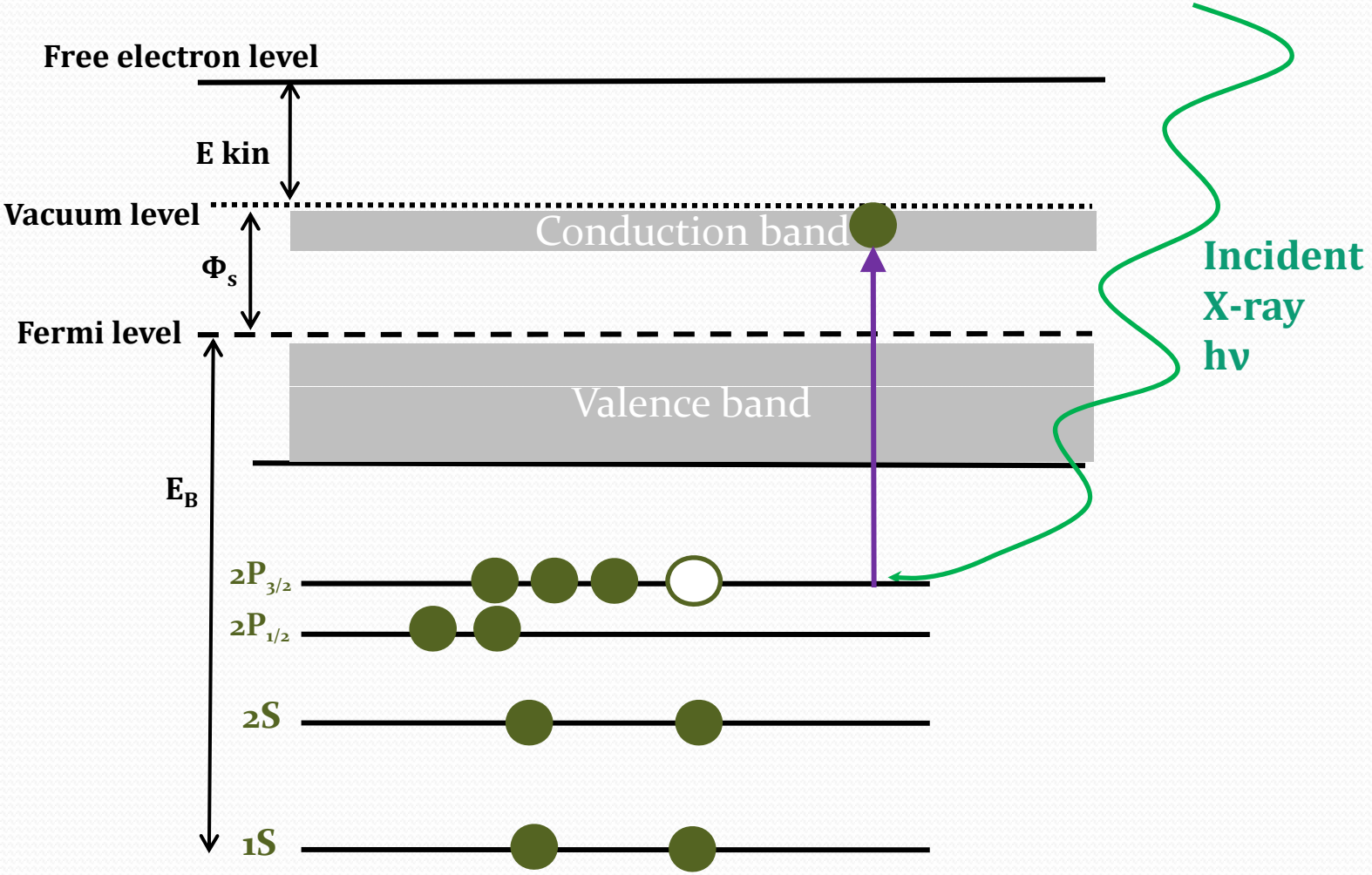
Two Photons process: Photon in Photon out

XES Cartoon Mechanism



XES:(Photon in Photon out) Fluorescent photon created by electron decay from valence band to core level

XAS Cartoon Mechanism



XAS: Electrons from core level to unoccupied conduction band, For example, A_1 for S_L edge

