Basic principles and applications of ARPES and Spin-ARPES

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AREA Science Park, Trieste, Italy
and NFFA Trieste

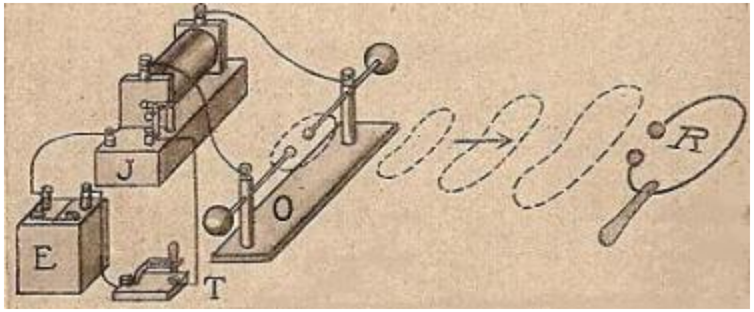
Outline

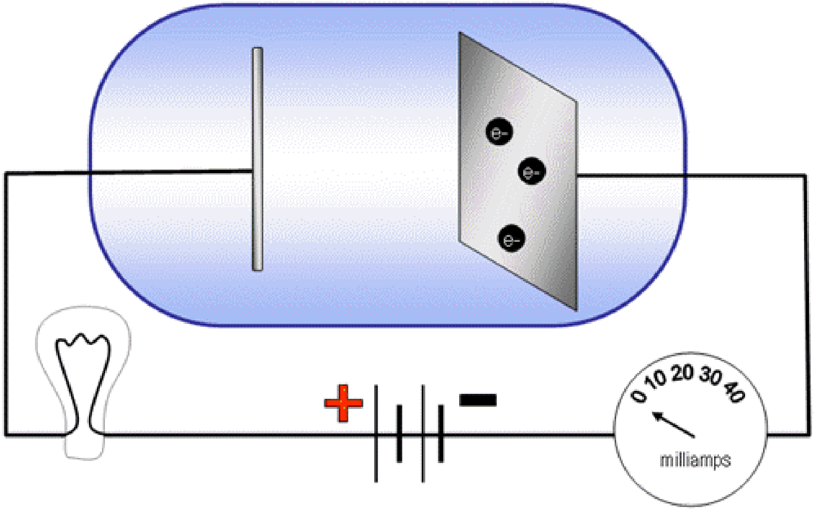
- A brief introduction to **photoemission**
  - History
  - Theory
  - Experimental requirements

- **Valence band** photoemission
  - Refreshing solid state physics concepts
  - **ARPES**
  - **Spin ARPES → complete photoemission experiment**

- **Complete photoemission** experiment @ Elettra
  - **ARPES** and **Spin-ARPES** station:  @ 

1887 - Photoelectric Effect





Observed by Heinrich Hertz 1887

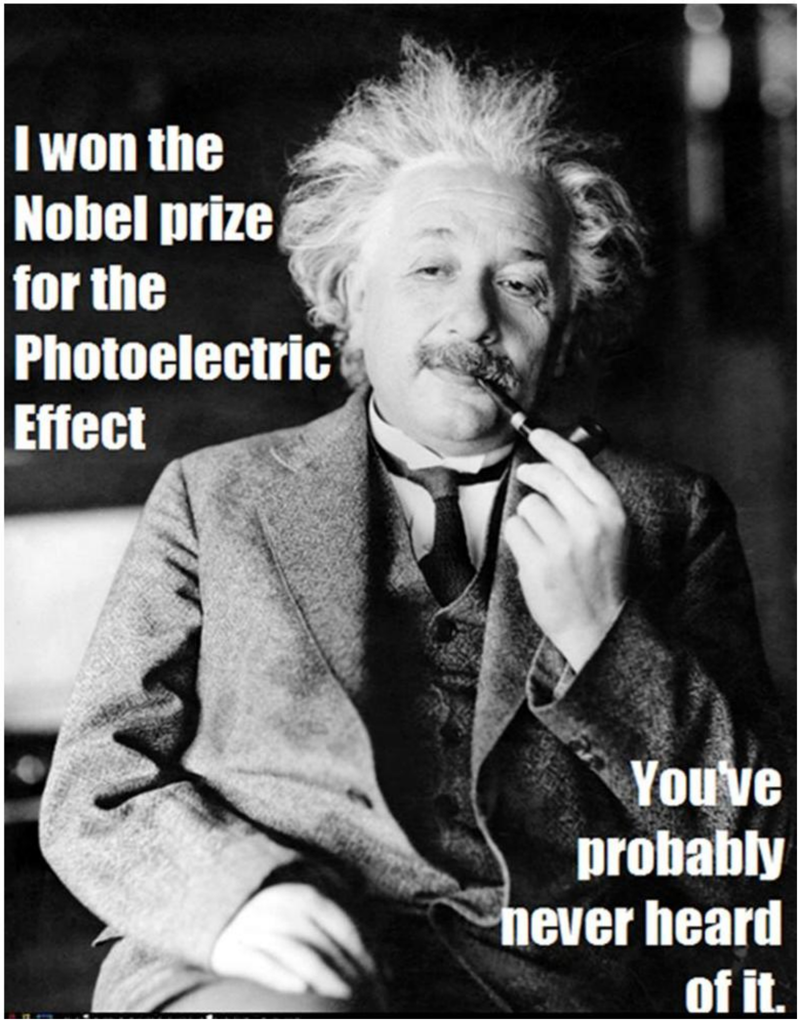
- P. Lenard: measuring kinetic energy of photoelectrons in retarding field

Experimental observations:

- Measured photoelectron current increases with photon intensity

- Maximum energy of the (photo)electrons **depends on light frequency** (contrary to classical expectation)

1905 – Explained by Albert Einstein



The Nobel Prize in Physics 1921
Albert Einstein

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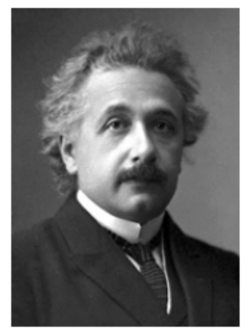
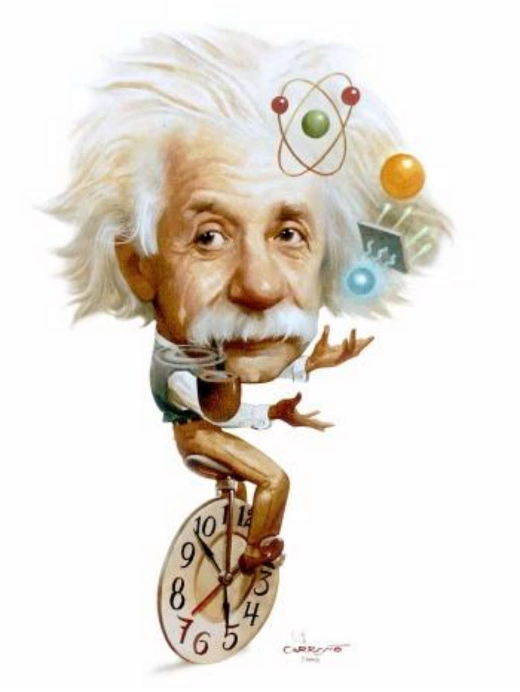
The Nobel Prize in Physics 1921

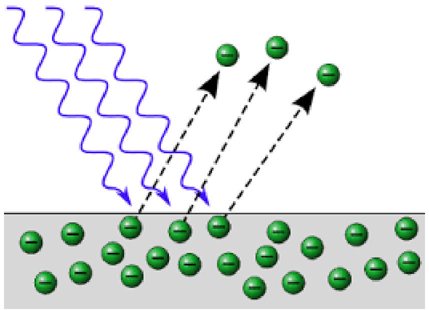


Albert Einstein
Prize share: 1/1

The Nobel Prize in Physics 1921 was awarded to Albert Einstein *"for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect".*

1905 – Photoelectric effect according to Einstein





- Electrons inside material absorb incoming light quanta - photons

- If their energy is sufficiently high they leave the material carrying info on their properties inside the material

Photoemission

Birth of photoemission 1950s

PHYSICAL REVIEW VOLUME 105, NUMBER 5 MARCH 1, 1957

Precision Method for Obtaining Absolute Values of Atomic Binding Energies

CARL NORDLING, EVELYN SOKOLOWSKI, AND KAI SIEGBAHN
Department of Physics, University of Uppsala, Uppsala, Sweden

(Received January 10, 1957)

WE have recently developed a precision method of investigating atomic binding energies, which we believe will find application in a variety of problems in atomic and solid state physics. In principle, the method is an old one: a magnetic analysis of electrons expelled from a substance exposed to x-radiation. Previous attempts in this direction have, however, given considerably less information about atomic structure than ordinary x-ray spectroscopic experiments, and some twenty years ago the method seems to have been definitely abandoned. We have introduced a number of improvements, both regarding the intensity and, in particular, the accuracy (a factor 100), which now enables us to measure atomic binding energies with an accuracy of one single electron volt from microgram quantities. The definition of the lines is essentially limited by the natural line widths of the atomic levels themselves. There is no shift of the lines due to electron scattering or similar causes, which could introduce systematic errors.

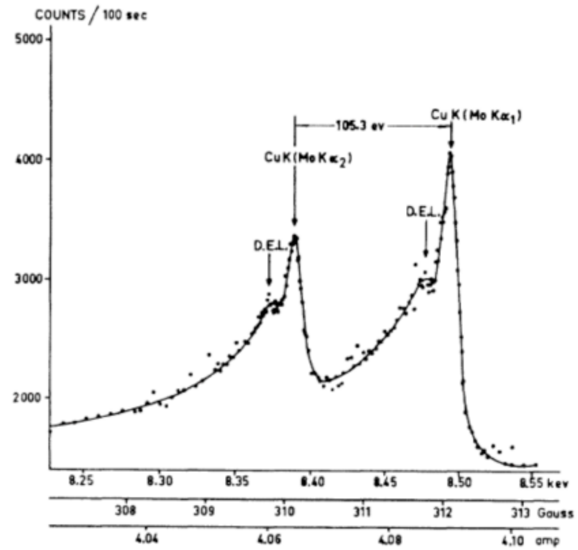


FIG. 1. Lines resulting from photoelectrons expelled from Cu by Mo $K\alpha_1$ and Mo $K\alpha_2$ x-radiation. The satellites marked D.E.L. are interpreted as due to electrons which have suffered a discrete energy loss when scattered in the source.

The Nobel Prize in Physics 1981
Nicolaas Bloembergen, Arthur L. Schawlow, Kai M. Siegbahn

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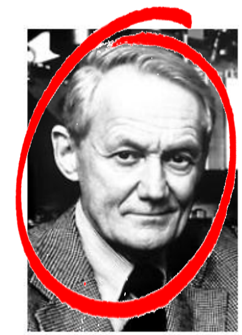
The Nobel Prize in Physics 1981

Nicolaas Bloembergen
Prize share: 1/4

Arthur Leonard Schawlow
Prize share: 1/4

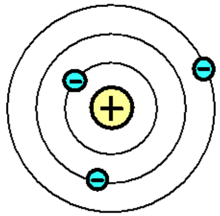


Kai M. Siegbahn
Prize share: 1/2

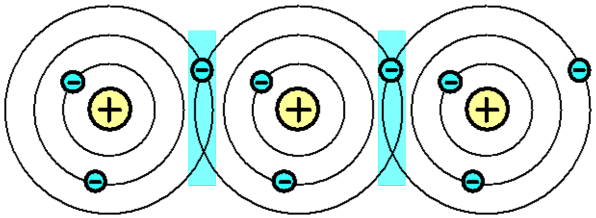
The Nobel Prize in Physics 1981 was divided, one half jointly to Nicolaas Bloembergen and Arthur Leonard Schawlow *"for their contribution to the development of laser spectroscopy"* and the other half to Kai M. Siegbahn *"for his contribution to the development of high-resolution electron spectroscopy"*.

ideal tool for the chemical investigation of surfaces and thin film, expressed in the famous acronym created by Siegbahn: **ESCA** (electron spectroscopy for chemical analysis)
or
XPS – X-ray Photoelectron/Photoemission Spectroscopy

