Курс:

Фізичні методи дослідження матеріалів

Тема:

Фотоемісійна спектроскопія з кутовим розділенням (ARPES)

Лектор: О. А. Кордюк
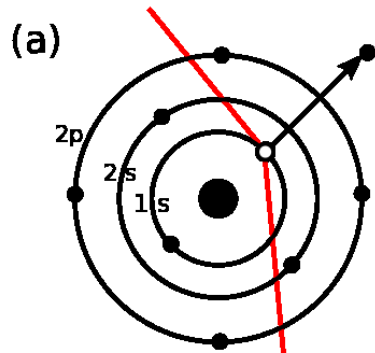
Spectroscopic Techniques

In \ Out	*hv*	*electrons*	*A*
hv	XD, IR, Raman	ARPES, Auger	LA
e	IPS, EDX (SEM)	SEM, LEED, EELS	ESD
A	BLE	IAES	RBS, SIMS
T			TDS
E		STM/STS, FEM	FIM

n-n: **ND, INS**
μ-e⁺: **μSR**

Auger electron spectroscopy

(a)

2p
2s
1s

Electron collision

2p
2s
1s
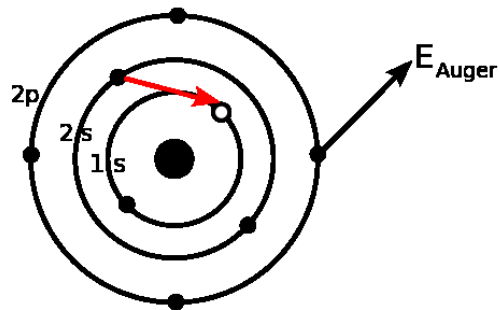
E_{Auger}

Auger electron emission

(b)

Vac

Valence Level

M, ...

$L_{2,3}$

L_1

K
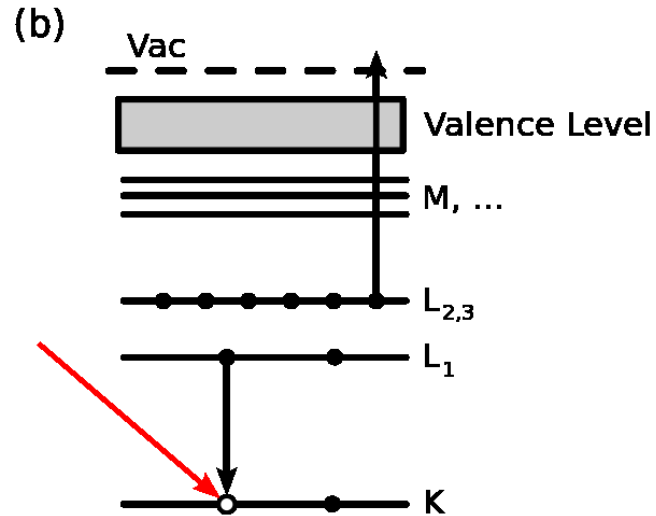
$$E_{\mathrm{kin}} = E_{\mathrm{Core\ State}} - E_B - E'_C$$

Spectroscopic Techniques

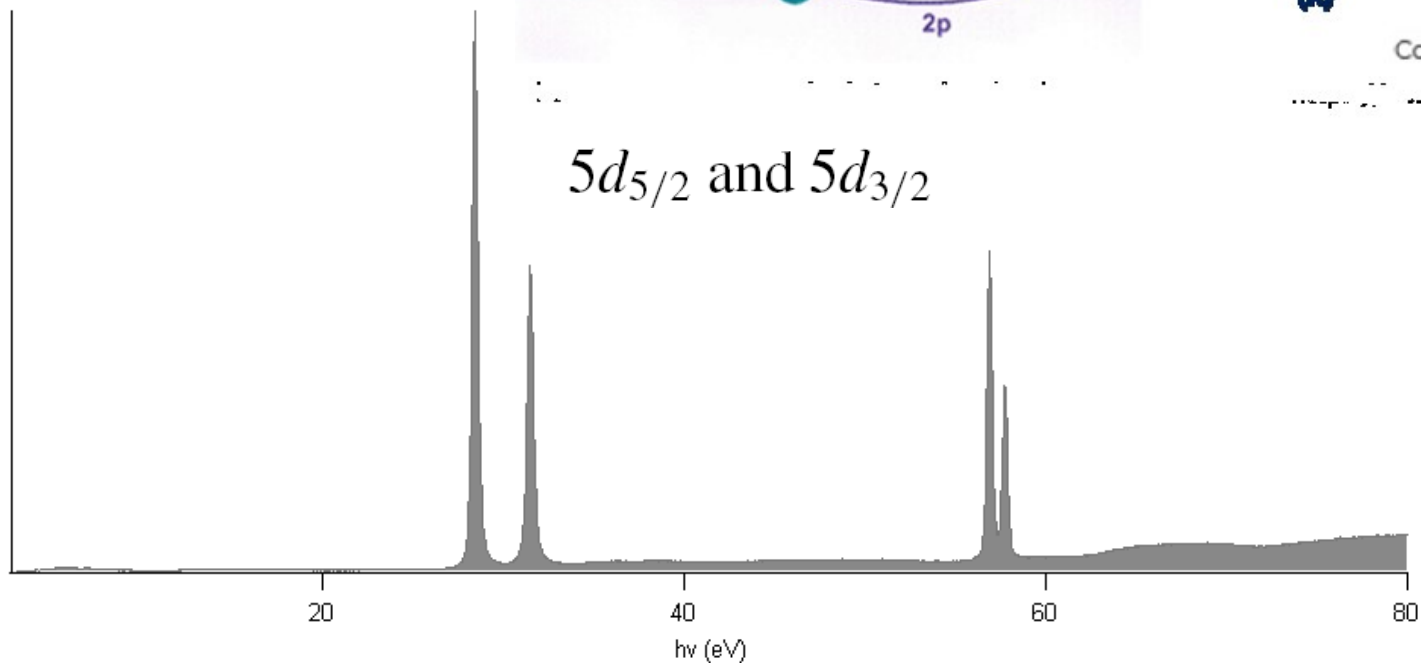| In \ Out	*hν*	*electrons*	*A*
hν	**XD, IR, Raman**	**XPS, ARPES**, **XPD**	**LA**
e	**IPS, EDX (SEM)**	**SEM, LEED, EELS**	**ESD**
A	**BLE**	**IAES**	**RBS, SIMS**
T			**TDS**
E		**STM/STS, FEM**	**FIM**