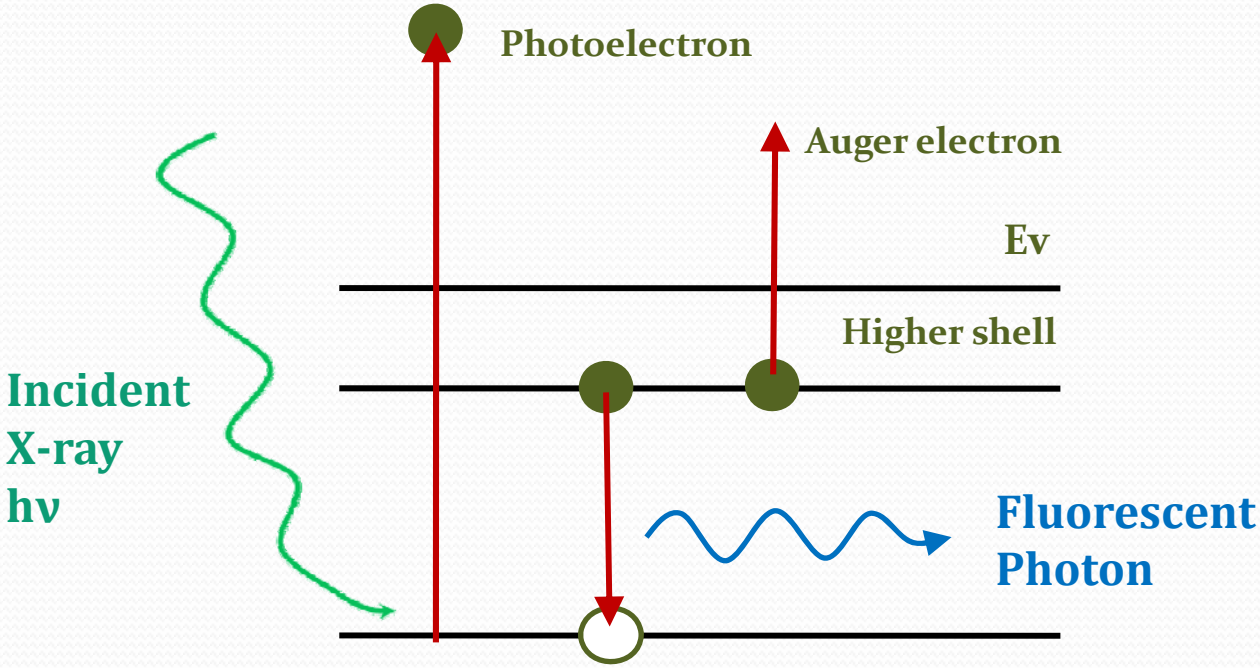
$E_A = h\nu - h\nu_T$ For example

Limitation

- **Traditional Measurement (Transmission)**
  - Signal-to-background ratios limited by thickness (~500Å)
  - Radiation damage
  - Reflection geometry experiment
  - Surface Sensitive?!
- **We can only collect electron not photon in beamline 11.0.2**