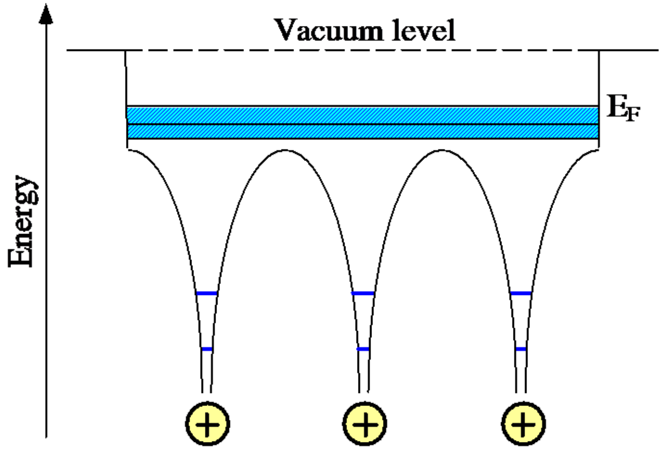
Atom → Solid Cartoon



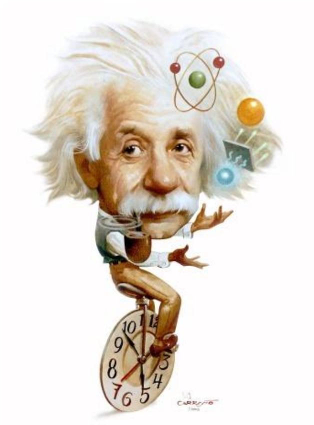
Localized core electrons

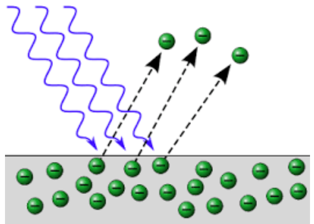


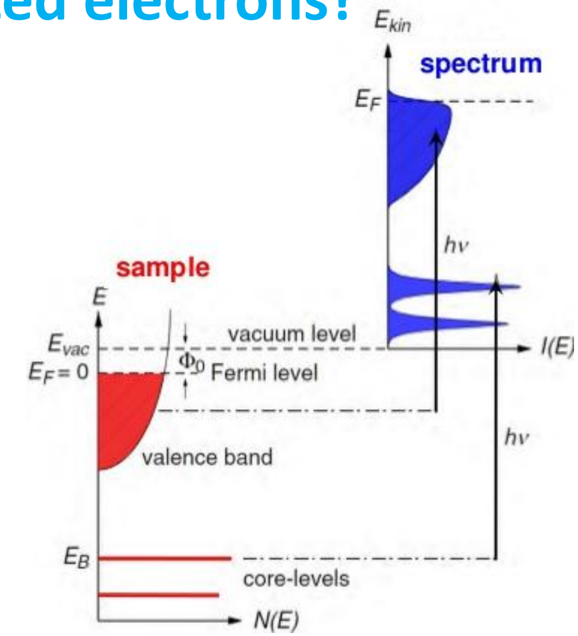
Localized core electrons
Delocalized valence electrons (energy bands)



What do we learn from photoemitted electrons?



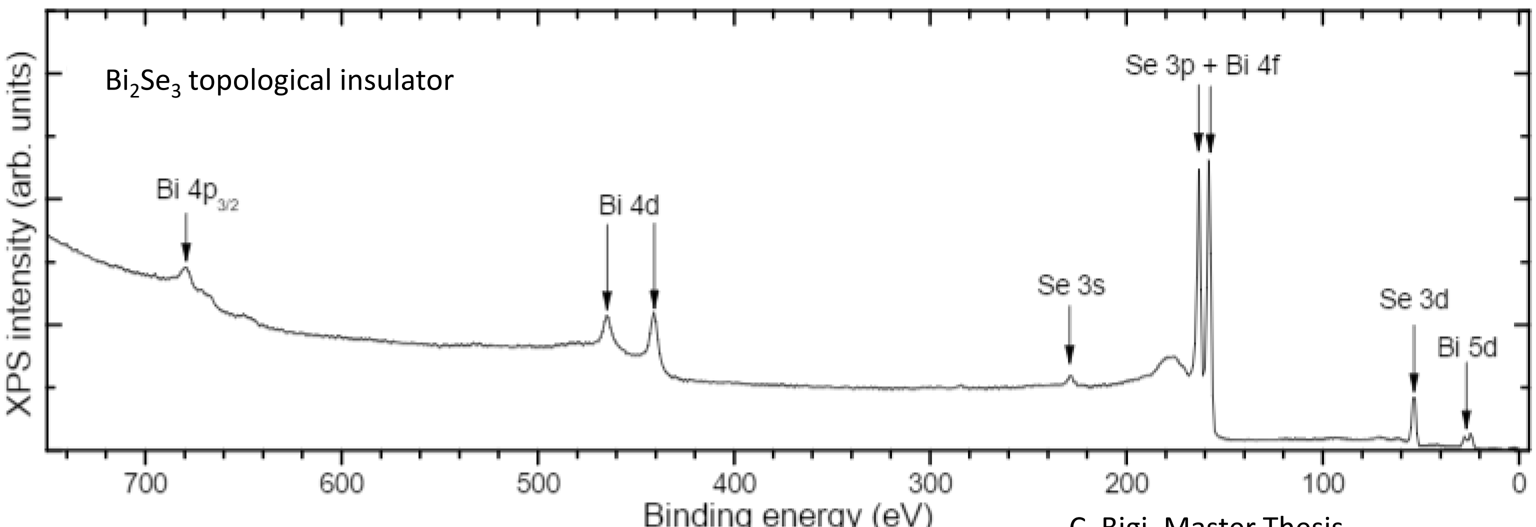




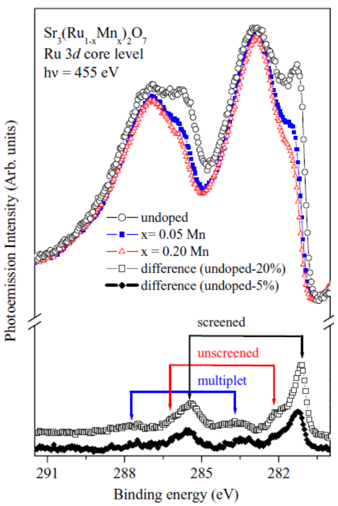
$$E_{kin} = h\nu - E_B - \Phi$$

Core electrons (XPS):

composition, chemical bonding, valence, density of states, electronic correlations



C. Bigi, Master Thesis
Uni. Milano 2016



G. Panaccione et al.
New J Phys 2011

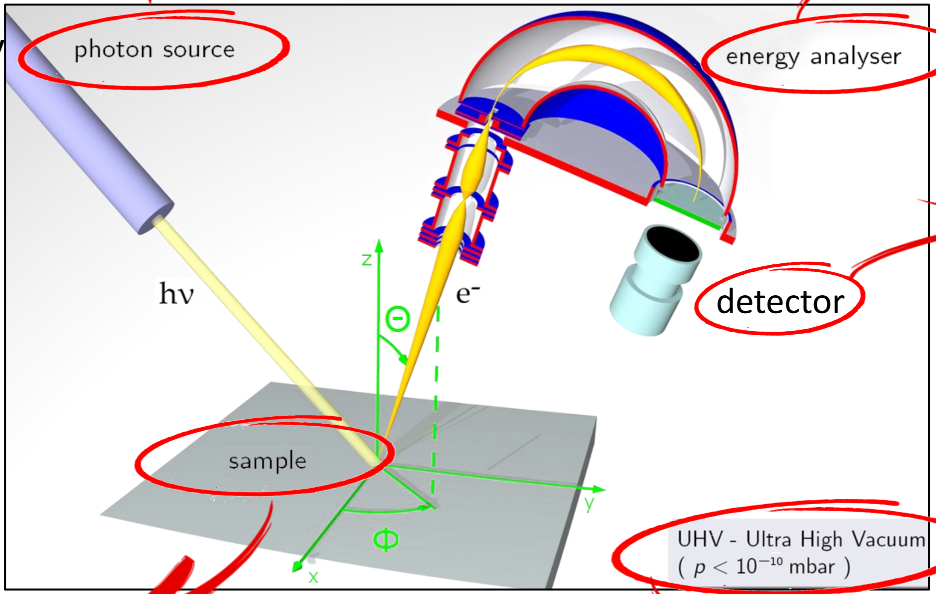
Experimental requirements for XPS (ESCA)

Laboratory

- **X-rays** - generated by bombarding a metallic anode with high-energy electrons
- **UV** - noble gas discharge lamps