n-n: **ND, INS**
μ-*e$^+$:* **µSR**

XPS: X-ray Photoelectron Spectroscopy – Density of States (DOS)
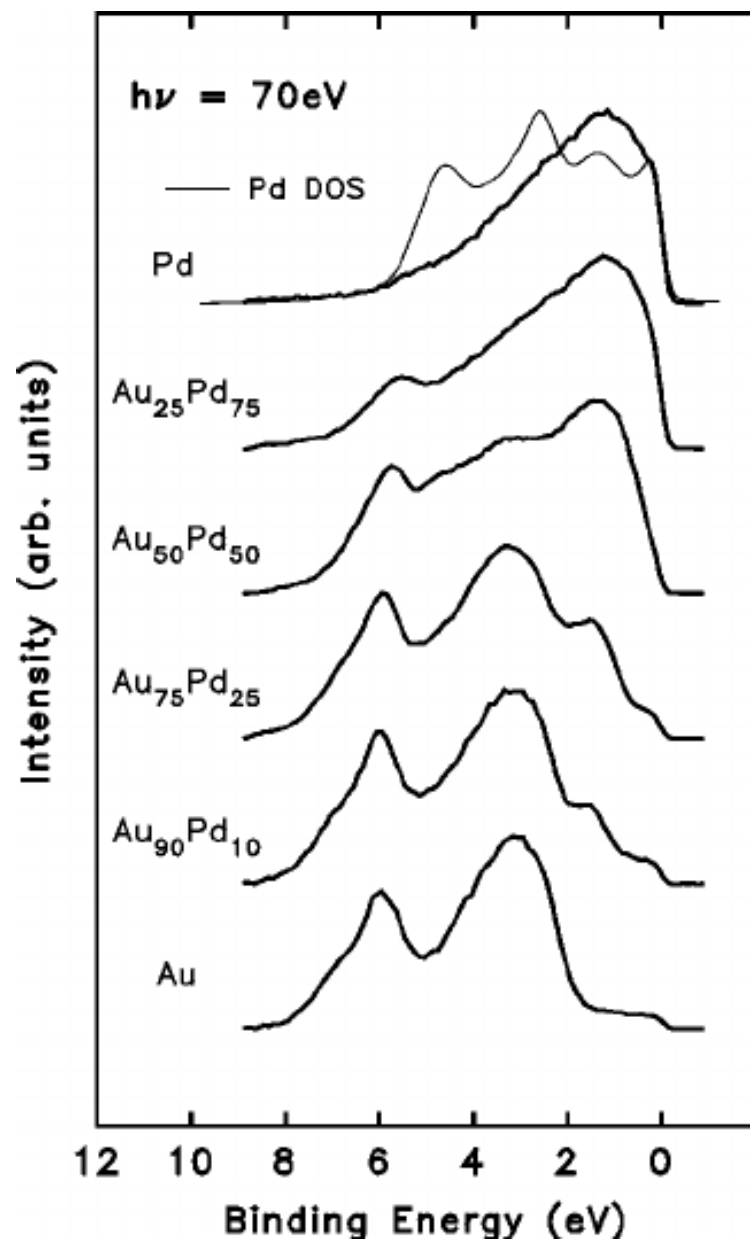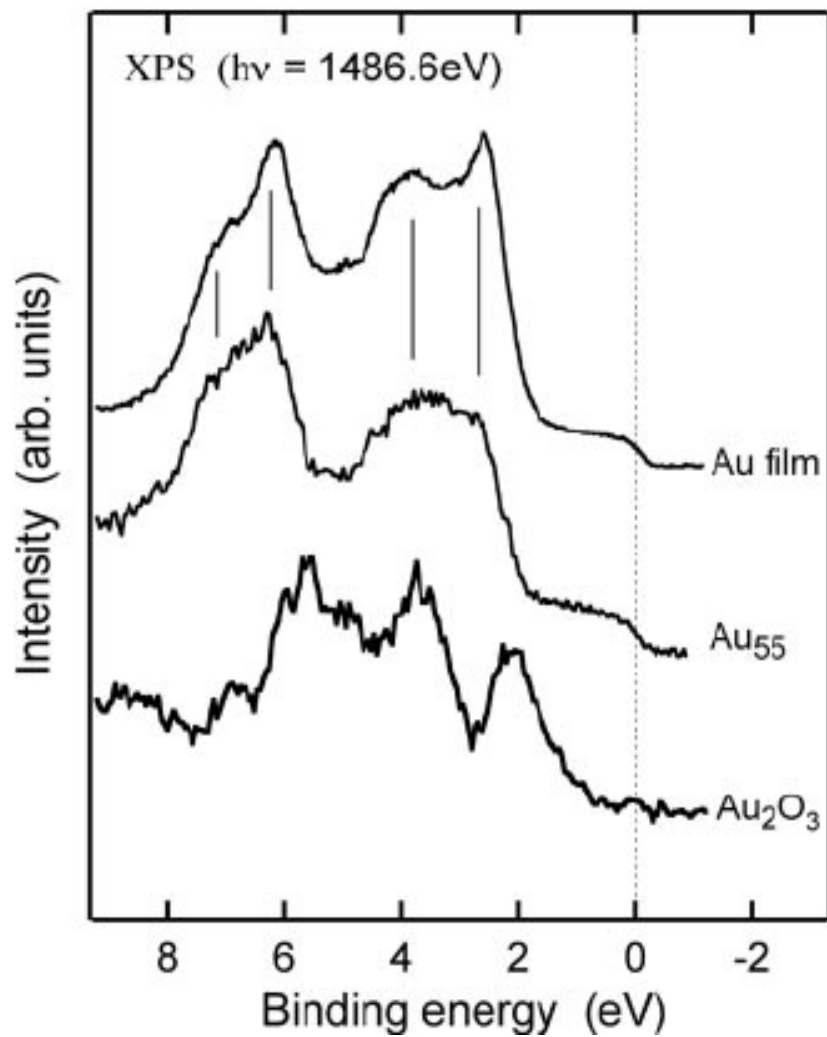
Bi$_2$Se$_3$
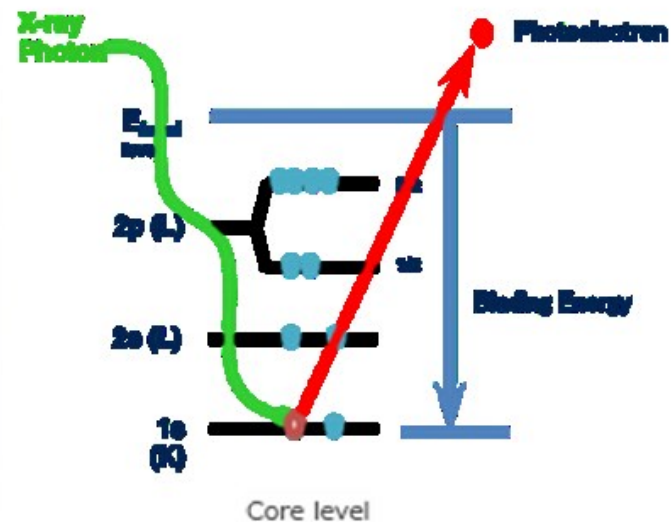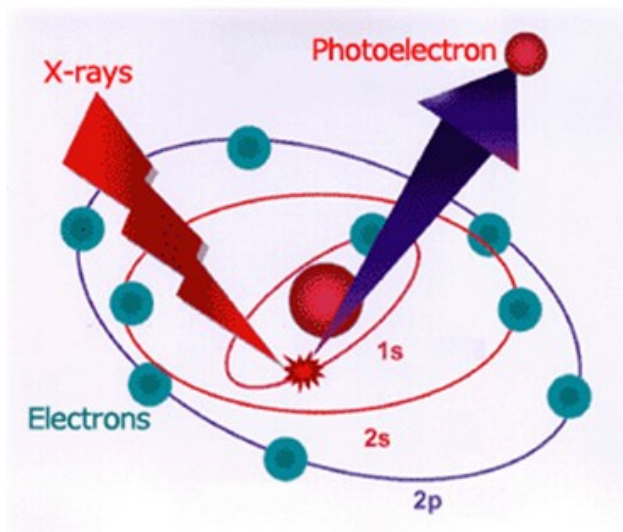
$5d_{5/2}$ and $5d_{3/2}$

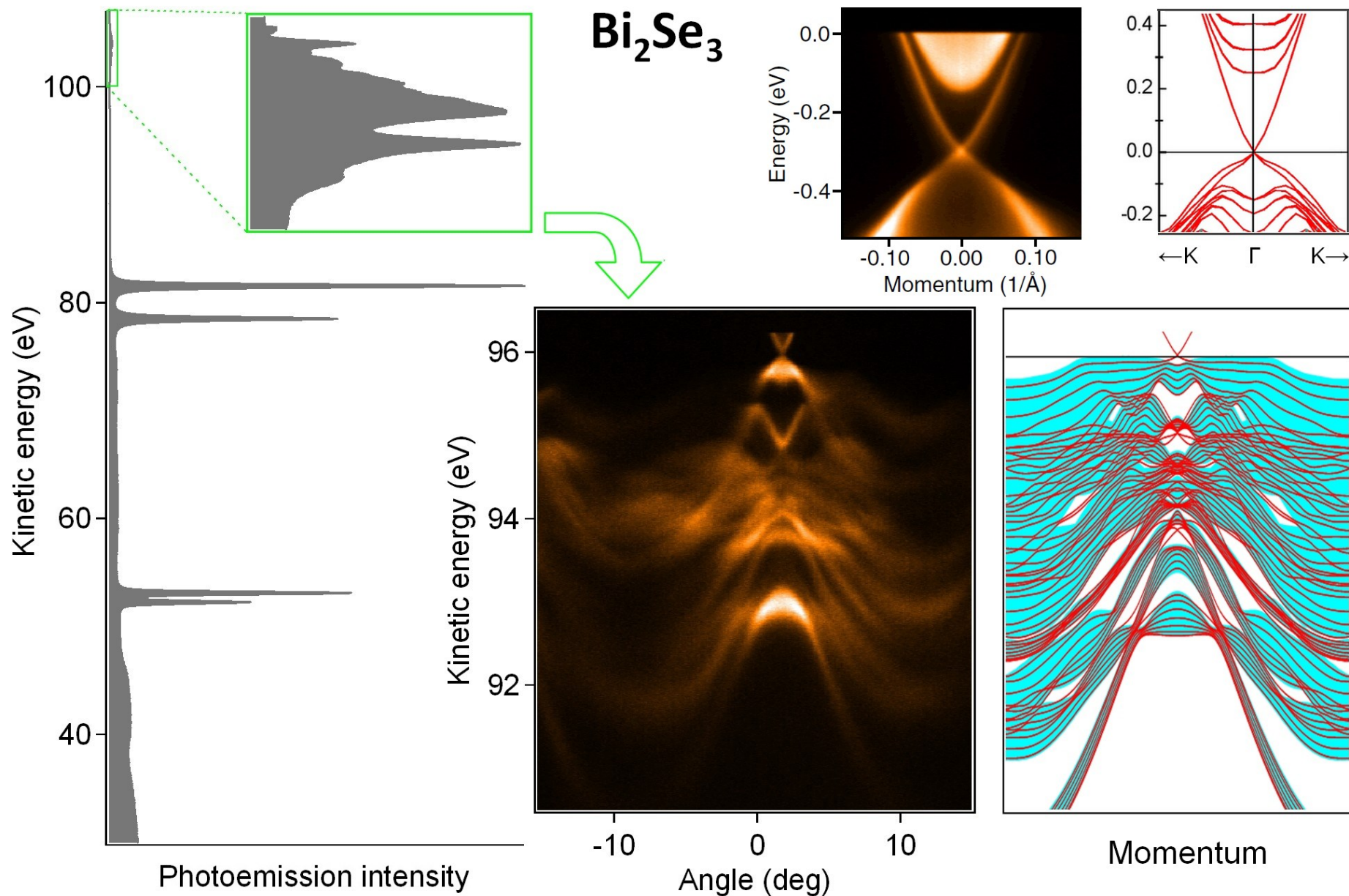# XPS: X-ray Photoelectron Spectroscopy – Density of States (DOS)
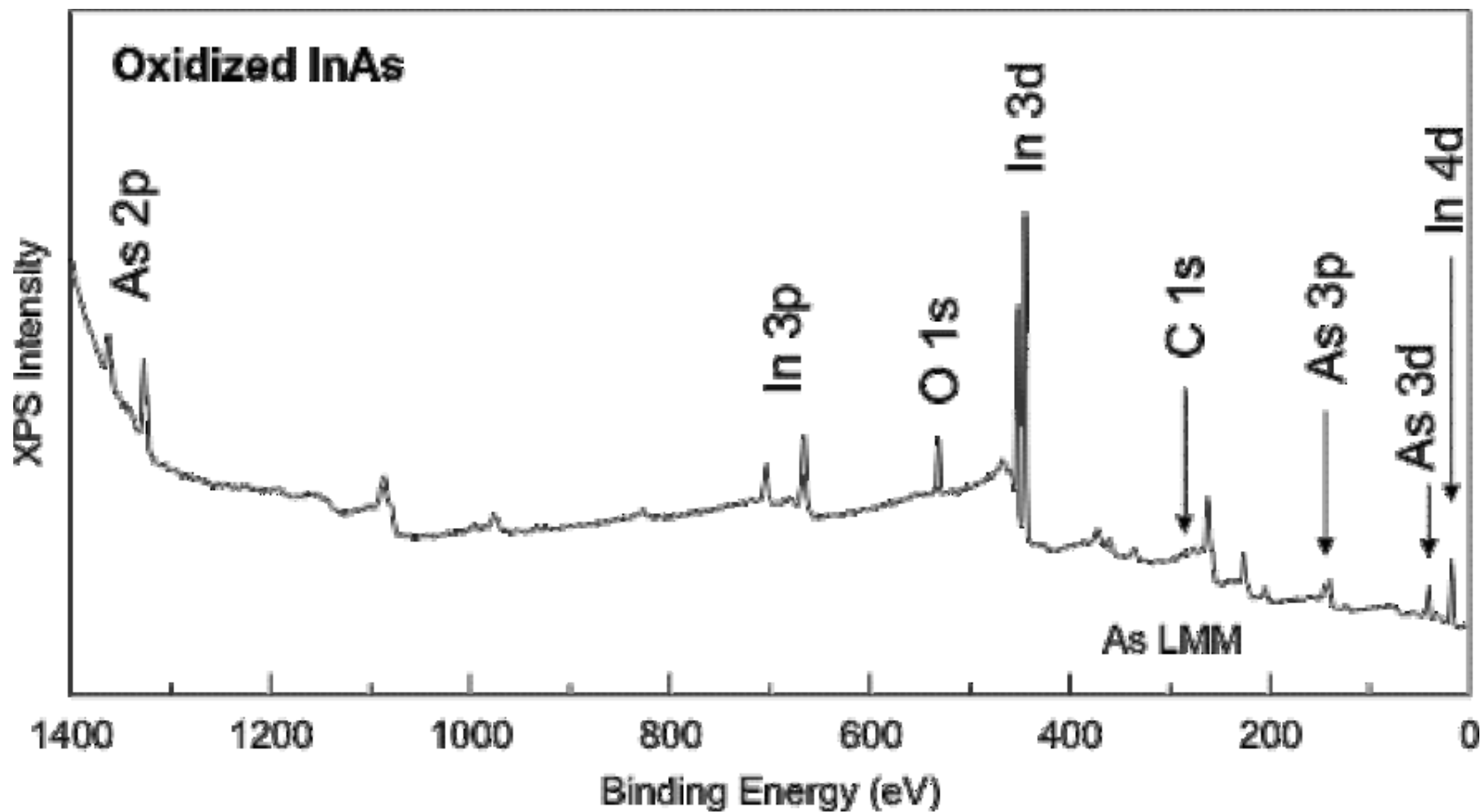
XPS – Valence band
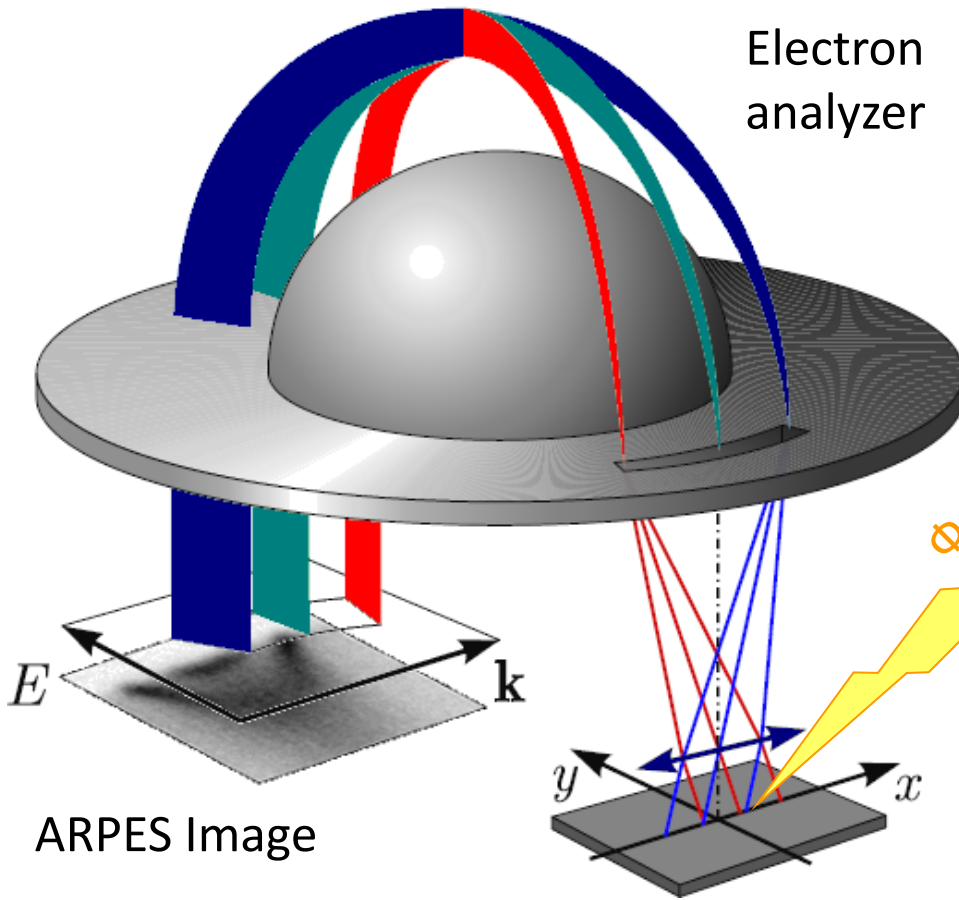
ARPES: Angle Resolved Photoemission Spectroscopy