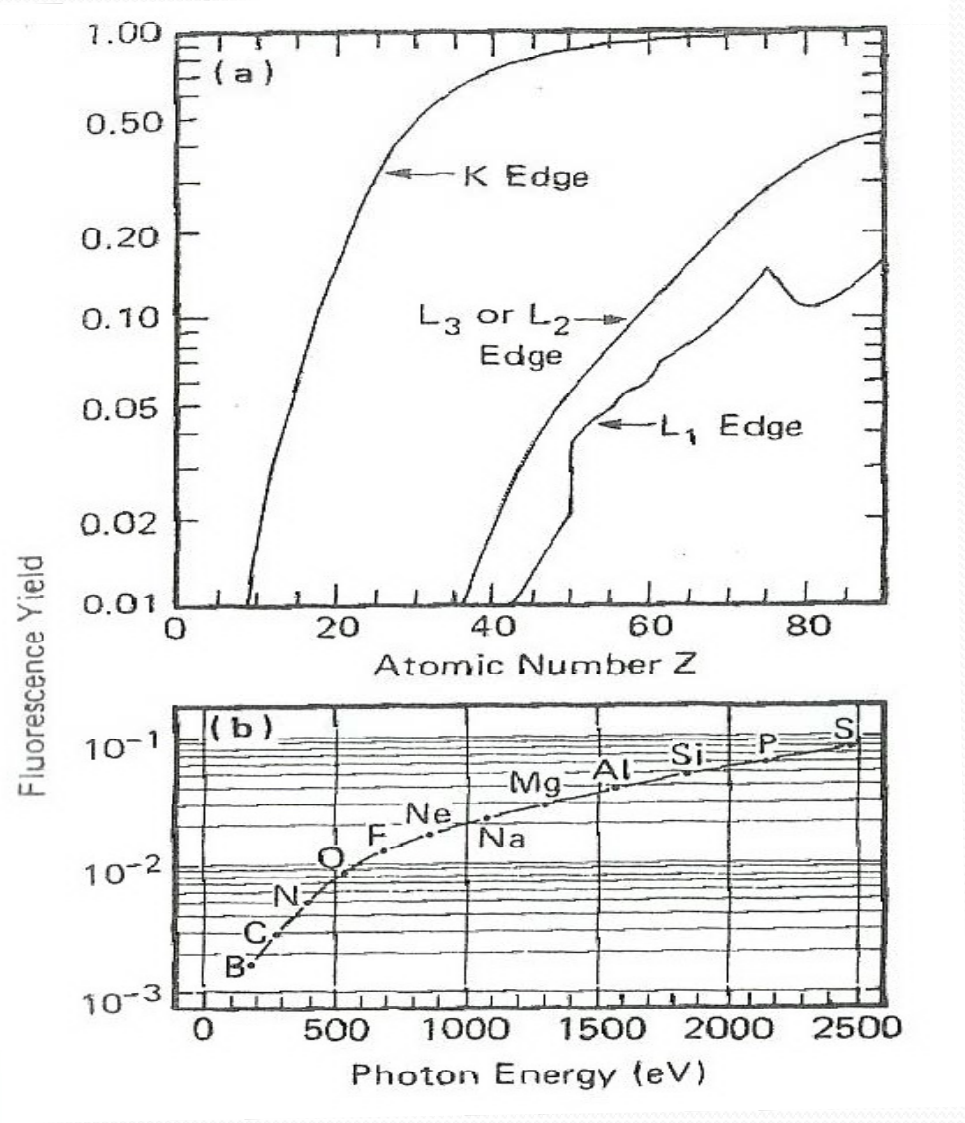
Electron Yield

- **Electron Yield or Secondary Electron**
  - Auger electron & Fluorescent Photon



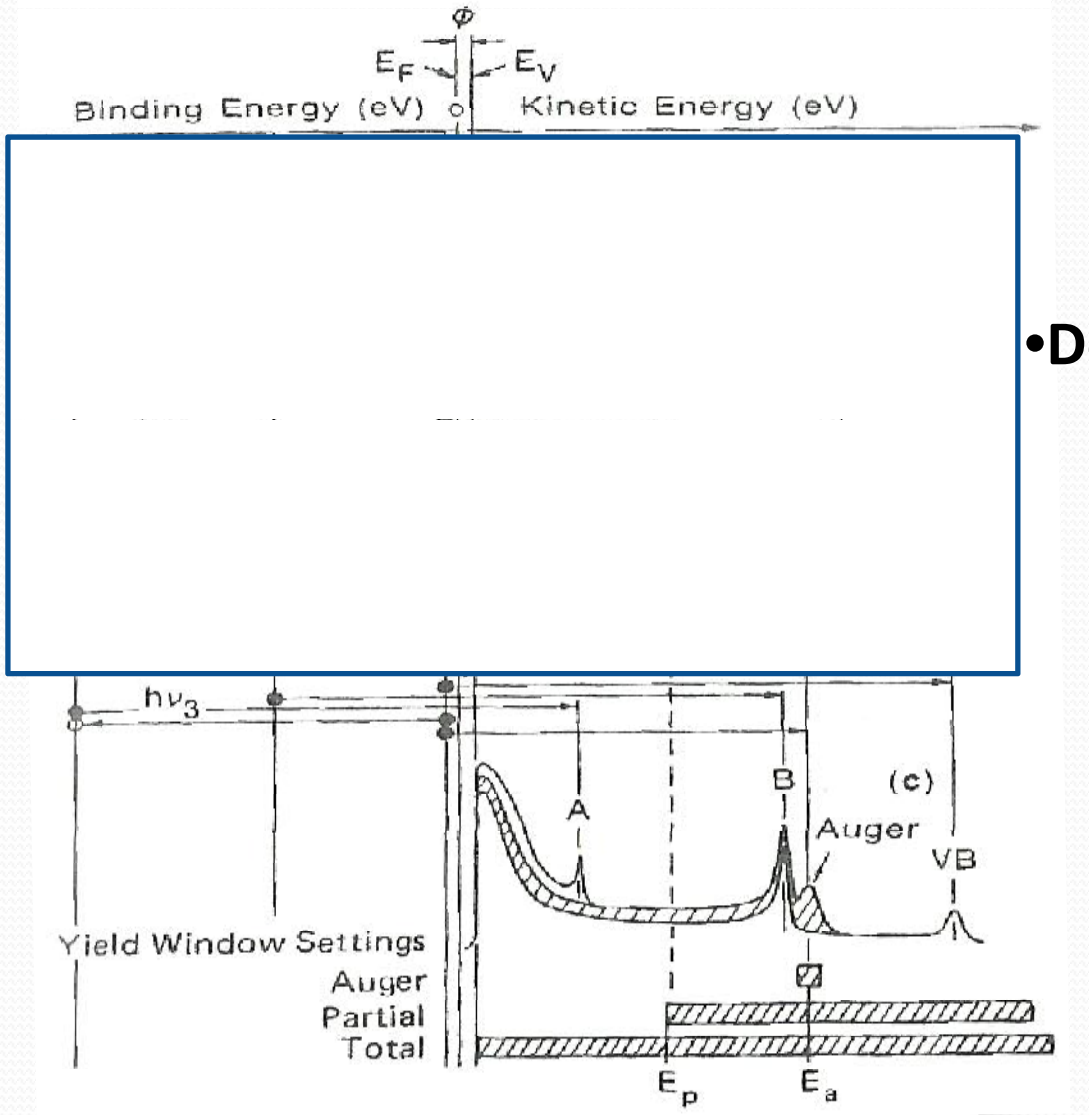
Electron Yield

- **Auger electron yield dominate**
  - For K shell excitation of low-Z atoms
  - For L shell excitation of all Z <90
  - C, N O, S, Si