Synchrotrons

-**Tunable and polarized UV→hard X-rays**



Hemispherical electron energy analyzer

Channeltron
MCP

Whatever you wish as long as sufficiently conductive…

Surface sensitivity - surfaces are an issue…

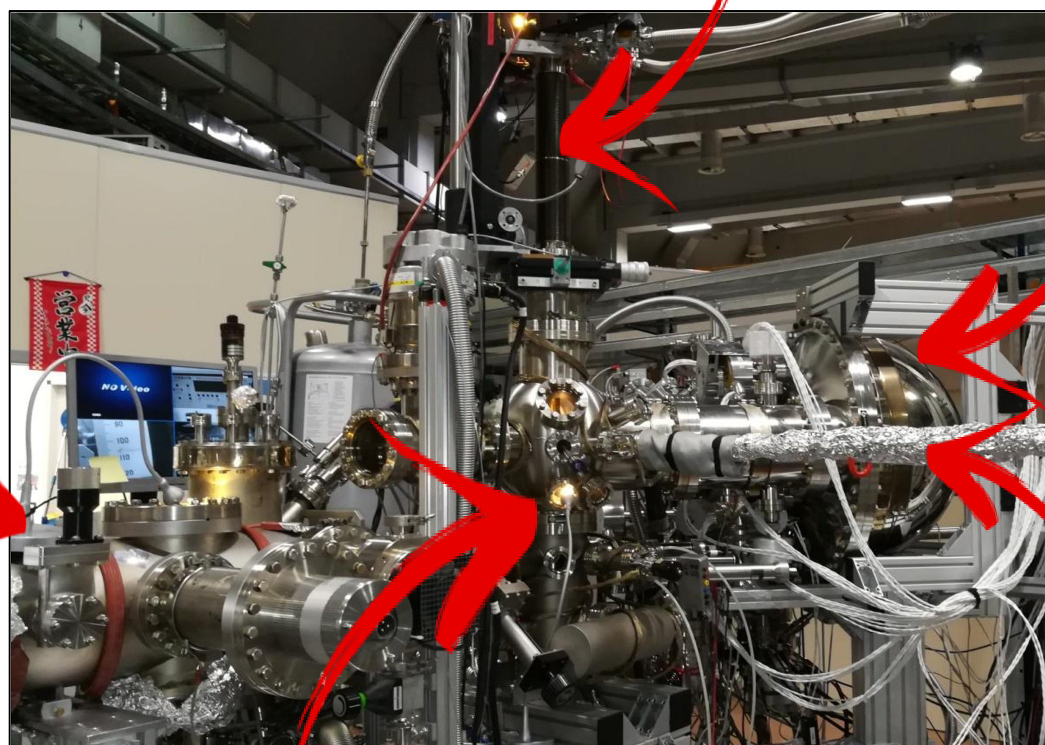
Experimental requirements – real life

End station of APE – LE beamline at Elettra

Sample manipulator

Hemispherical electron energy analyzer

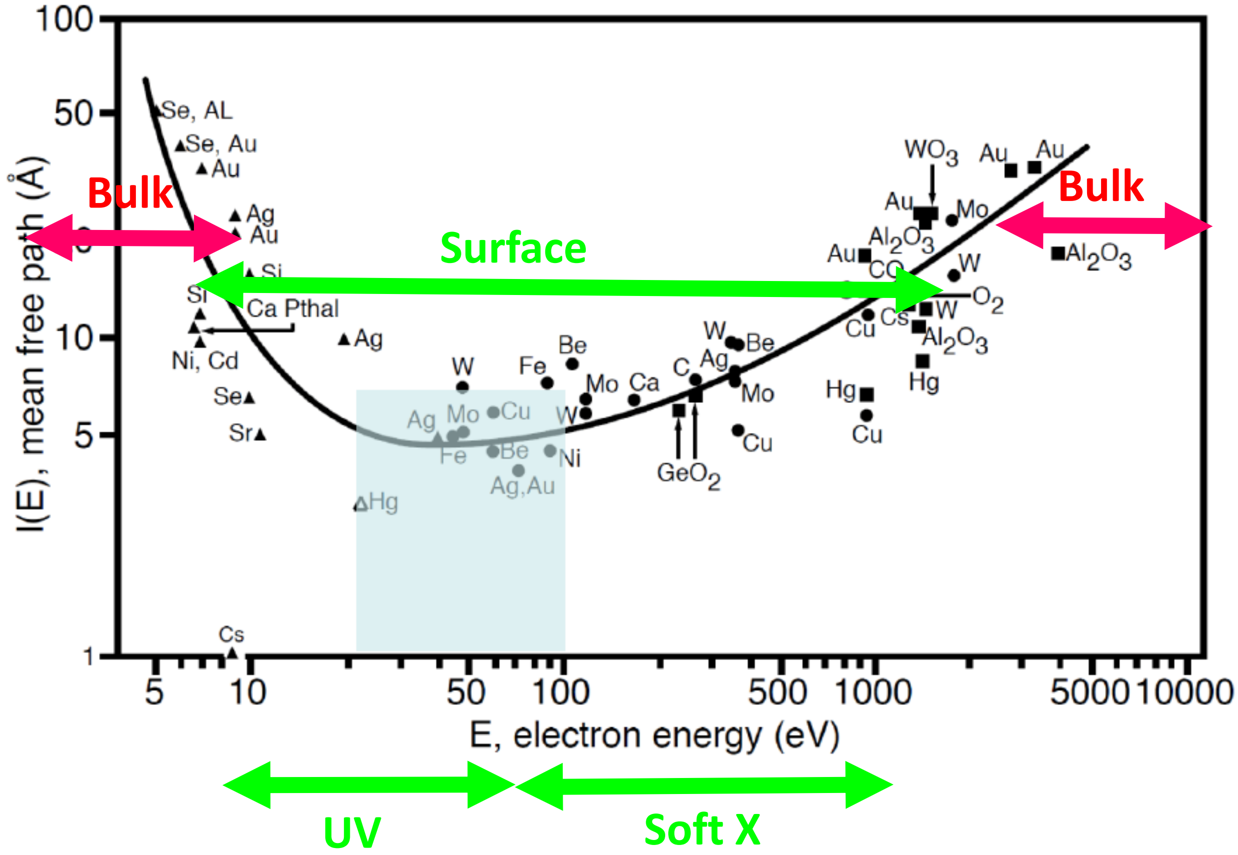
Sample surface preparation chamber



Photons

ARPES chamber

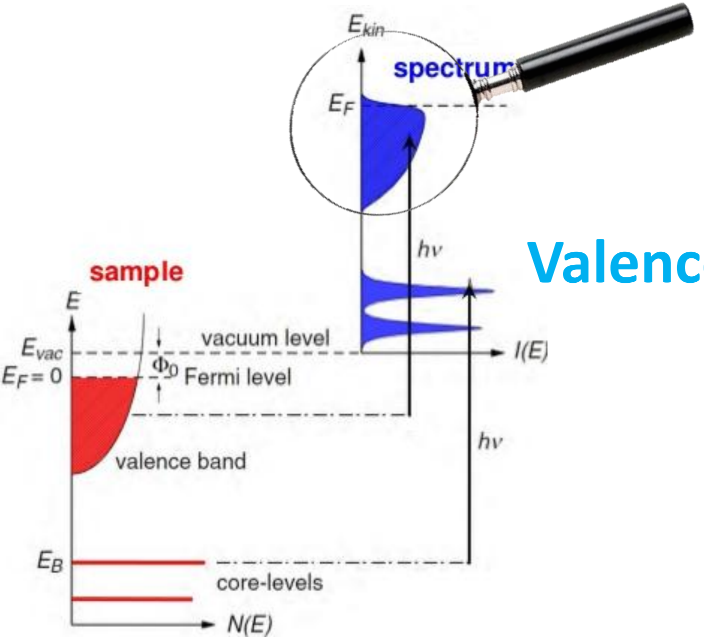
Surface sensitivity – electron mean free path



- Number of electrons reaching the surface is reduced by electron-electron scattering

→**Only sensitive to first couple of atomic layers!!** →**Clean surfaces** and **UHV** needed

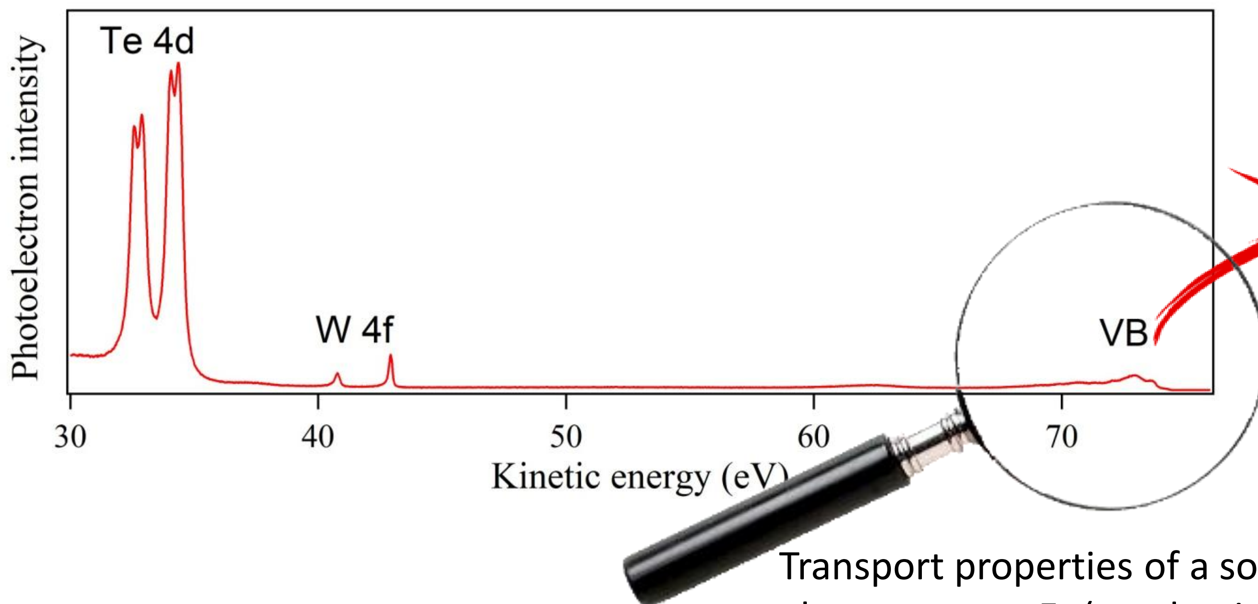
- Scattered electrons with lower kinetic energies form background (secondaries)

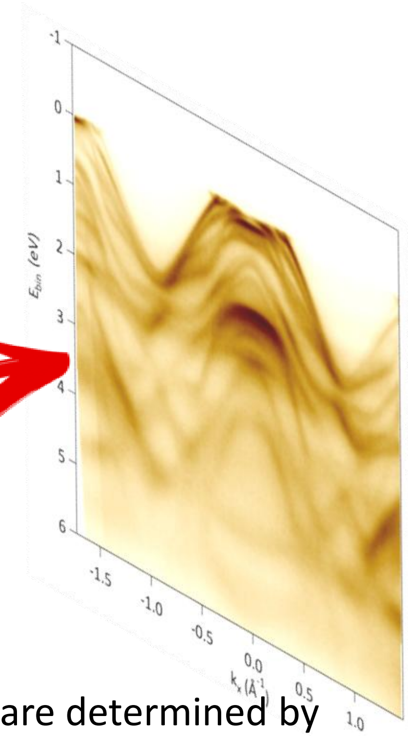


Valence electron photoemission

ARPES

Spin-ARPES

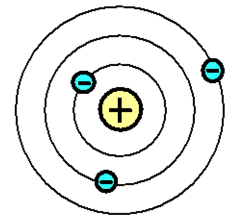




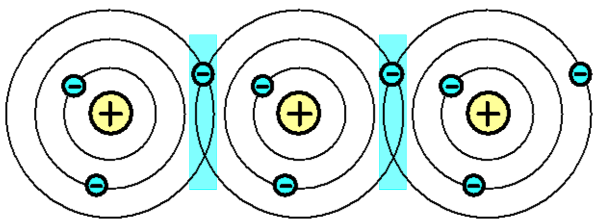
Transport properties of a solids are determined by electrons near E_F (conductivity, magnetoresistance, superconductivity, magnetism)

Valence band photoemission

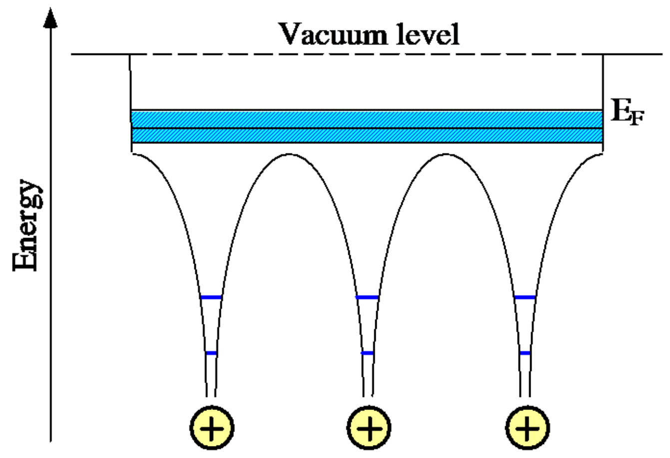
Atom → Solid Cartoon



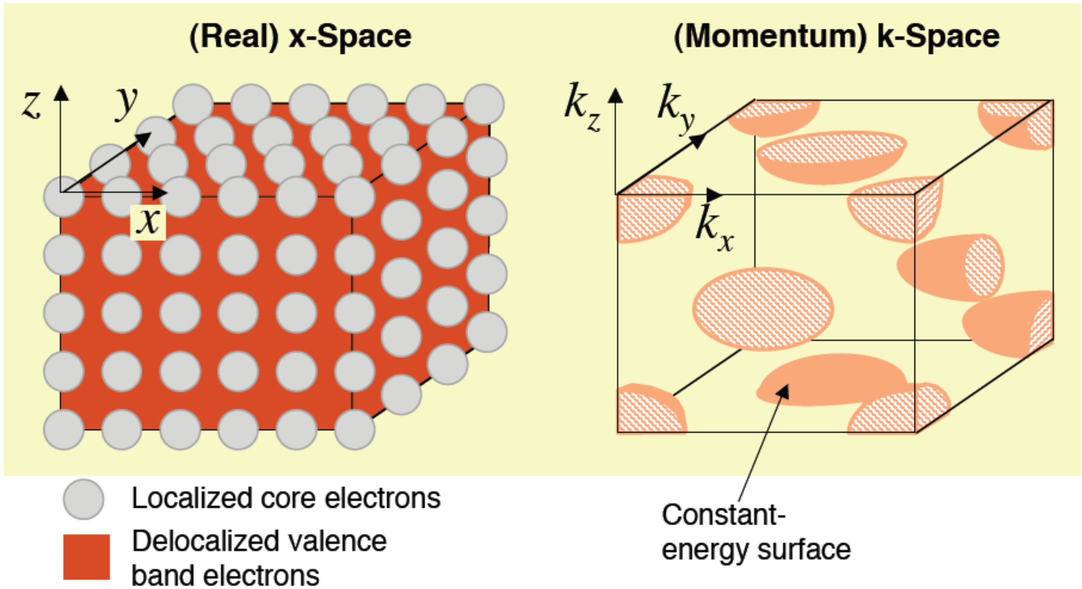
Localized core electrons

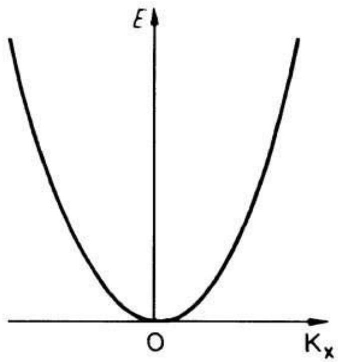


Localized core electrons
Delocalized valence electrons (energy bands)



Real vs. reciprocal (momentum or *k*-)space

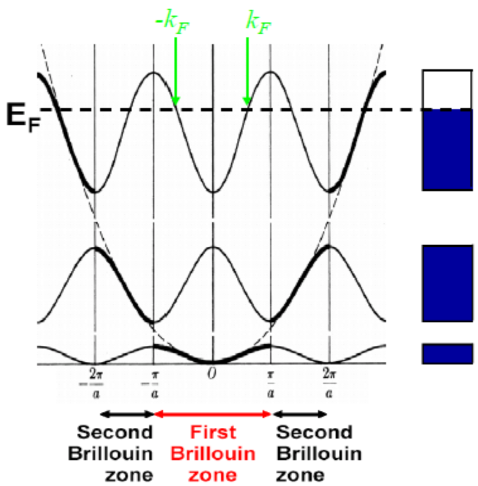




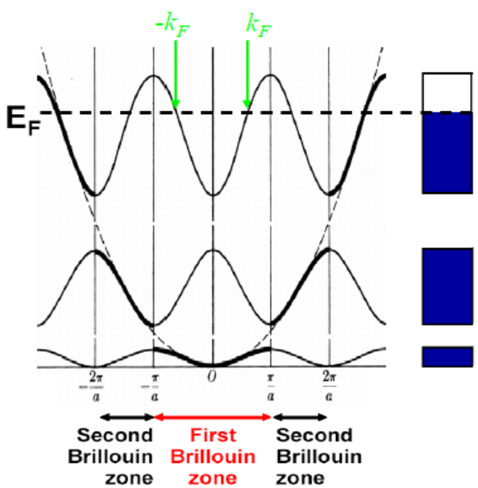
$$E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}$$