Bi₂Se₃

ARPES: Angle Resolved Photoelectron Spectroscopy
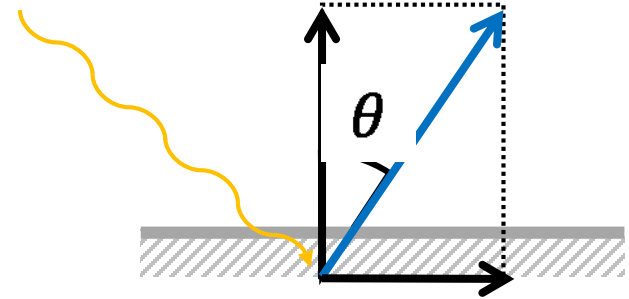
$$h\nu = \phi + E_B + E_K$$

$$E_K = \frac{p^2}{2m}$$
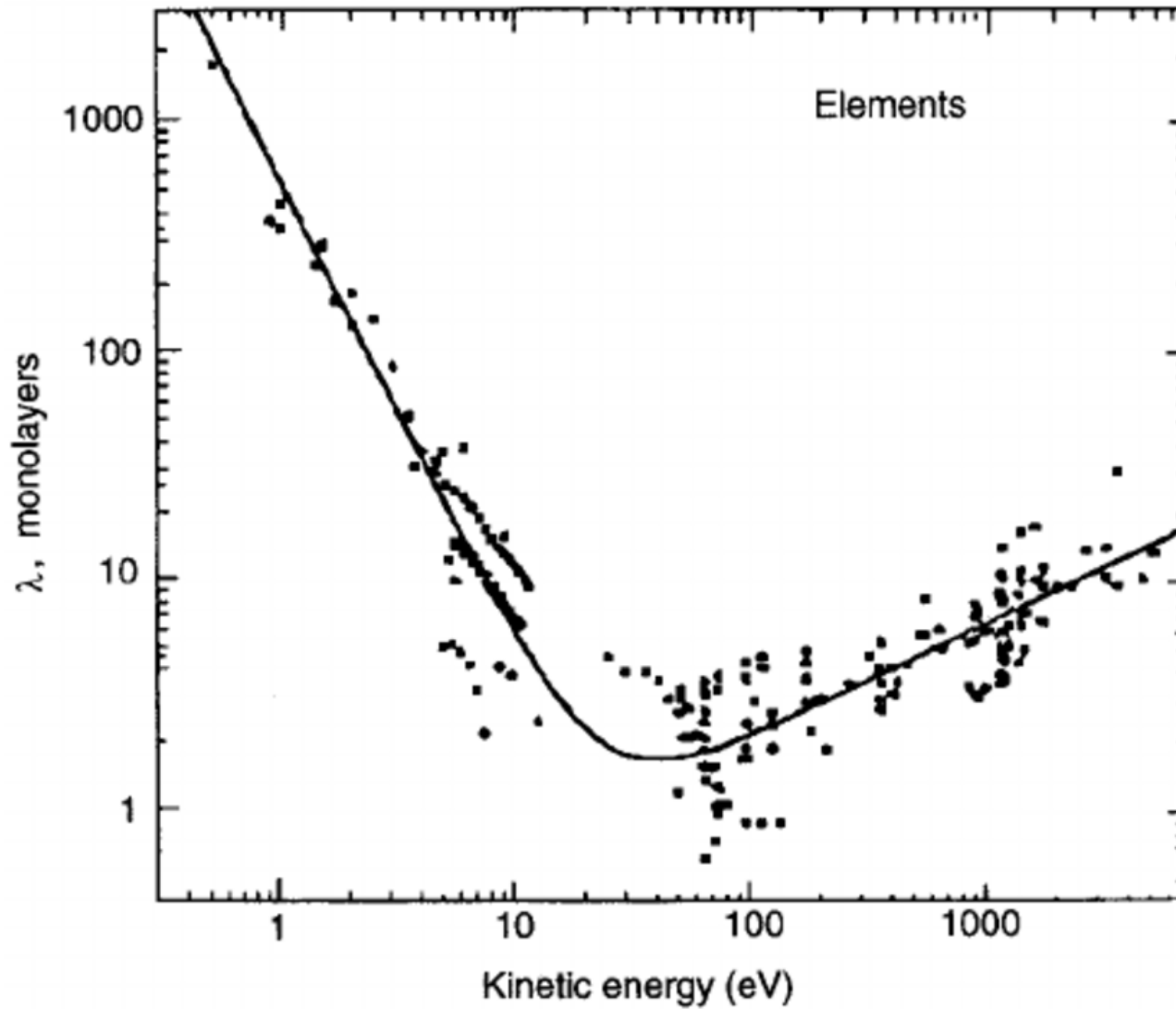
$$p = \sqrt{2mE_K}$$