J. Phys. Chem. Ref. Data 8, 307 (1979)

Electron Yield



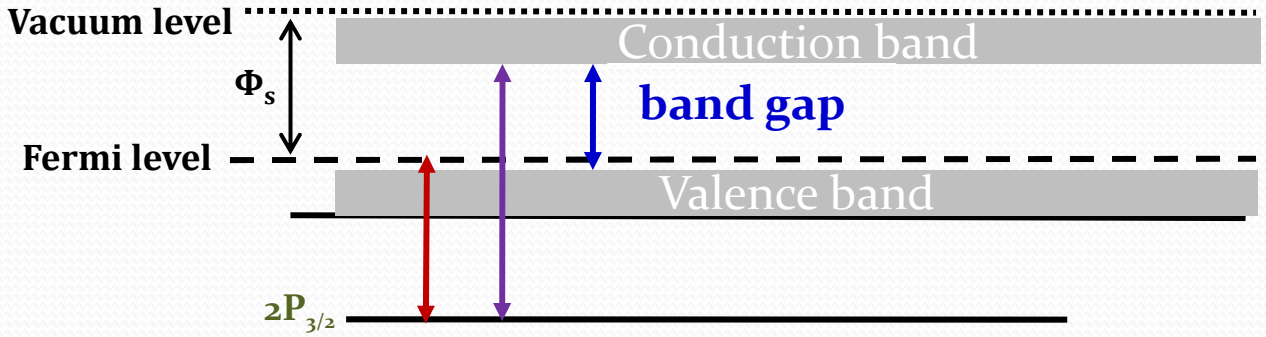
- **Detection Mode**
  - Auger Electron Yield (AEY)
  - Partial Electron Yield (PEY)
  - Total Electron Yield (TEY)

Stöhr, Joachim, NEXAFS Spectroscopy, Springer-Verlag 1996

Reviews:
XPS & Electron Yield XAS
Band Gap Determination

Fermi Surface Determination

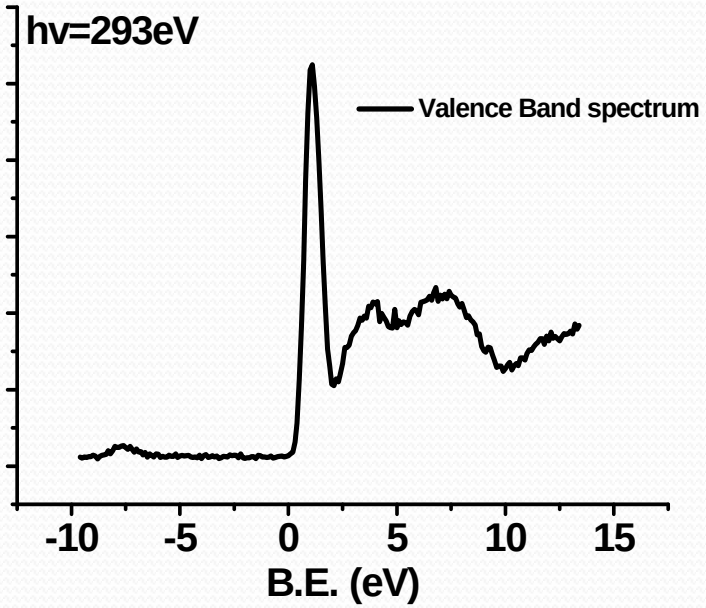
- Testing Experiment on Si (band gap 1.11eV)



- Binding Energy calibration
  - Au $4f_{7/2}$=84.00 eV
  - Ag $3d_{5/2}$=368.27 eV
  - Cu $2p_{3/2}$=932.67 eV

M. P. Seah, Surf. Interface Anal. 14, 488 (1989)

- Valence Band Spectrum



Take-home messages

- **Band Gap Determination by XPS+XAS**
  - ➢Fermi Surface Determination by Valence Band Spectrum
  - ➢Fermi Surface Determination by Binding Energy Calibration
  - ➢Testing Experiment on Si

- **Band Gap Determination by Electron Yield XES+XAS**
  - ➢Density of State Information of Valence band and Conduction band
  - ➢Core Hole Effect Analysis