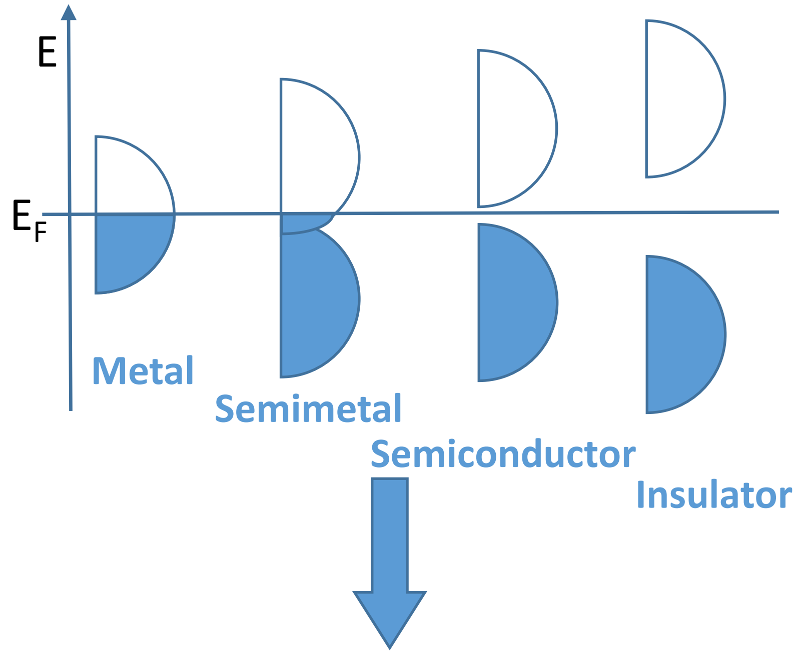
Free electron vs. electron in a lattice:

Periodic potential → **electronic bands and band gaps**

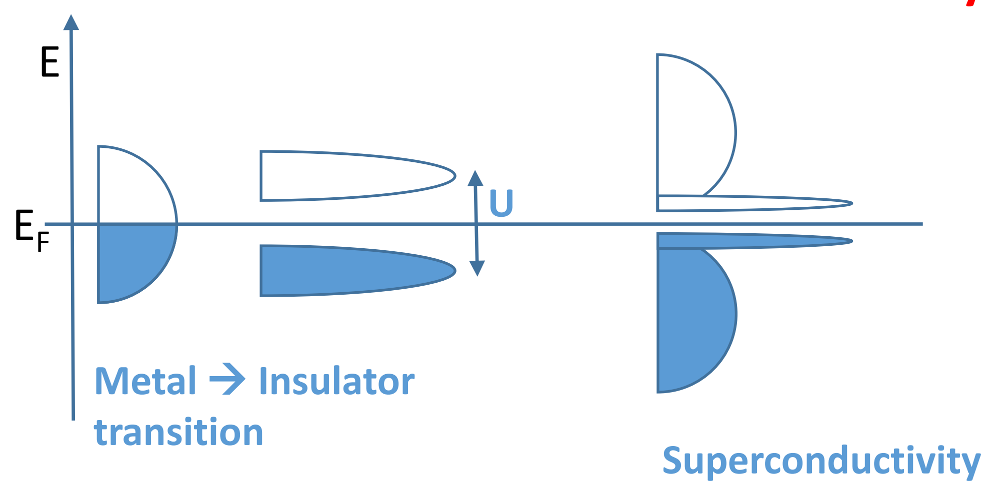


Classification of materials according to the filling of the electronic bands





All this from E vs. k relation! And not only…



…when things get more complicated and electrons interact: **fingerprints of electronic correlations**

The question is…

Can E vs. k (i.e., **the electronic band structure of solids**) be directly **measured**?

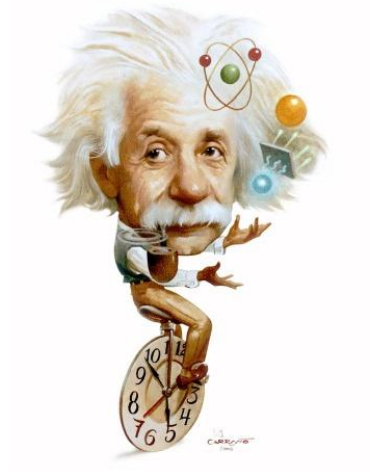
… and the answer…

Yes!

Valence band photoemission with angular resolution:

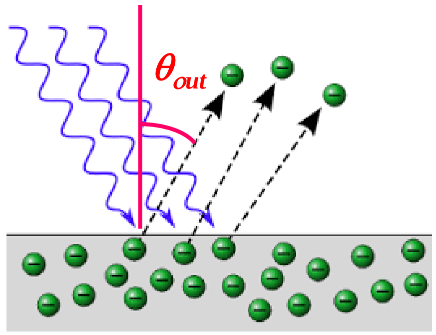
Angle-Resolved PhotoEmission Spectroscopy - **ARPES**

What do we learn from photoemitted *valence* electrons?



Energy conservation

$$E_{kin} = h\nu - E_B - \Phi$$



Momentum conservation

Inside the crystal:

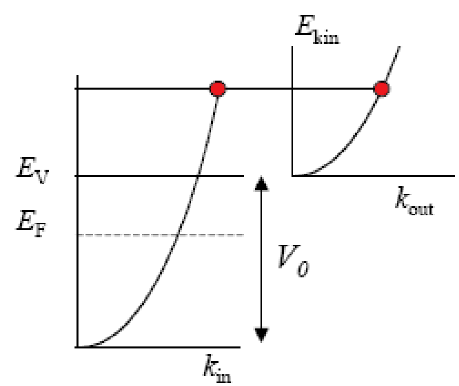
$$\vec{k}_f = \vec{k}_i + \vec{k}_{h\nu}$$

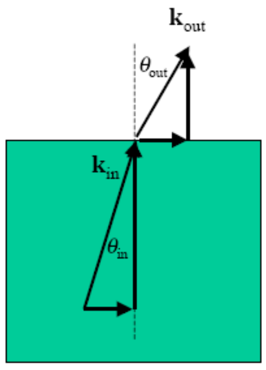
$$\vec{k}_f = \vec{k}_i$$

Refraction on the surface (Snell's law):

$$k_{out} = \sqrt{\frac{2m}{\hbar^2} E_{kin}}$$

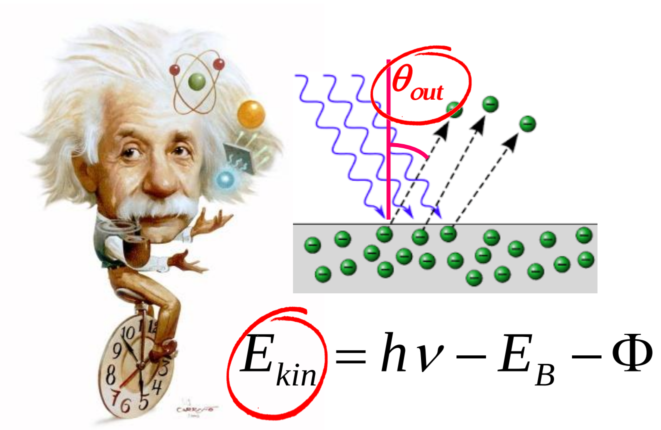
$$k_{in} = \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$





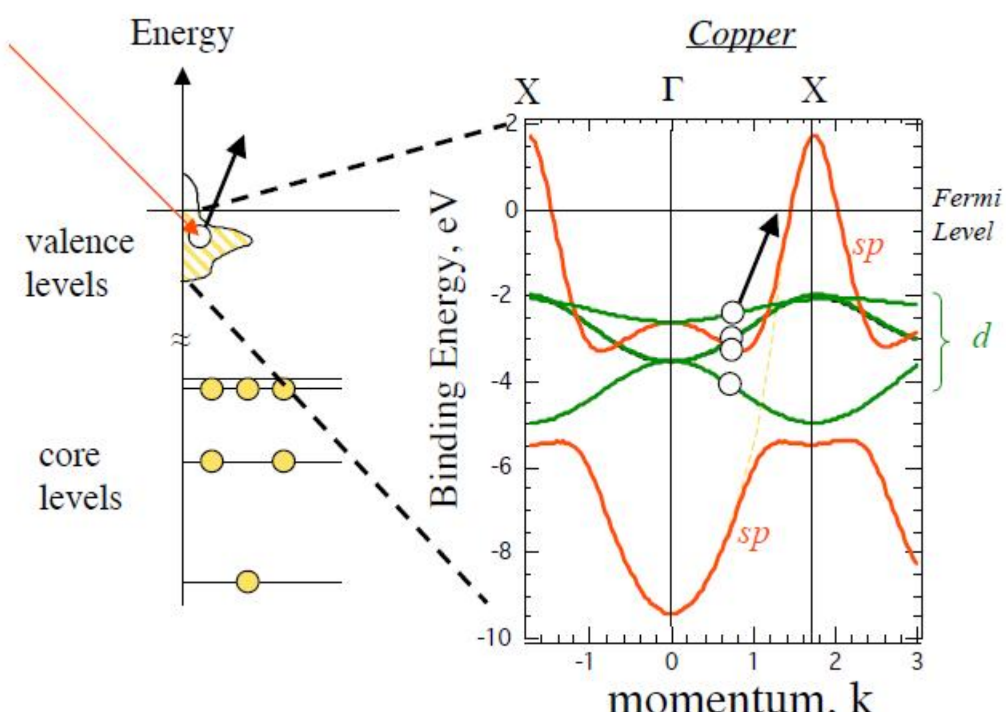
$$k_{in\parallel} = k_{out\parallel} \equiv k_{\parallel} = \sin\vartheta_{out} \sqrt{\frac{2m}{\hbar^2} E_{kin}} = \sin\vartheta_{in} \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$

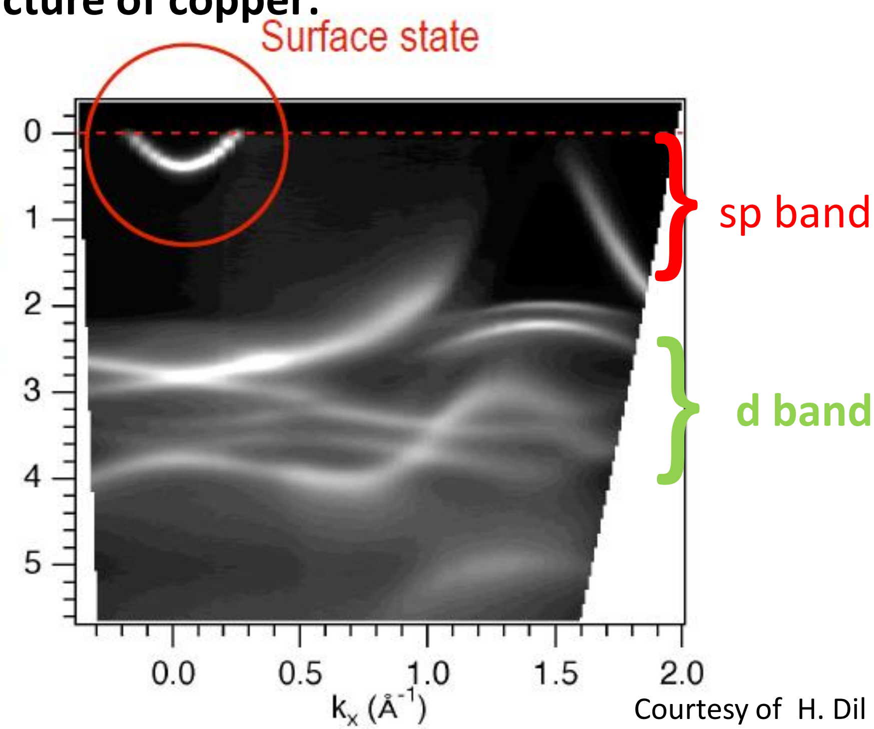
What do we learn from photoemitted *valence* electrons?