θ

$$p_{||} = p \sin\theta$$

Electron analyzer

$$\mathbf{p}_{||} = \hbar\mathbf{k}_{||} + \hbar\mathbf{G}$$

Фотони

E $\mathbf{k}$

ARPES Image

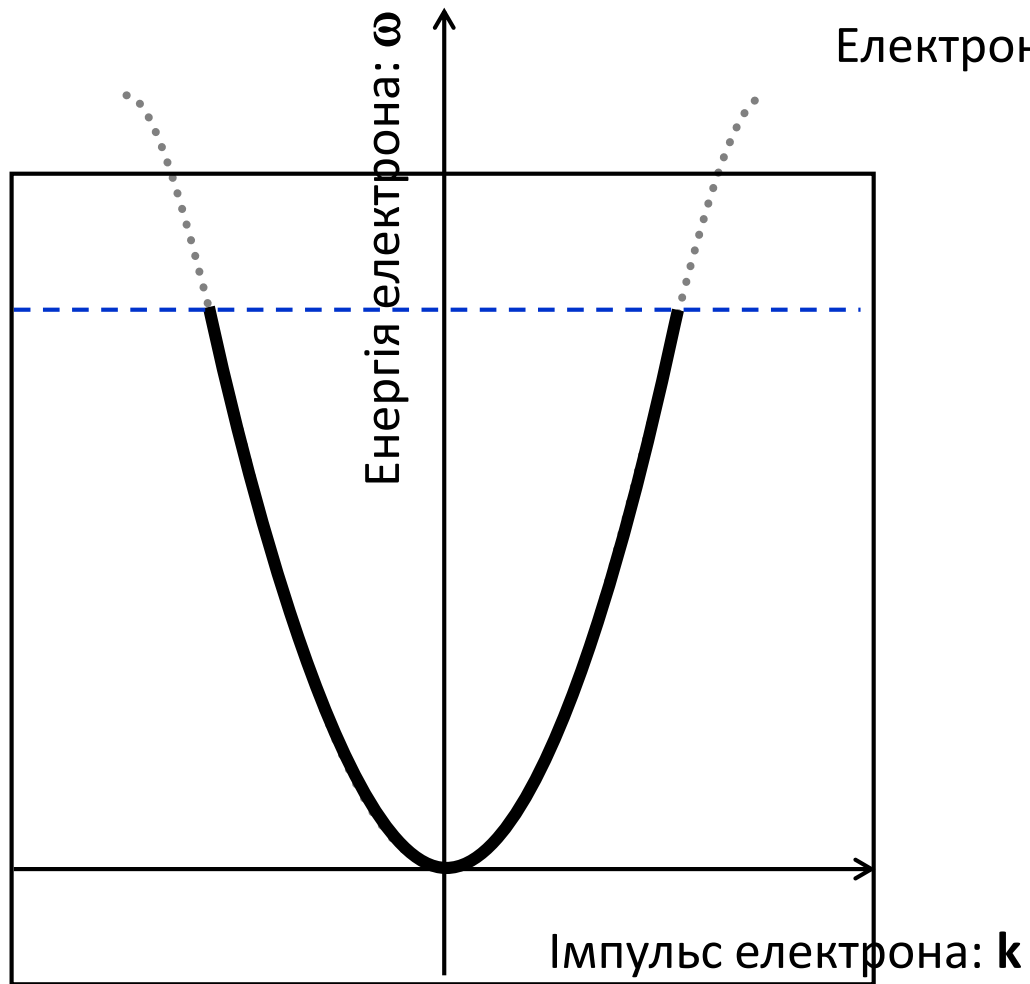y x

Sample

Fermi's golden rule

$$T_{i \to f} = \frac{2\pi}{\hbar}\left|\langle i|\hat{V}|f\rangle\right|^2 \delta(E_f - E_i \pm \hbar\omega)$$

Three step model

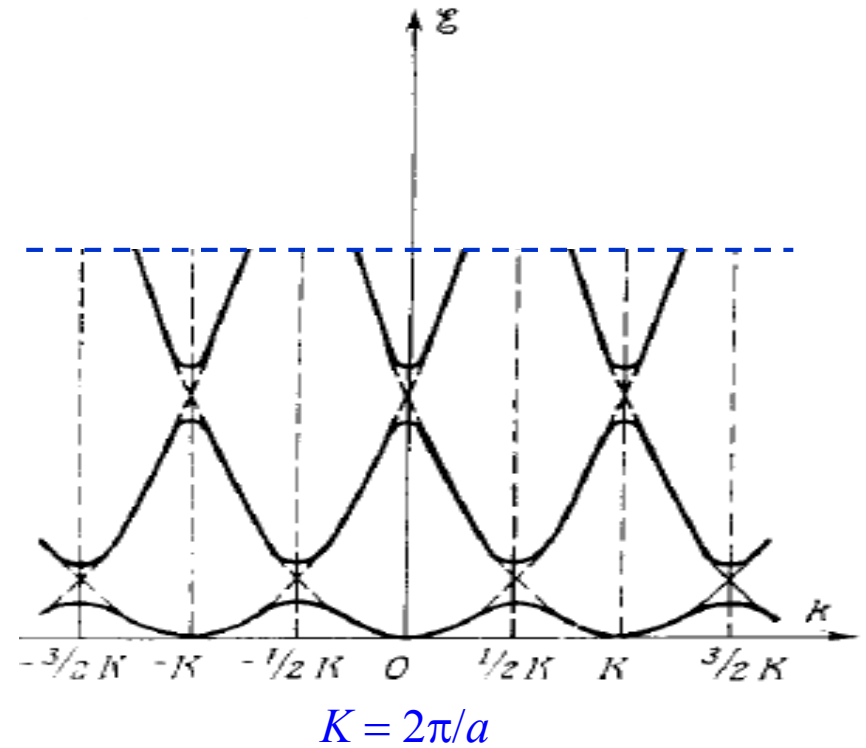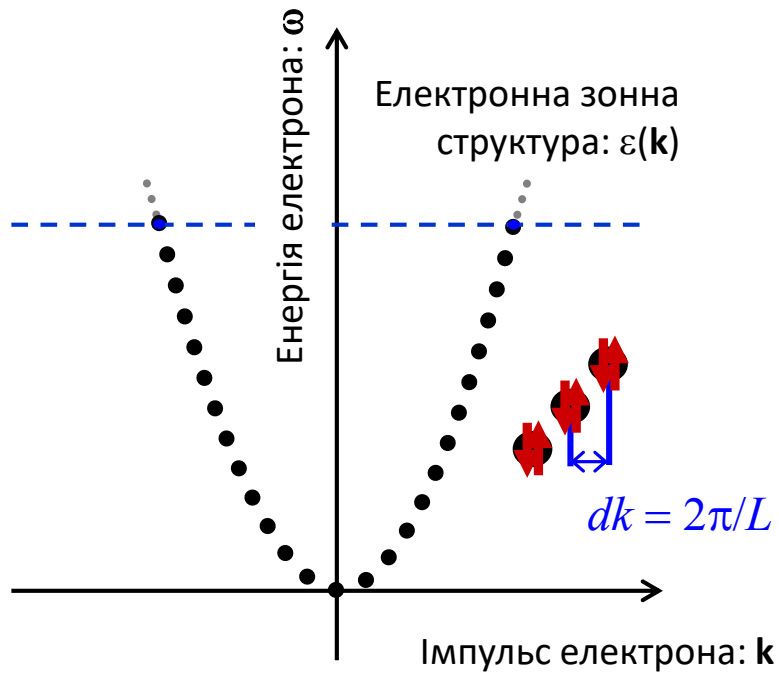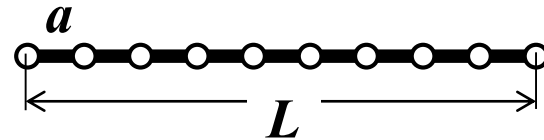# Photoelectron escape depth

Electronic structure

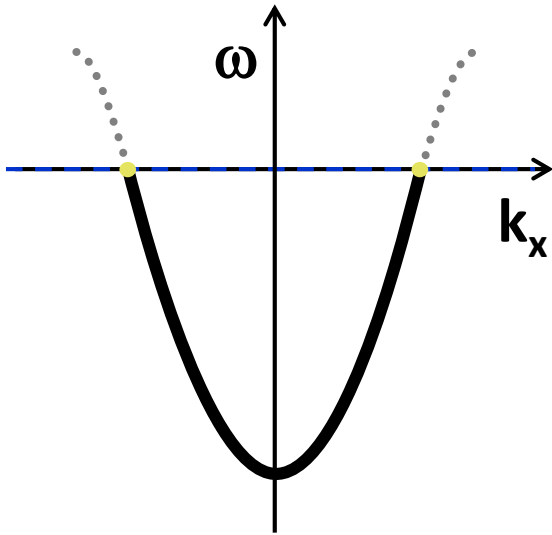Електронна зонна структура: $\varepsilon(\mathbf{k})$
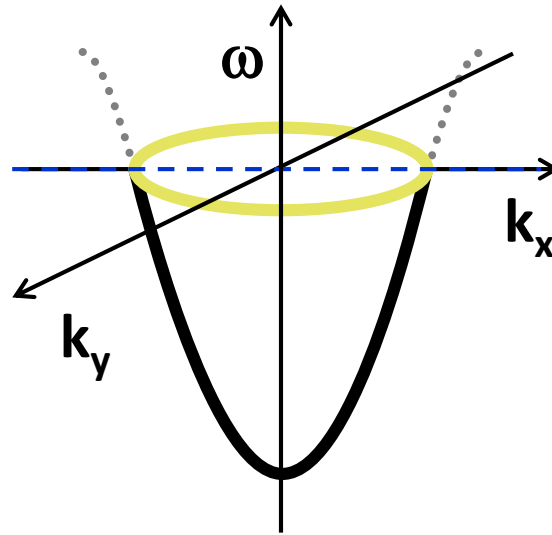
$$E = \frac{p^2}{2m}$$