Measure:
- **Kinetic energy** of the photoemitted electrons
- **Angle** at which they are emitted

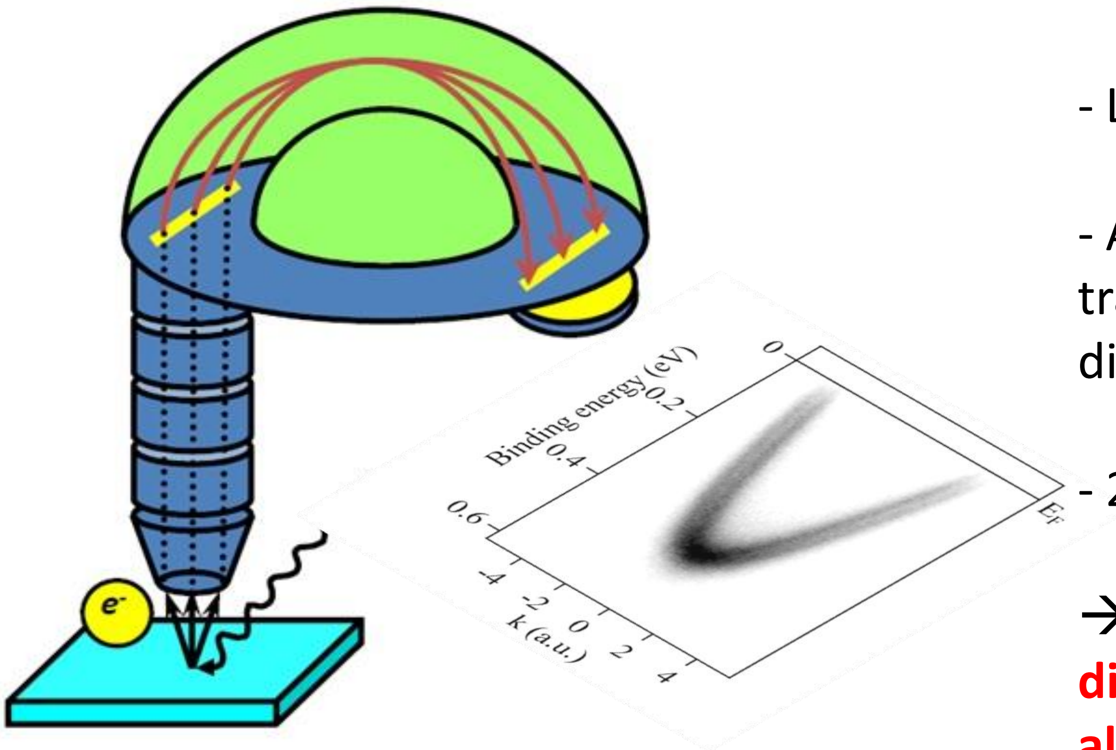
Textbook example – the electronic band structure of copper:





Courtesy of H. Dil

How do we handle the angle of the photoemitted electrons?



- Large angular acceptance (~30°)

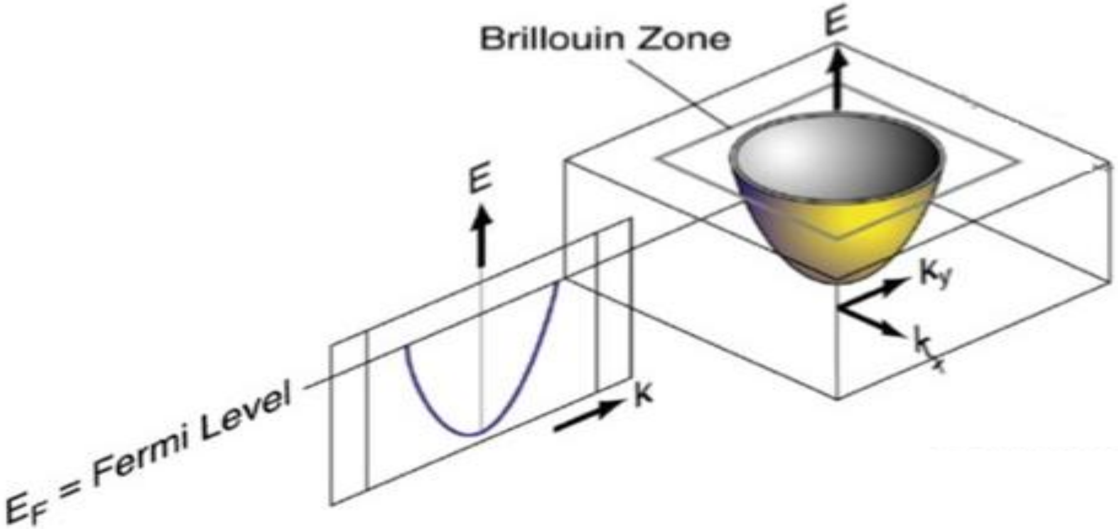
- Analyzer electronic lenses keep track of the electrons emitted at different angles

- 2d detection (MCP)

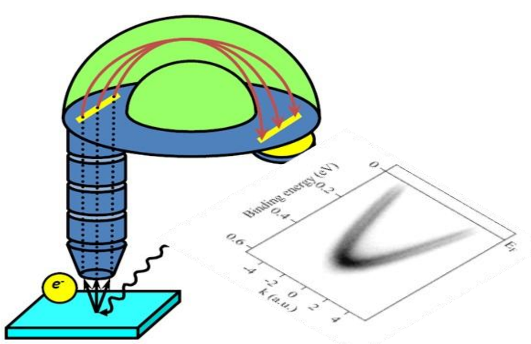
→ **Dispersion along the analyzer slit directly measured (i.e. dispersion along one line in k space)**

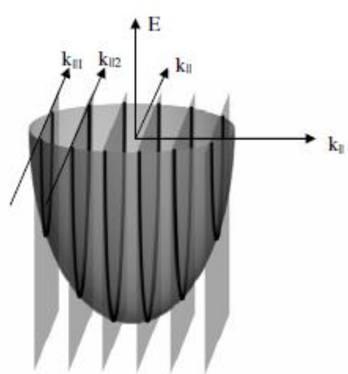
Band mapping: 2d surface state on Au(111) surface

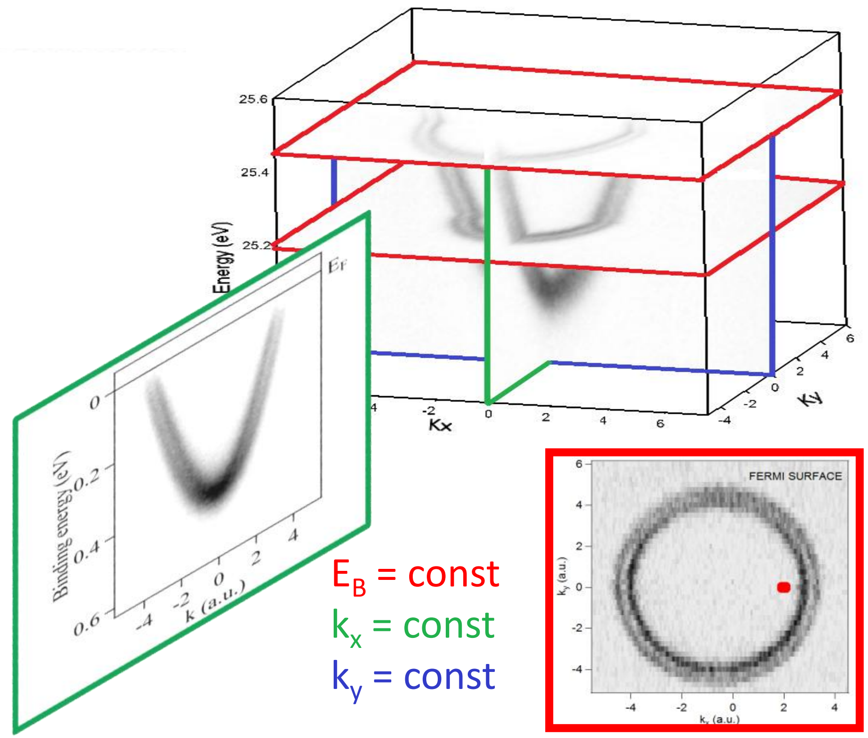
- 2d electron gas – parabolic disperion, circular Fermi contour - expected



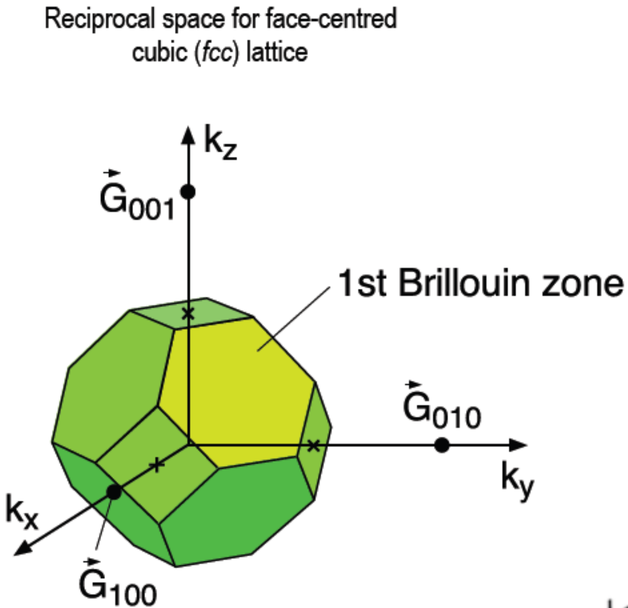
- and measured by ARPES







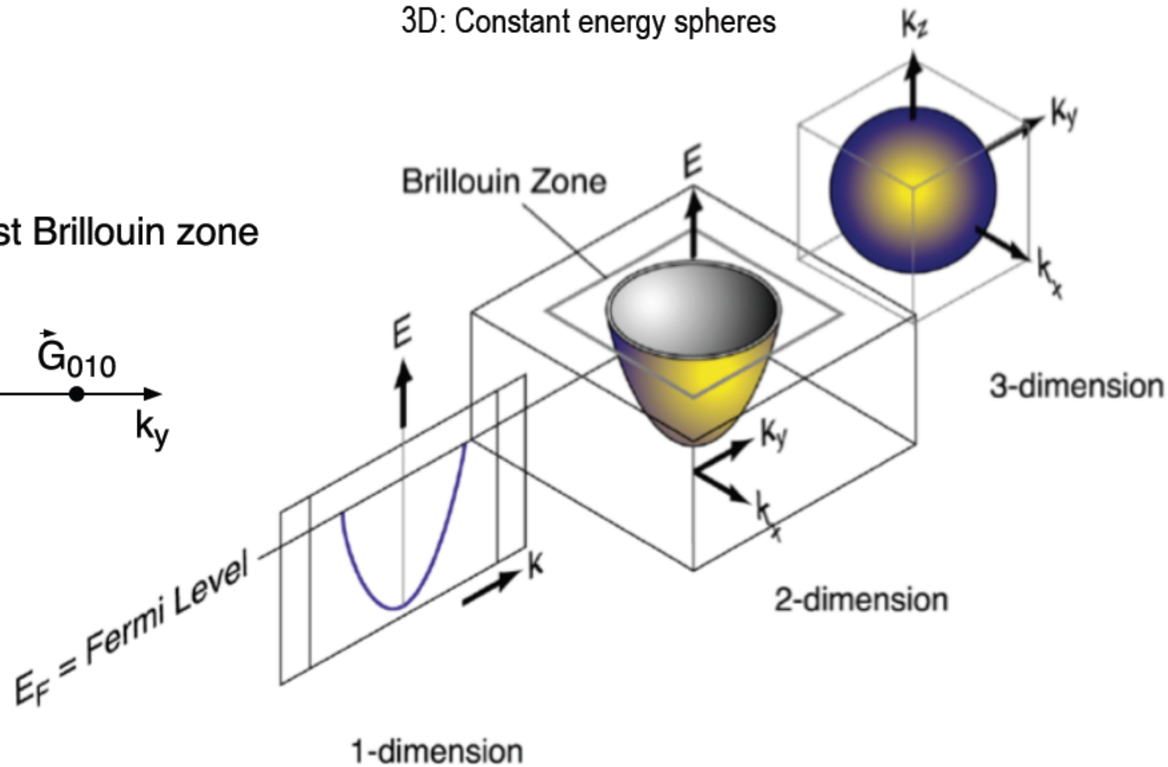
Back to textbooks: 1D → 2D → 3D



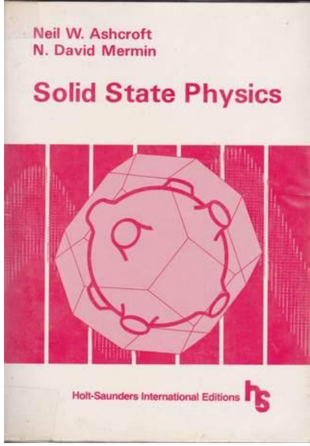
1D: Constant energy points

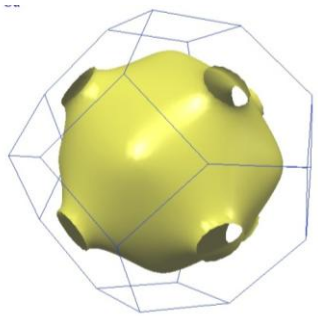
2D: Constant energy circles

3D: Constant energy spheres

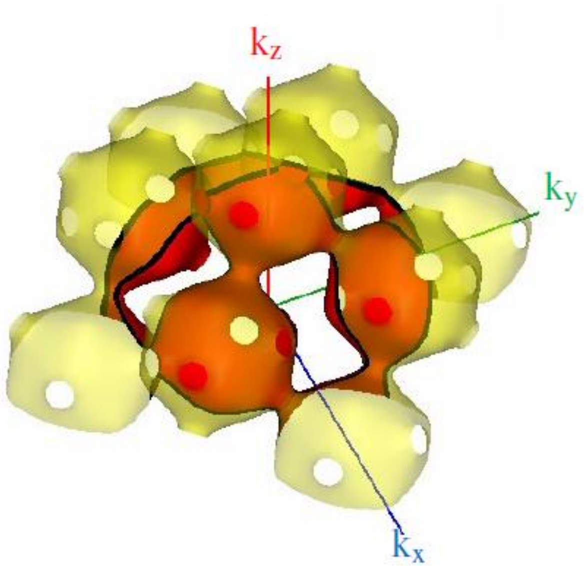


Fermi surface mapping – Fermi surface of copper





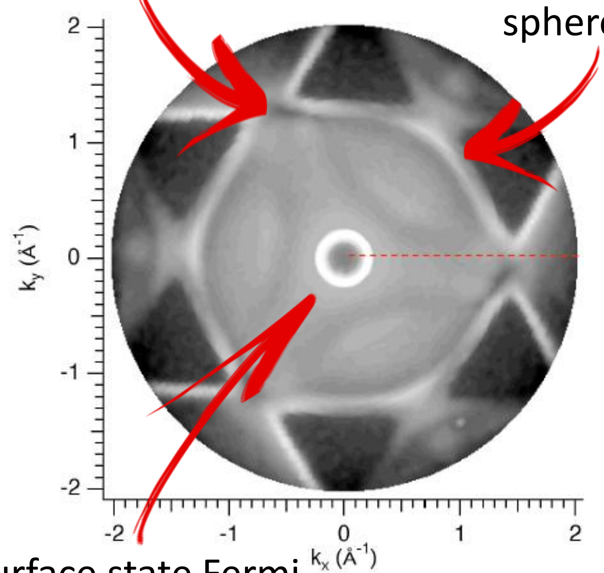
- 3d Fermi surface of Cu:
Almost (but not really) free electrons: the **sphere is not perfect** – the **necks** connect the spheres in the subsequent Brillouin zones



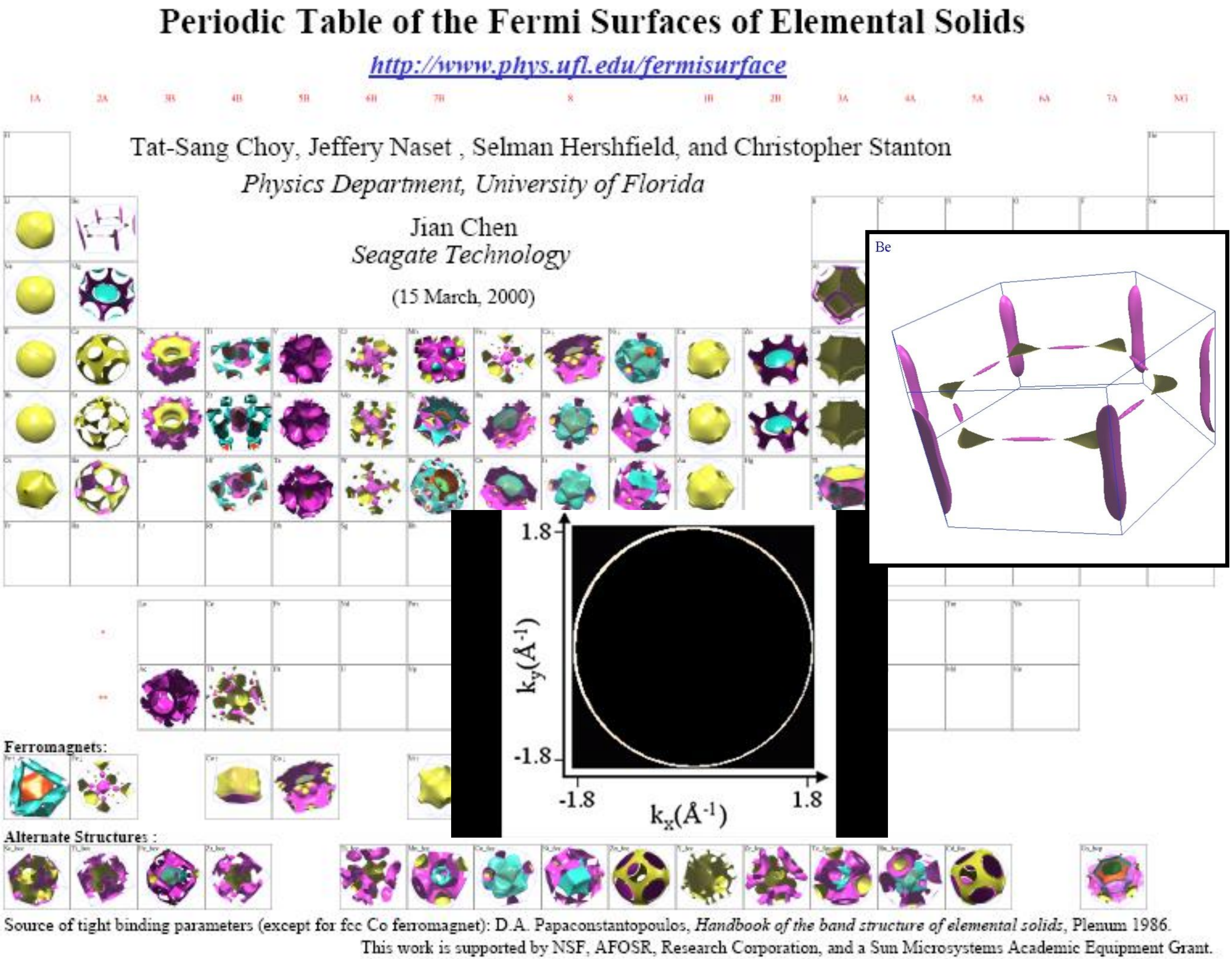
- With single photon energy ARPES measures a spherical cut through the 3d Fermi surface

Neck

Distorted sphere



Surface state Fermi contour (perfect circle)



Periodic Table of the Fermi Surfaces of Elemental Solids
http://www.phys.ufl.edu/fermisurface
Tat-Sang Choy, Jeffery Naset , Selman Hershfield, and Christopher Stanton
Physics Department, University of Florida
Jian Chen
Seagate Technology
(15 March, 2000)
Ferromagnets:
Alternate Structures :
Source of tight binding parameters (except for fcc Co ferromagnet): D.A. Papaconstantopoulos, Handbook of the band structure of elemental solids, Plenum 1986.
This work is supported by NSF, AFOSR, Research Corporation, and a Sun Microsystems Academic Equipment Grant.
Be
1.8
-1.8
$k_y(Å^{-1})$
-1.8
1.8
$k_x(Å^{-1})$

Principal boost to ARPES development

The Nobel Prize in Physics 1987
J. Georg Bednorz, K. Alex Müller

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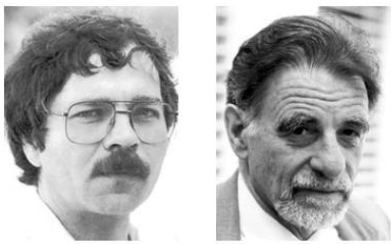
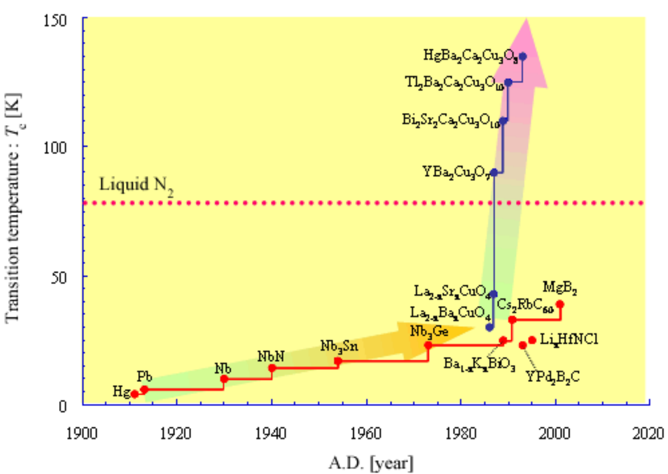
The Nobel Prize in Physics 1987

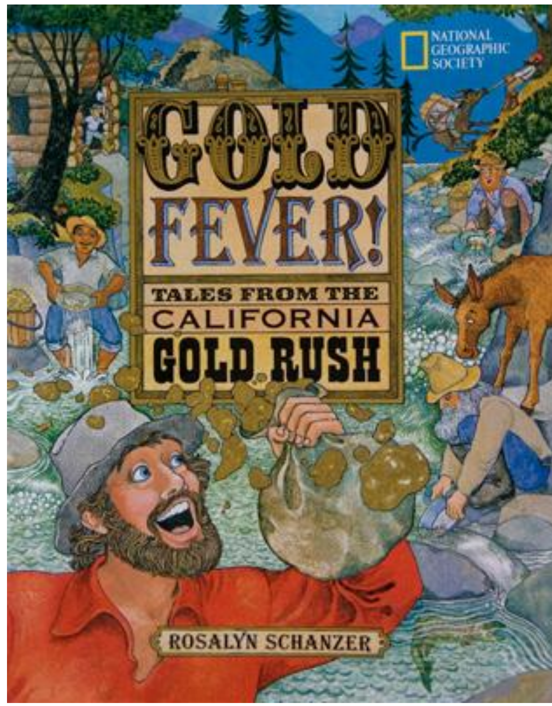


J. Georg Bednorz
Prize share: 1/2

K. Alexander Müller
Prize share: 1/2

The Nobel Prize in Physics 1987 was awarded jointly to J. Georg Bednorz and K. Alexander Müller *"for their important break-through in the discovery of superconductivity in ceramic materials"*





SUPERCONDUCTIVITY FEVER
PHYSICS GOLD RUSH 1990S

The Nobel Prize in Physics
XXXXXXXX

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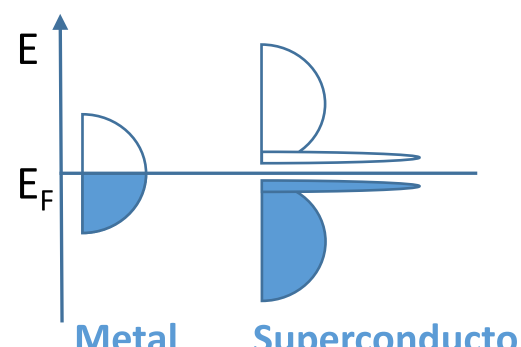
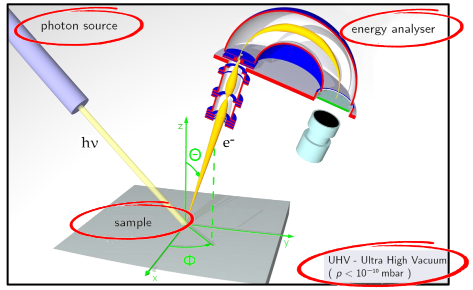
The Nobel Prize in Physics 20??

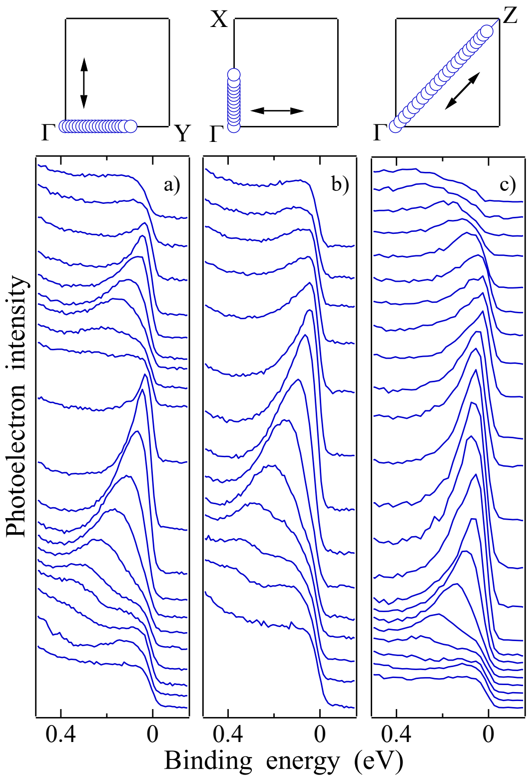
Searching for the mechanism of high Tc superconductivity → room temperature superconductivity!!!