$$p = \hbar k$$

Енергія електрона: ω

Імпульс електрона: $\mathbf{k}$

Electronic dispersion, electronic structure, Fermi surface

L

Електронна зонна структура: $\varepsilon(\mathbf{k})$

Енергія електрона: ω

$dk = 2\pi/L$

Імпульс електрона: $\mathbf{k}$

a

L

$\mathscr{E}$

k

$-\tfrac{3}{2}K \quad -K \quad -\tfrac{1}{2}K \quad O \quad \tfrac{1}{2}K \quad K \quad \tfrac{3}{2}K$
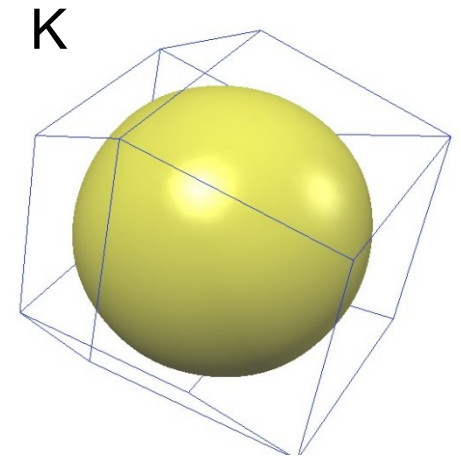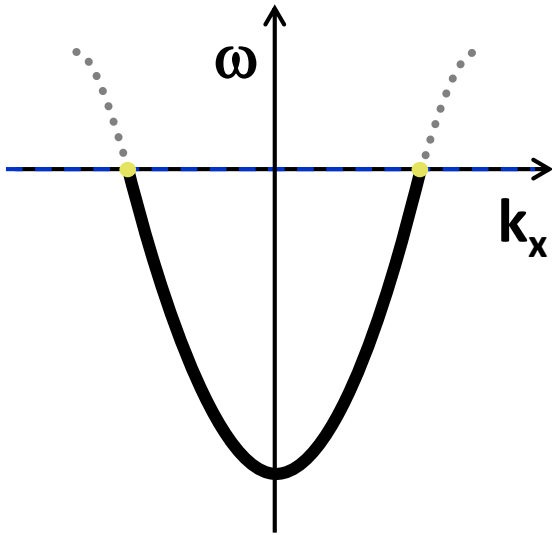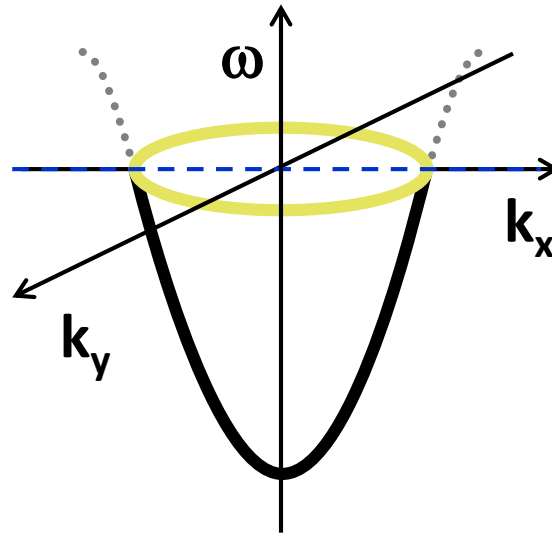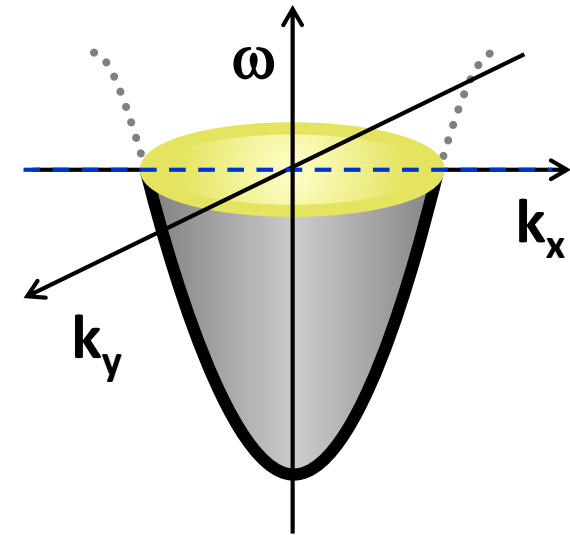
$K = 2\pi/a$

... Fermi surface

1D   2D   3D

... Fermi surface

1D

2D

3D projected on 2D
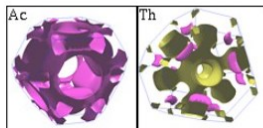
Nb

Cu

The Fermi Surface Database

(click icons)
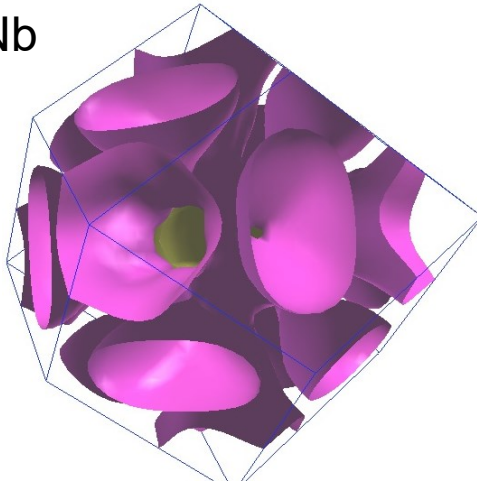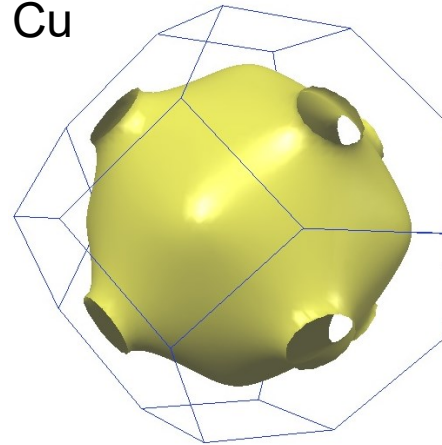
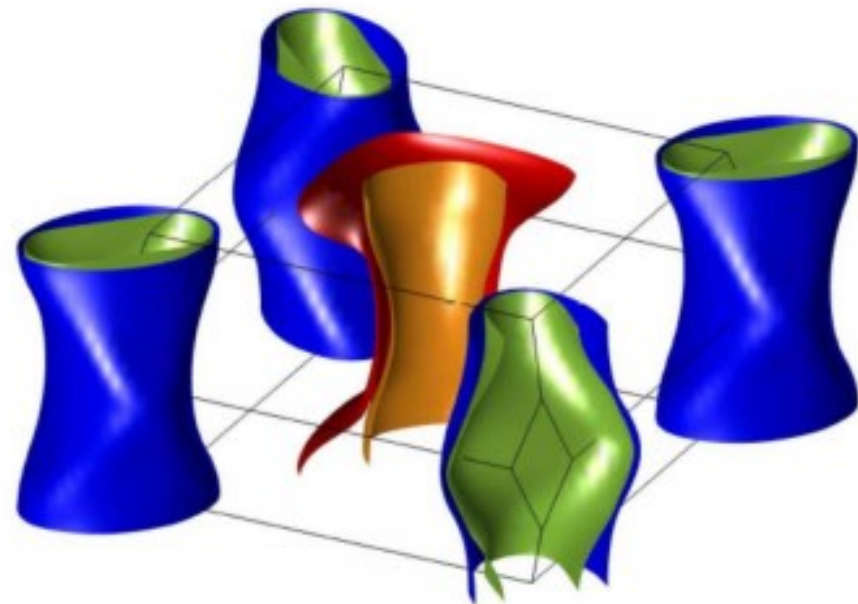| Li	Be											B	C
Na	Mg											Al	Si
K	Ca	Sc	Ti	V	Cr	Mn	Feup	Coup	Niup	Cu	Zn	Ga	Ge
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb

**

Ac	Th
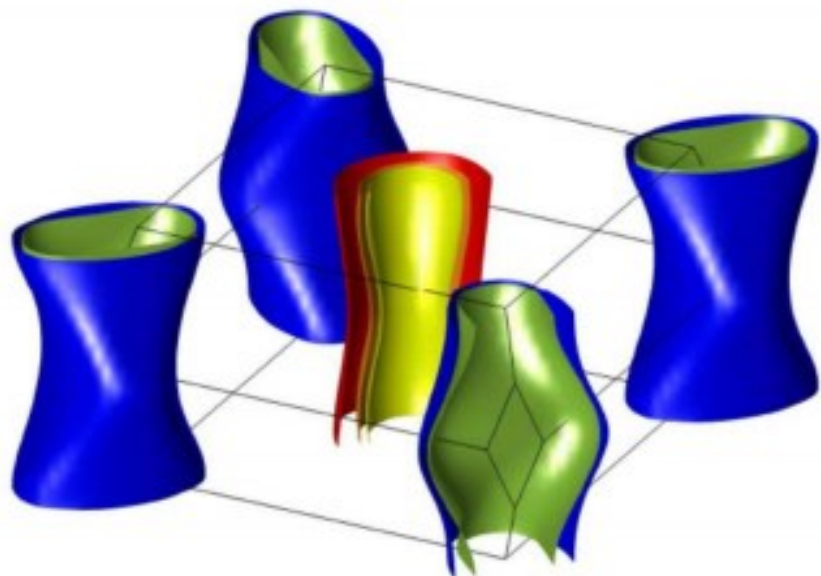
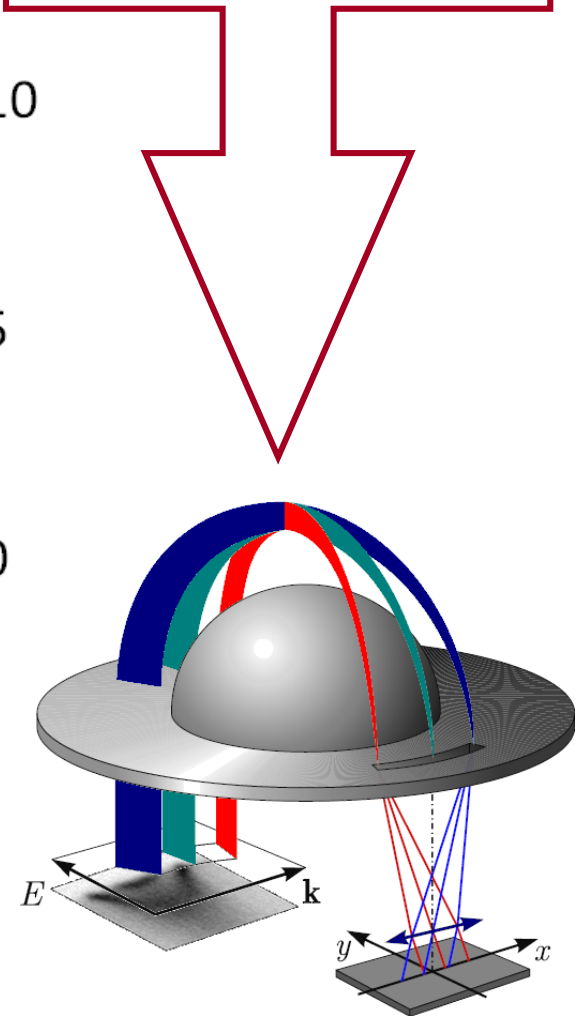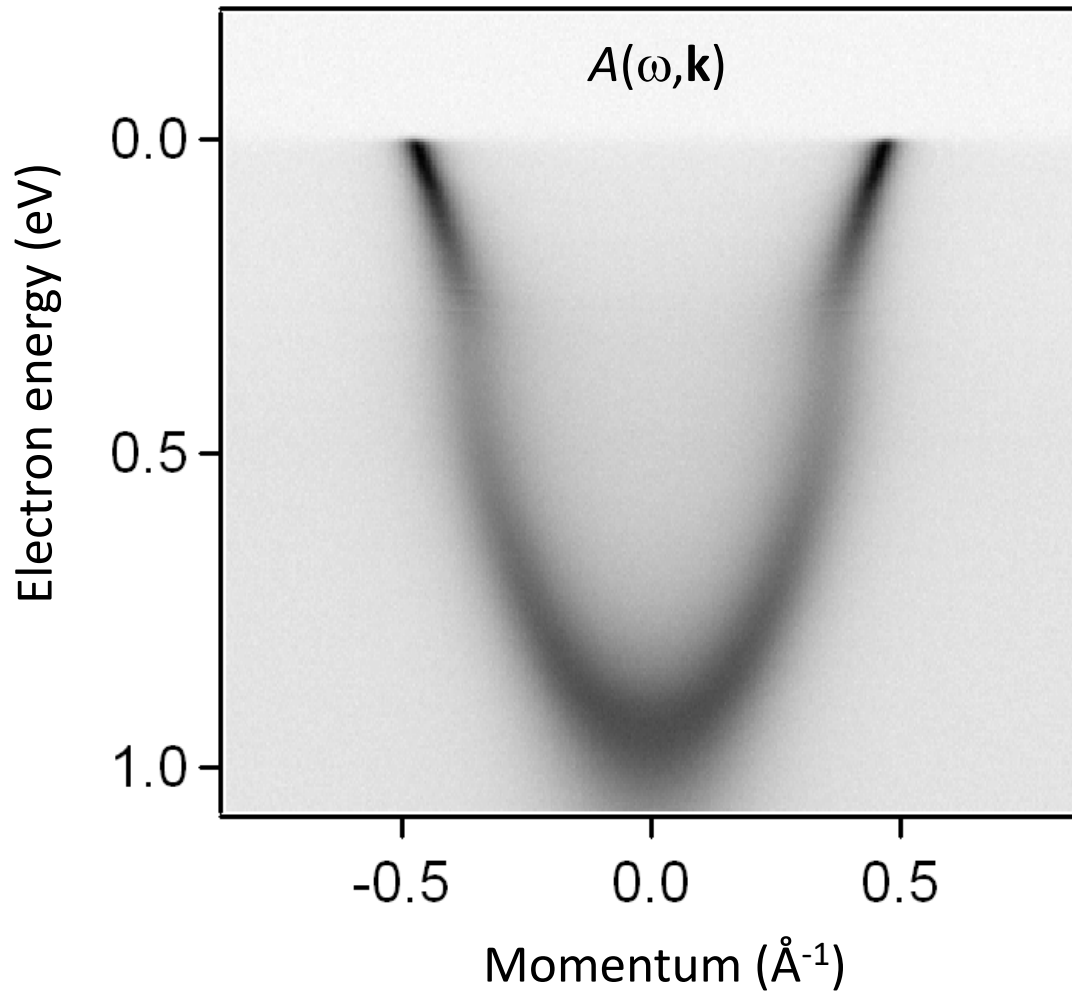BaFe$_2$As$_2$ BaFe$_2$P$_2$