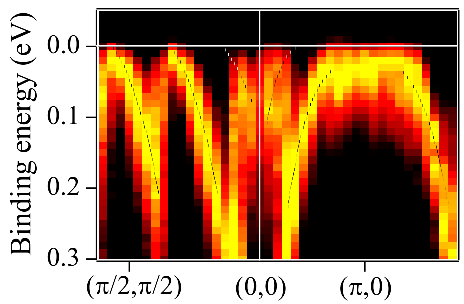


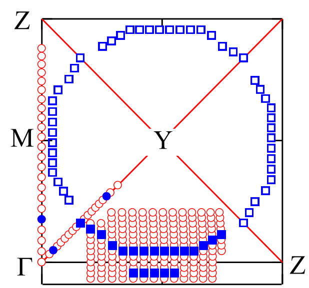
ARPES – stone age



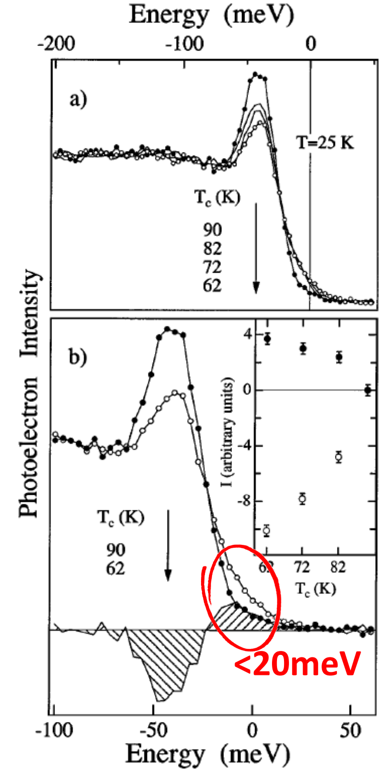
High Tc cuprates:
Band mapping and Fermi surface mapping… by hand

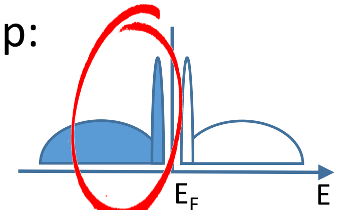


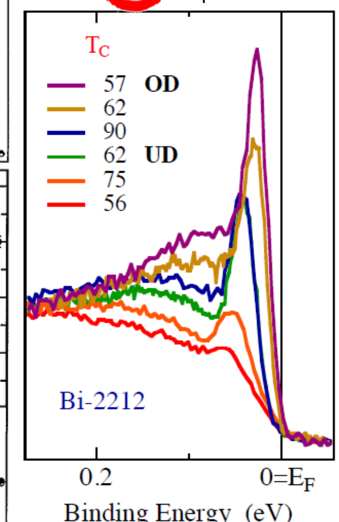




Superconducting gap:





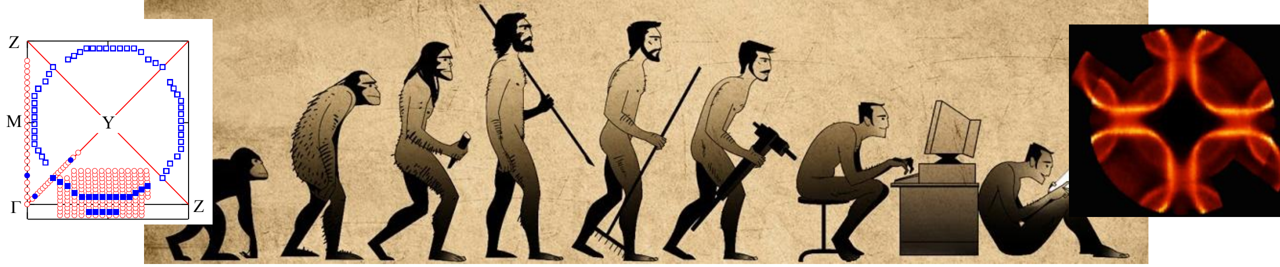


I. Vobornik *et al.*,
Phys. Rev. Lett. **82**, 3128 (1999)

Energy resolution < 10 meV; angular resolution ~1°

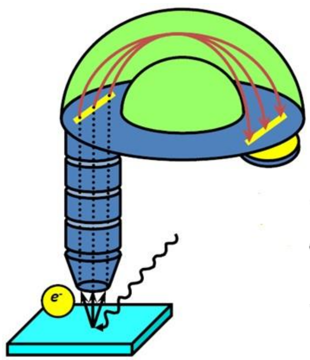
I. Vobornik, PhD thesis, EPFL, Lausanne, 1999

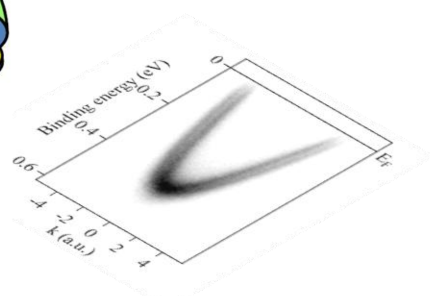
ARPES evolution

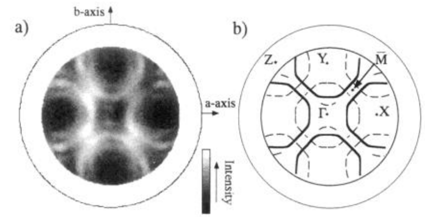


Milestone: Development of **two dimensional detectors**

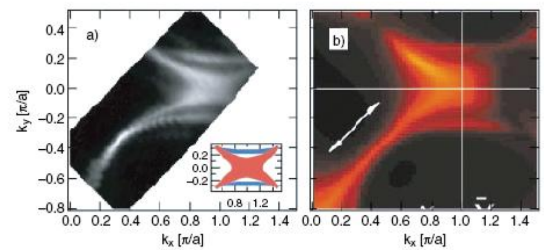
1994





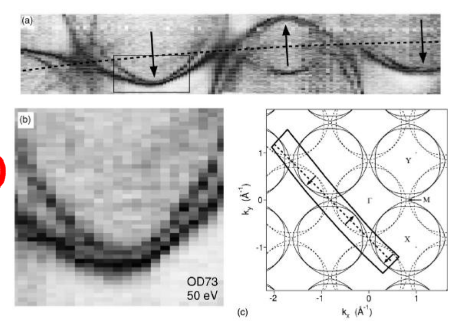


P. Aebi *et al.*, Phys. Rev. Lett. **72**, 2757 (1994)



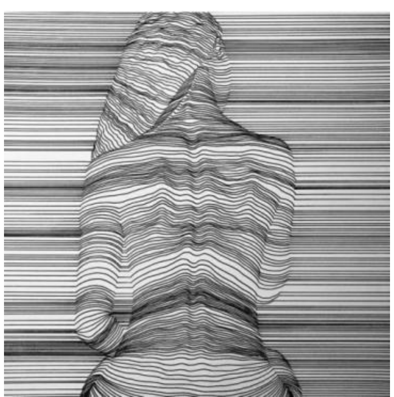
P.V. Bogdanov et al., Phys. Rev. B 64 180505 (R) (2001), A. Bansil, M. Lindroos *Phys. Rev. Lett.* **83** 5154 (1999)

→**Images** rather than spectra, **BUT** still composed of spectra!!!



A.A. Kordyuk et al., Phys. Rev. B **70**, 214525 (2004)

2004

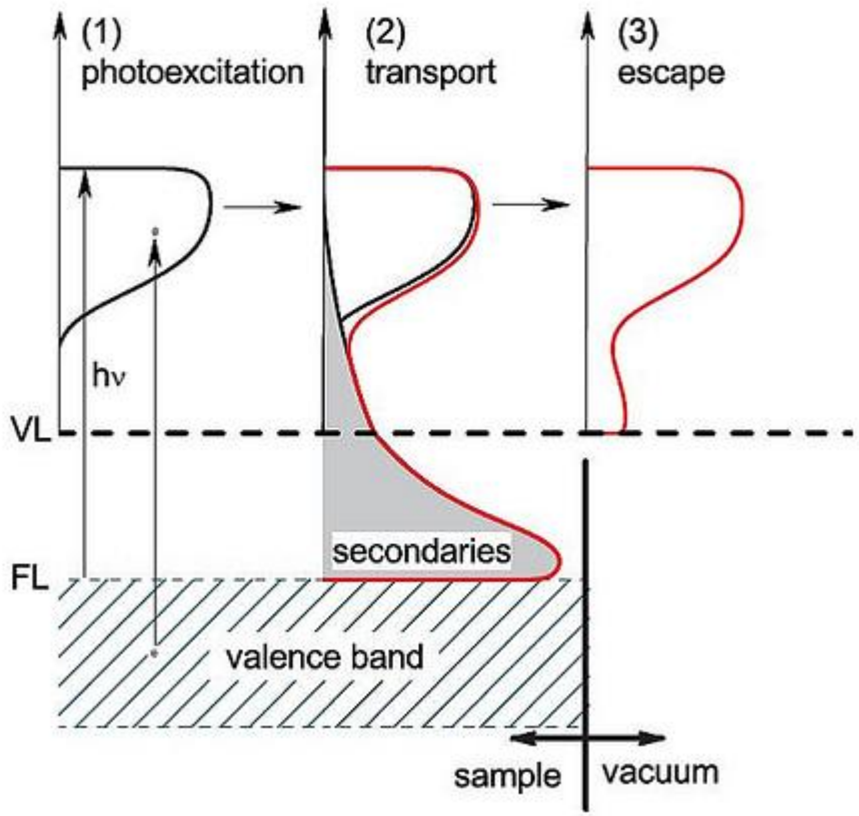


20XX ?

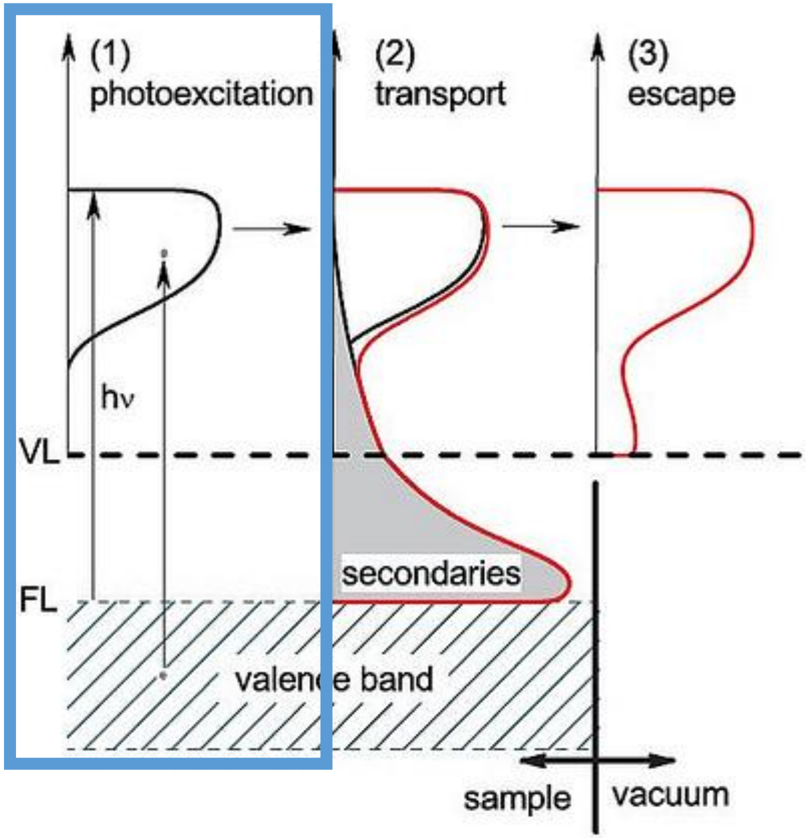
Energy resolution ~1 meV; angular resolution ~0.1°

What do we learn from the ARPES SPECTRA?