Electronic structure

Electronic structure ≡ Electronic excitation spectrum ≡

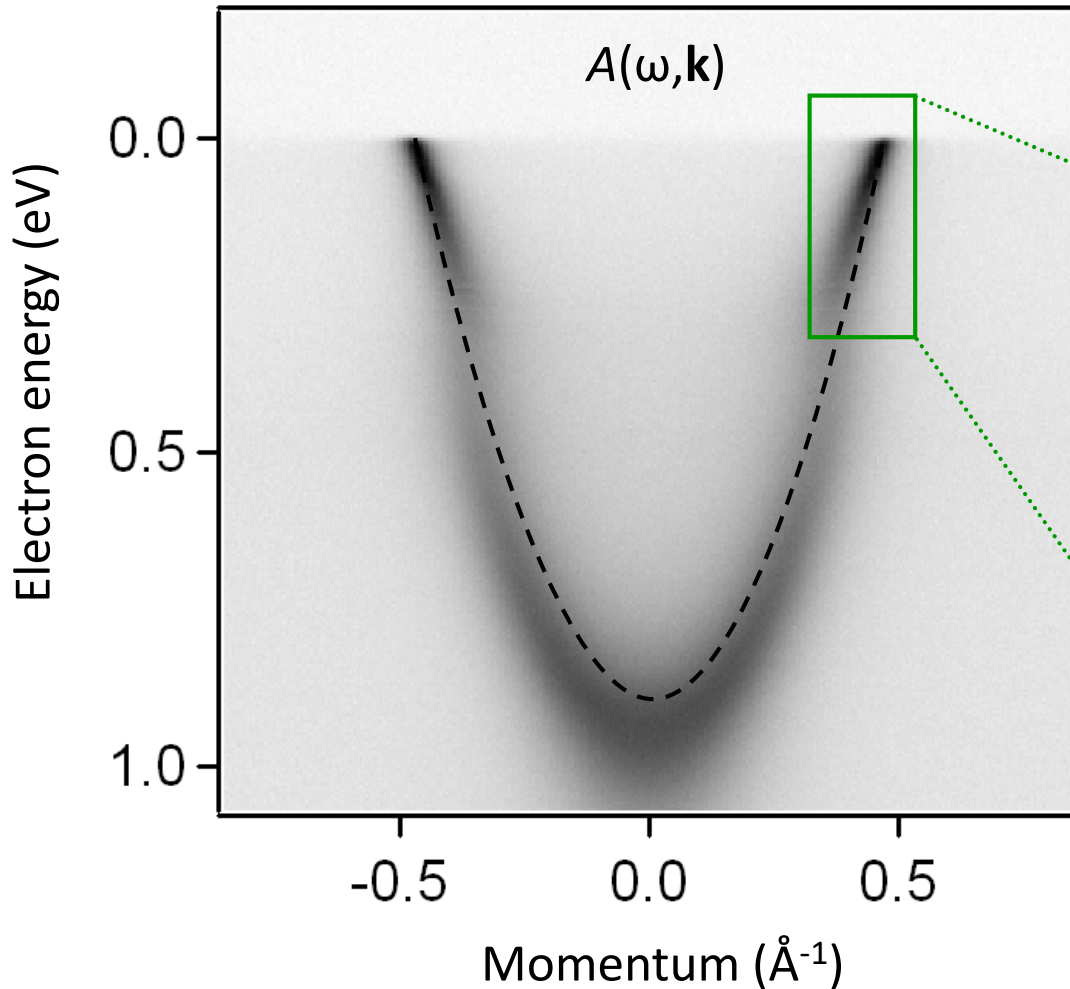Probability to find electron with momentum **k** and energy ω
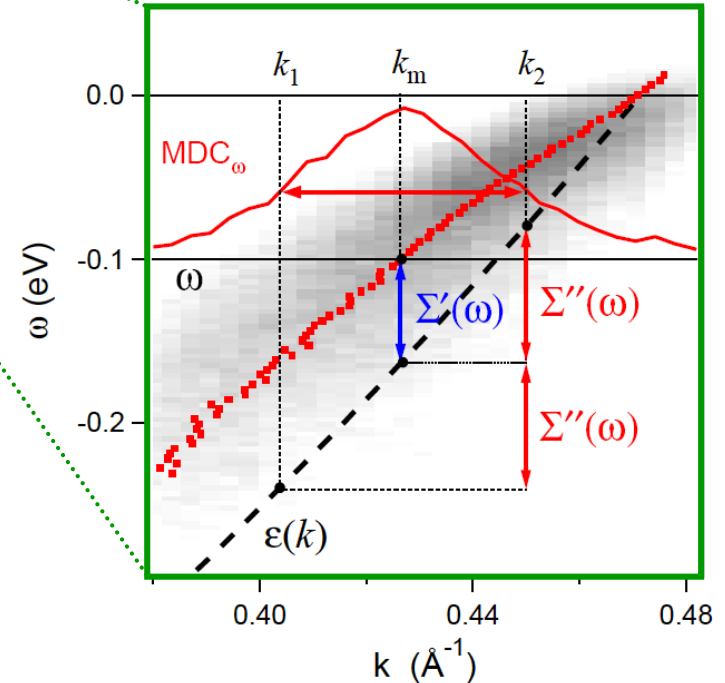
Structure of electronic spectrum

Spectral function

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(\mathbf{k}) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$
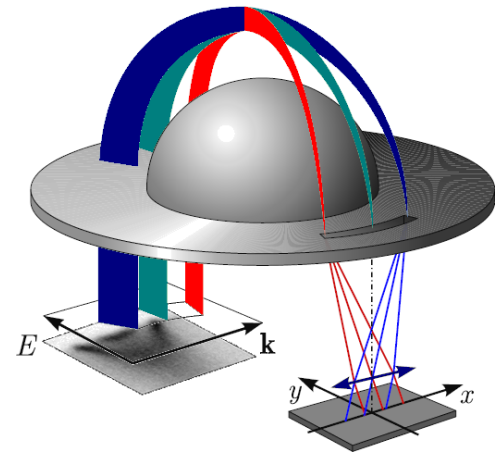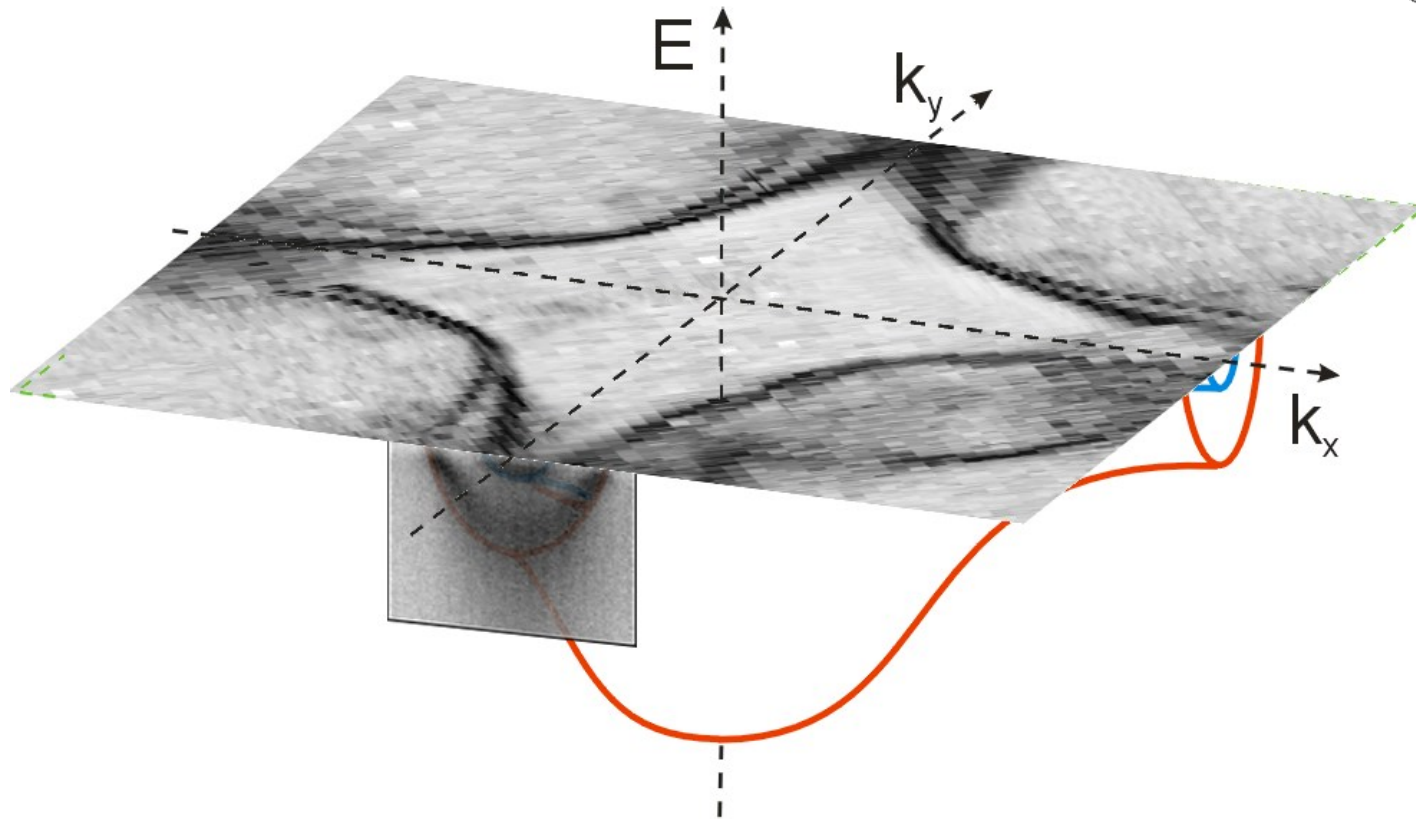
$\varepsilon(\mathbf{k})$ – "bare" electronic band structure

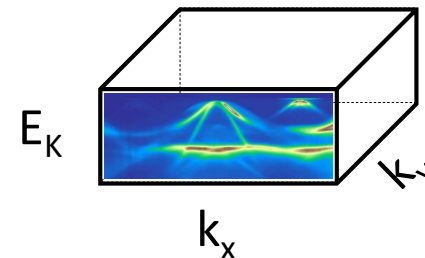$\Sigma(\omega, \mathbf{k})$ – self-energy

$A(\omega, \mathbf{k})$

Electron energy (eV)

Momentum (Å⁻¹)

Kordyuk *PRB* 2005

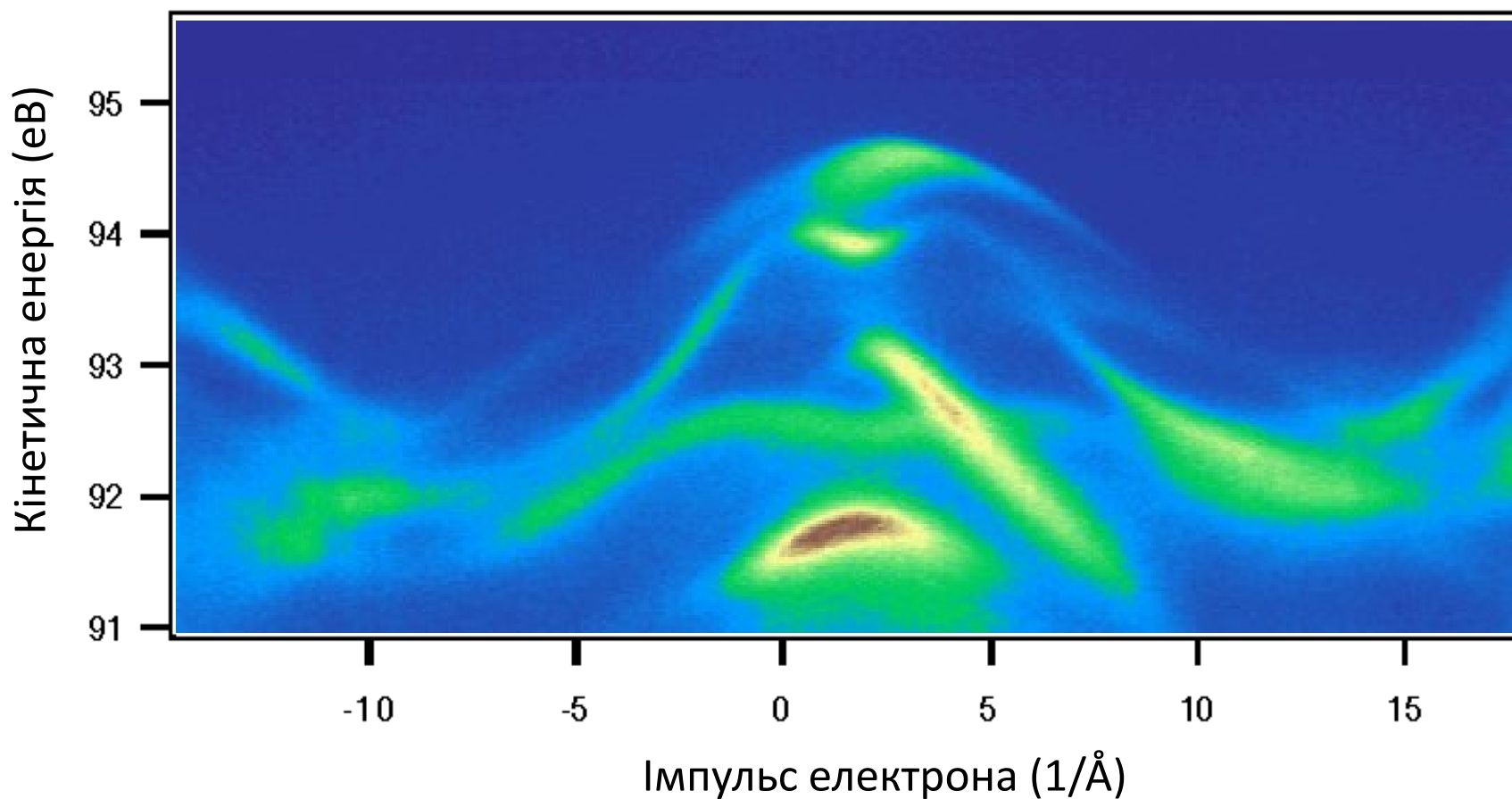# Electronic spectrum of quasi-2D crystals

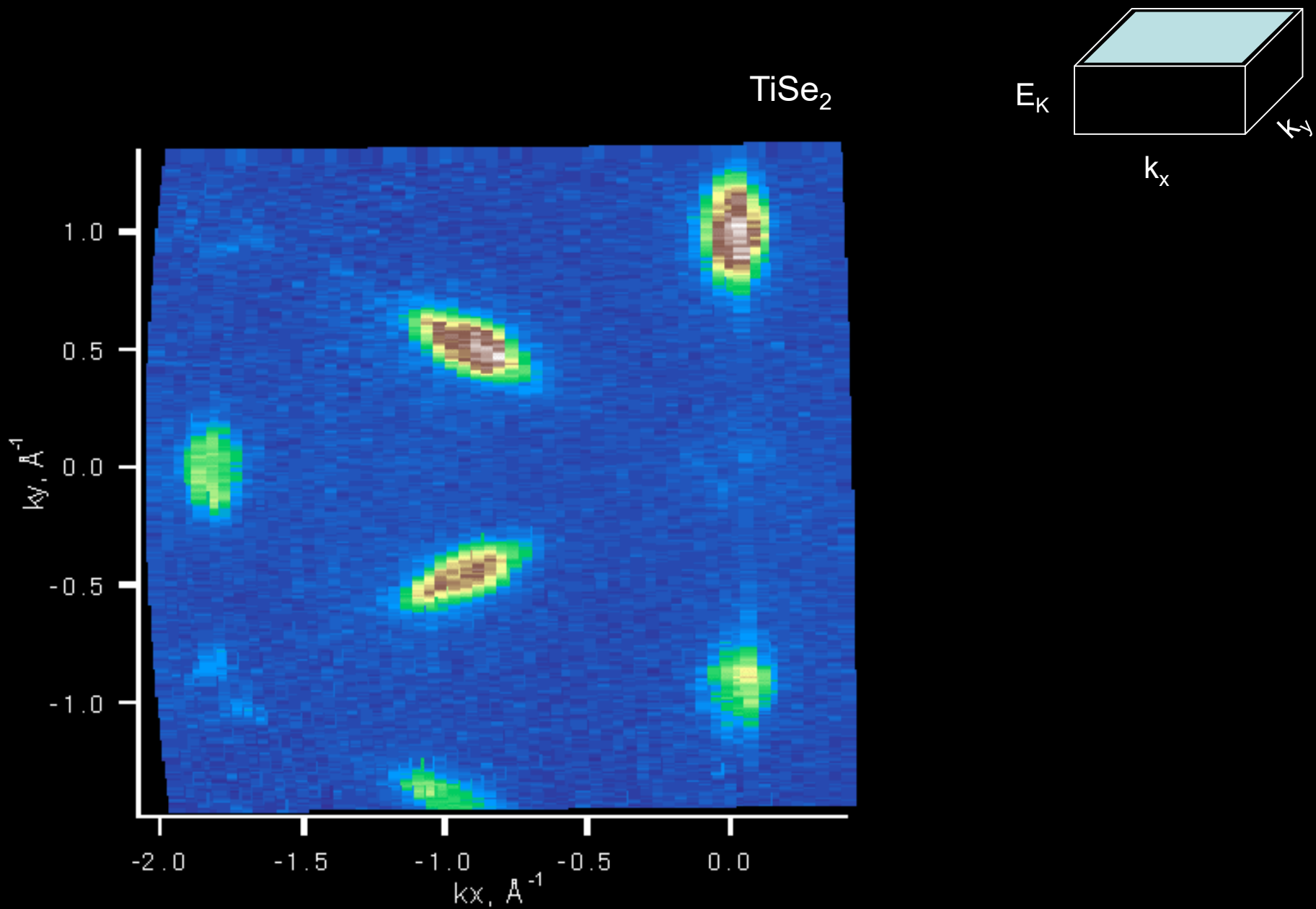$$\varepsilon(k_x, k_y) \quad \Rightarrow \quad A(\omega, k_x, k_y)$$

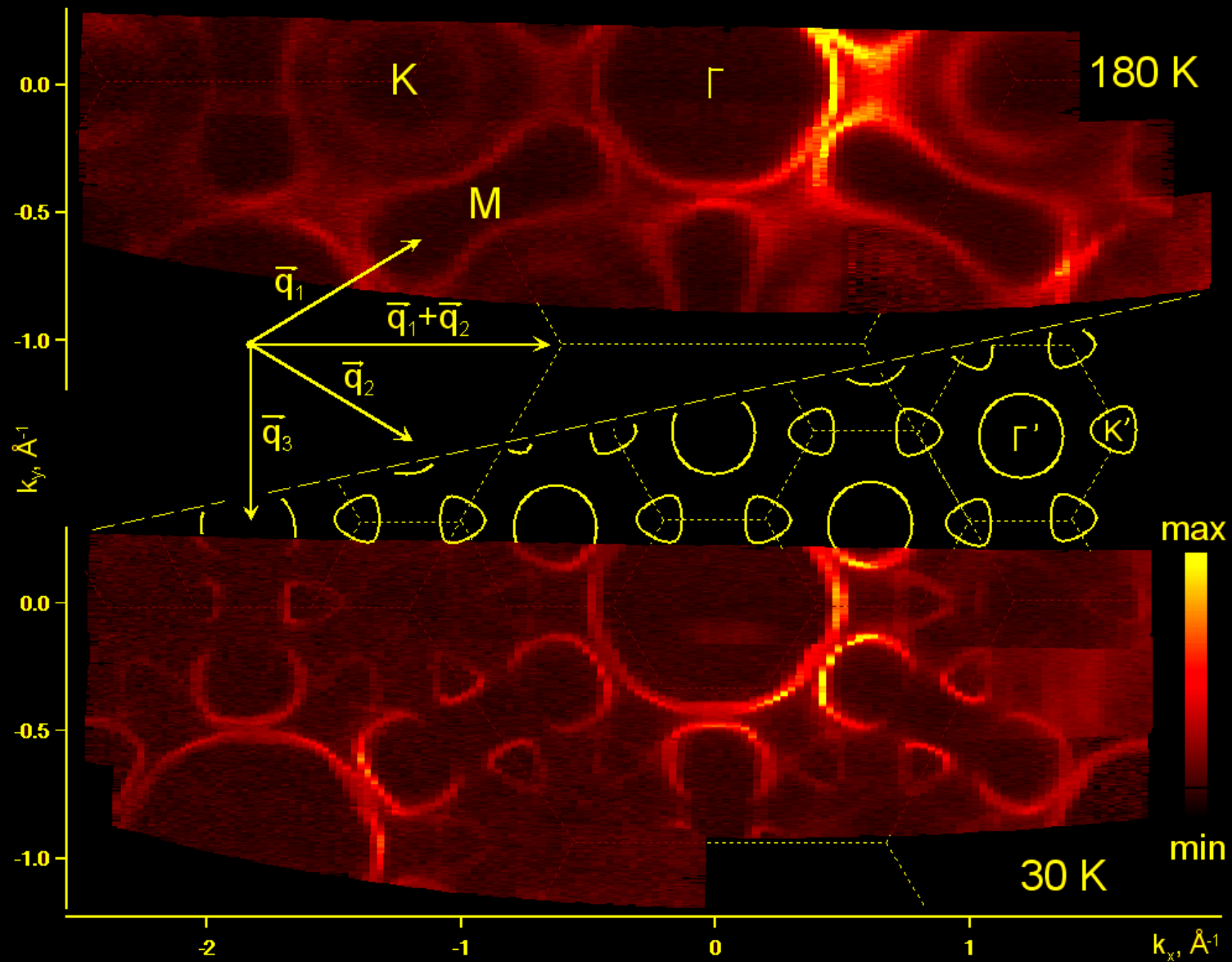# Electronic spectrum in momentum-energy 3D space
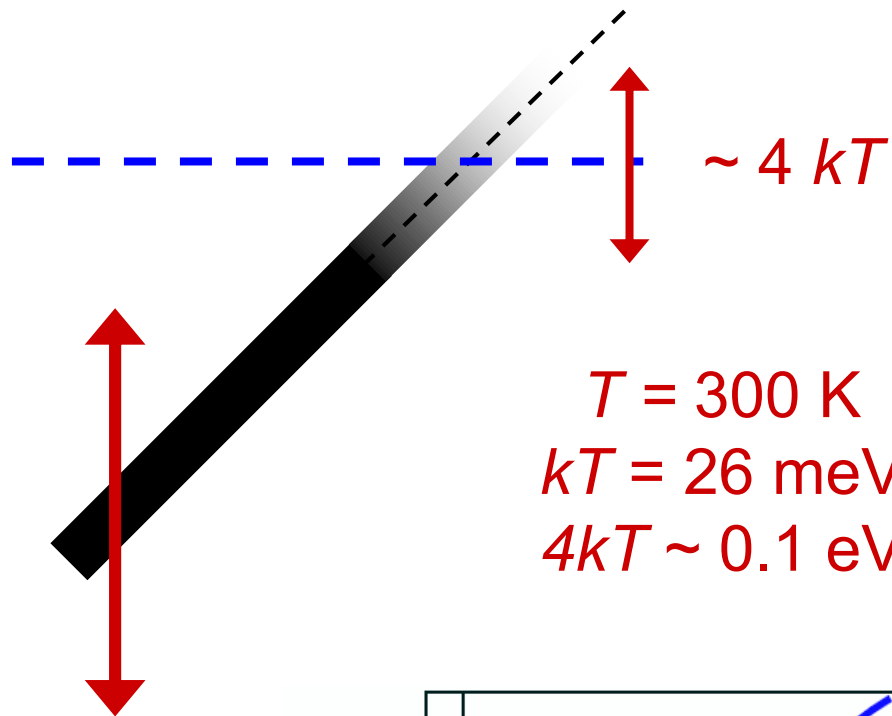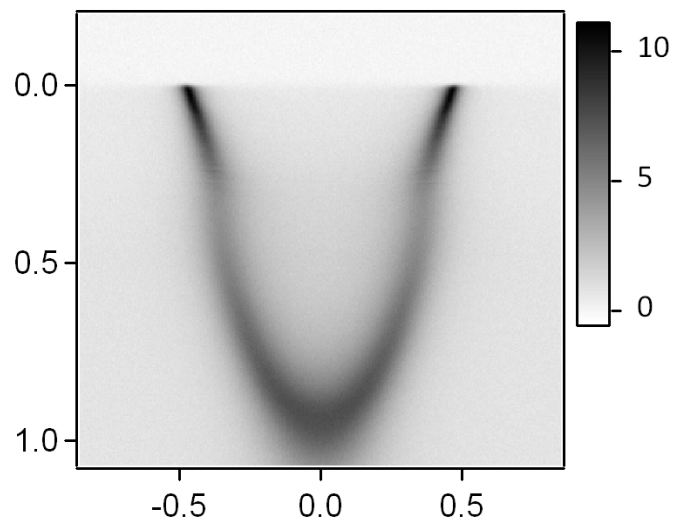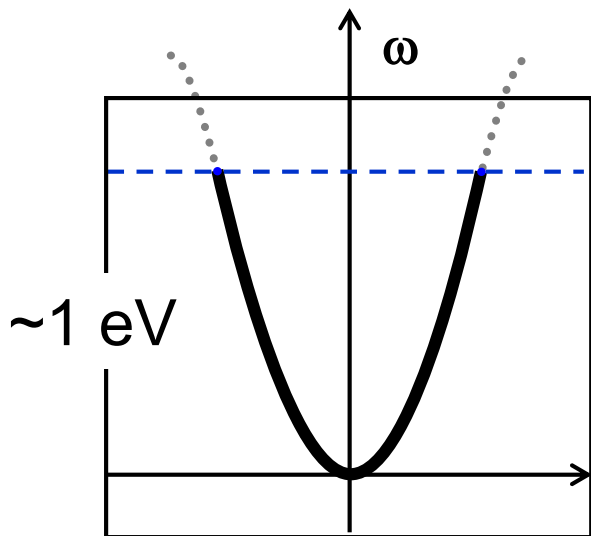

TiSe₂ - «excitonic insulator»

Кінетична енергія (eB) / Імпульс електрона (1/Å)

Fermi surface (energy distribution) map

TiSe$_2$

CDW y TaSe$_2$: commensurate CDW state

Energy scales

~ 1 eV

ω

$\sim 4\ kT$

$T = 300$ K
$kT = 26$ meV
$4kT \sim 0.1$ eV

$2\Sigma'' \sim \alpha\,\omega^2 + \beta T^2$

$-\Sigma''$ (eV)

— $< T^*$
-- $> T^*$

-- Σ_1
■ Σ_2

ω (eV)
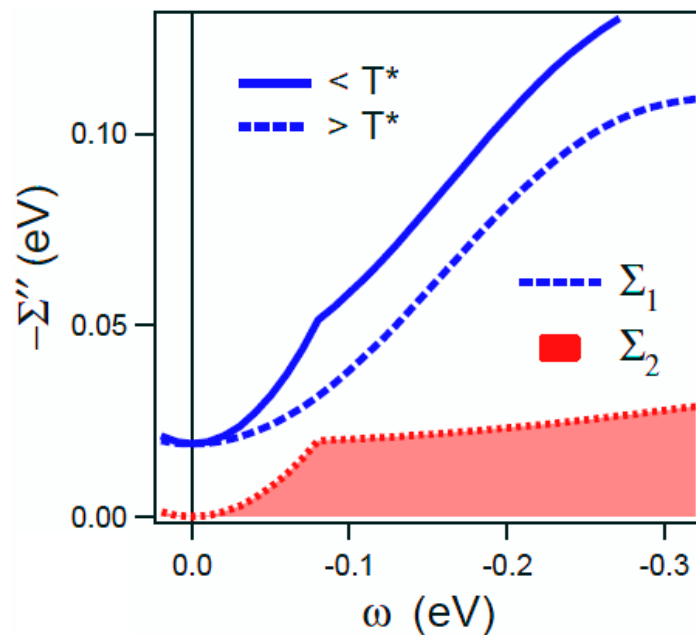
Spectroscopic Techniques

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e	IPS, EDX (SEM)	SEM, LEED, EELS	ESD
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$n\text{-}n:$ **ND, INS**

$\mu\text{-}e^+:$ **μSR**