Intuitive (NOT exact) **three-step model** of the photoemission process:



Three-step model: step 1



Transition probability from initial to final state under the excitation by the photon with vector potential ***A***

$$w_{fi} = \frac{2\pi}{\hbar} \left| \langle f | H_{\text{int}} | i \rangle \right|^2 \delta(E_f - E_i - h\nu) \qquad H_{\text{int}} = \frac{e}{mc} \vec{A} \bullet \vec{p}$$

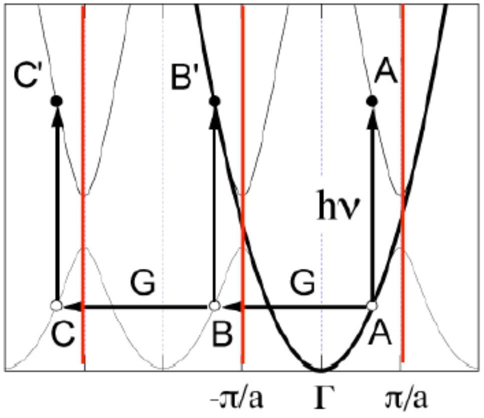
Optical transition in the solid:

- Energy is conserved

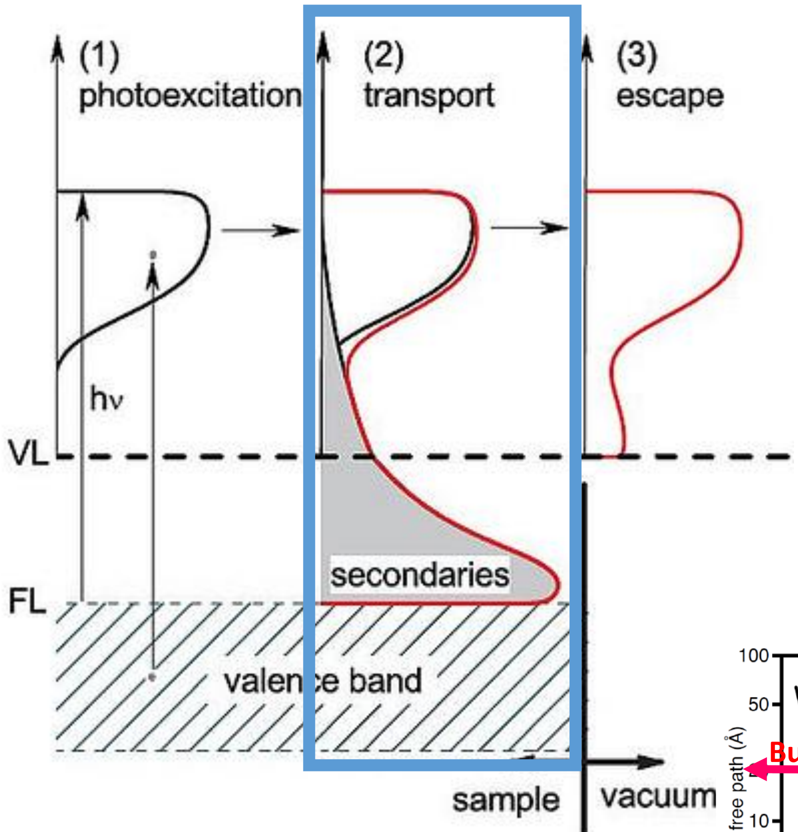
$$E_f = E_i + h\nu$$

- Wave vector is conserved modulo ***G***

$$\vec{k}_f = \vec{k}_i + \vec{G}$$



Three-step model: step 2



Inelastic scattering of the photoelectron with

- other electrons

(excitation of e-h-pairs, plasmons)

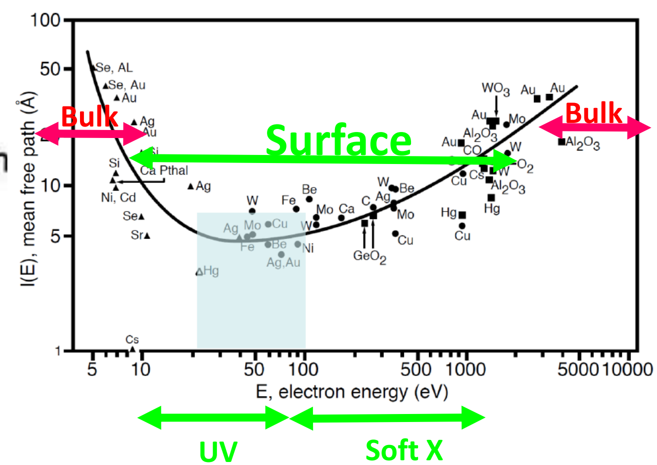
- phonons

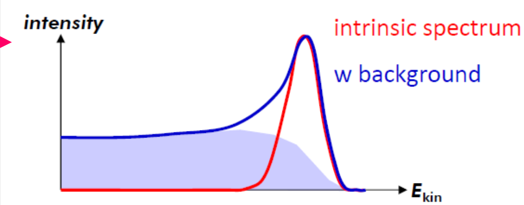
- Generation of secondary electrons

"inelastic background"

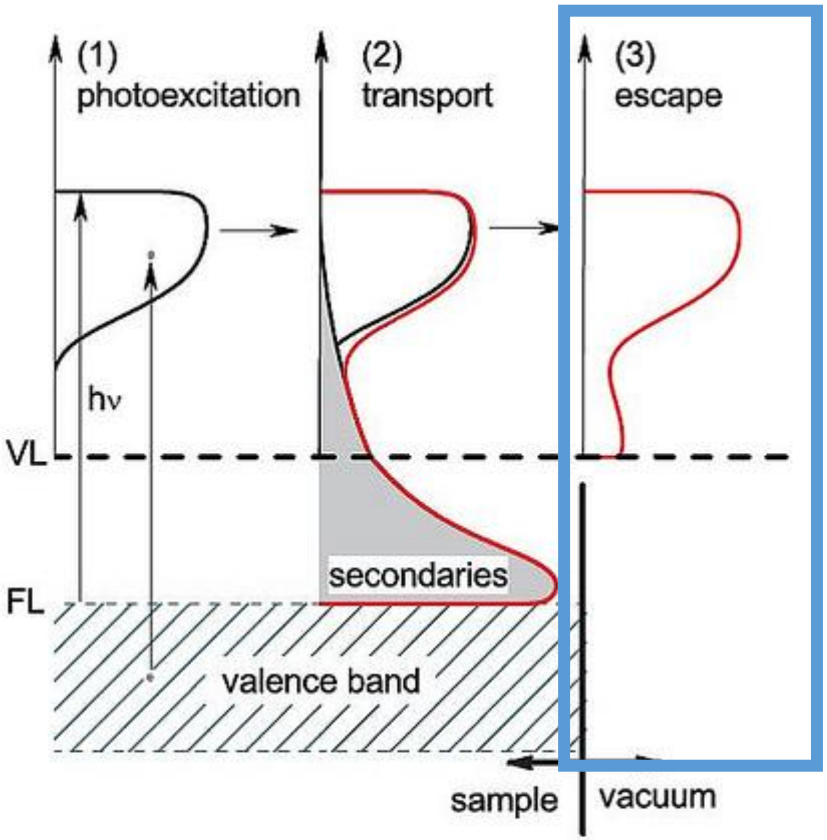
- Loss of energy and momentum information in the photoelectron current:

inelastic mean free path





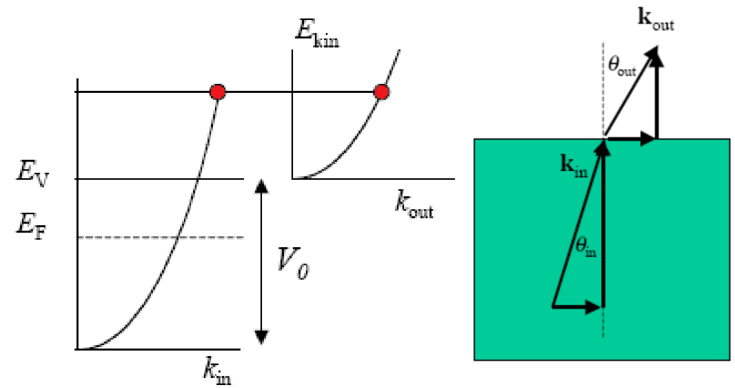
Three-step model: step 3



The lowest energy electrons can't exceed the work function potential

$$E_{kin} = h\nu - E_B - \Phi$$

Surface breaks crystal symmetry
$k_{\perp}$ is not a good quantum number

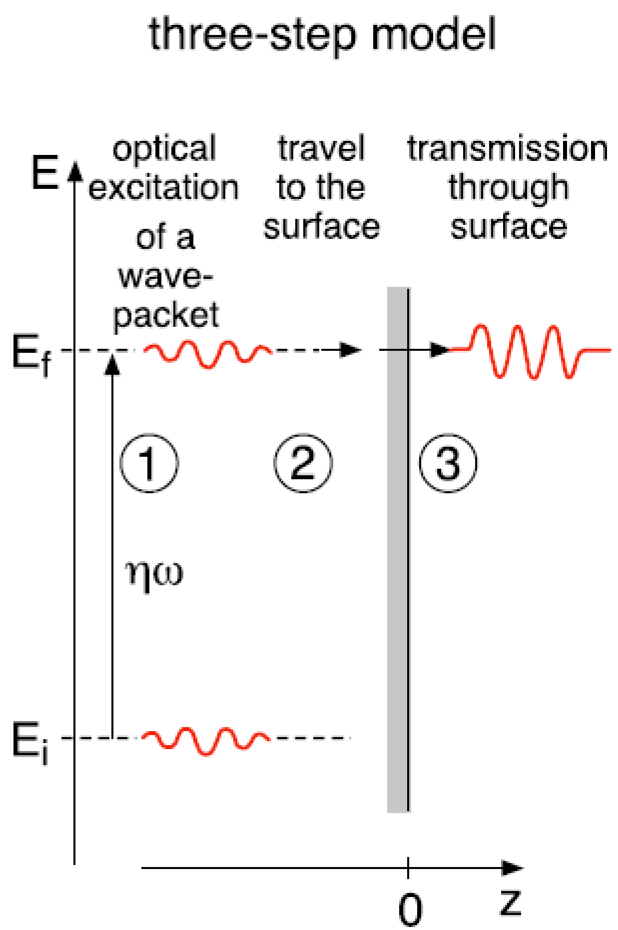


$$k_{out} = \sqrt{\frac{2m}{\hbar^2} E_{kin}}$$

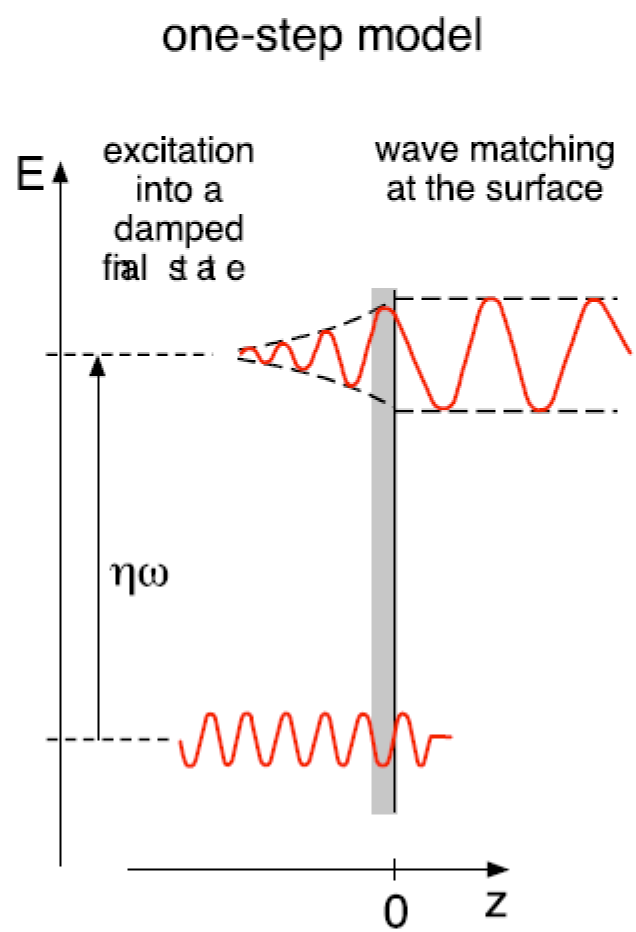
$$k_{in} = \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$

$$k_{out\parallel} = k_{in\parallel} \equiv k_{\parallel} = \sin \vartheta_{out} \sqrt{\frac{2m}{\hbar^2} E_{kin}} = \sin \vartheta_{in} \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$

Exact one-step vs. intuitive three-step model



3 step model is strong simplification; **quantitative description** only possible by matching wave function of initial and final state



Photoemission intensity is directly related with...

One particle Green's function

➔ describes the propagation of an extra electron (t>t') (hole, t<t') added to the many body system

$$G(xt, x't') = -i\left\langle N,0 \middle| T[\Psi(xt)\Psi^{+}(x't')] \middle| N,0 \right\rangle$$

How?

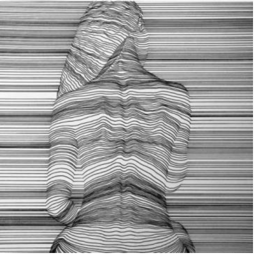
Starting from the **Fermi golden rule**

➔ the transition probability from the initial state $|N,0\rangle$ to a final state $|N,s\rangle$ with a photoelectron of energy ε_{κ} and momentum $\boldsymbol{\kappa}$ is given by

$$p(\varepsilon_{\kappa}) = \frac{2\pi}{\hbar}\sum_{s}\left|\left\langle N,s \middle| H_{\mathrm{int}} \middle| N,0 \right\rangle\right|^{2} \delta(E_{s}^{N} - E_{0}^{N} - \hbar\omega) = \ldots$$

***Dipole** approximation, **Sudden** approximation - the photoelectron is instanteneously created and decoupled form the remaining N-1 electron system*

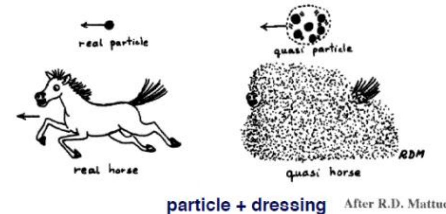
$$\ldots = \frac{2\pi}{\hbar}\left|M_{k\kappa}\right|^{2} A(\kappa,\omega) = \frac{2\pi}{\hbar}\left|M_{k\kappa}\right|^{2}\frac{1}{\pi}\left|\mathrm{Im}\, G^{<}(\kappa,\omega)\right|$$

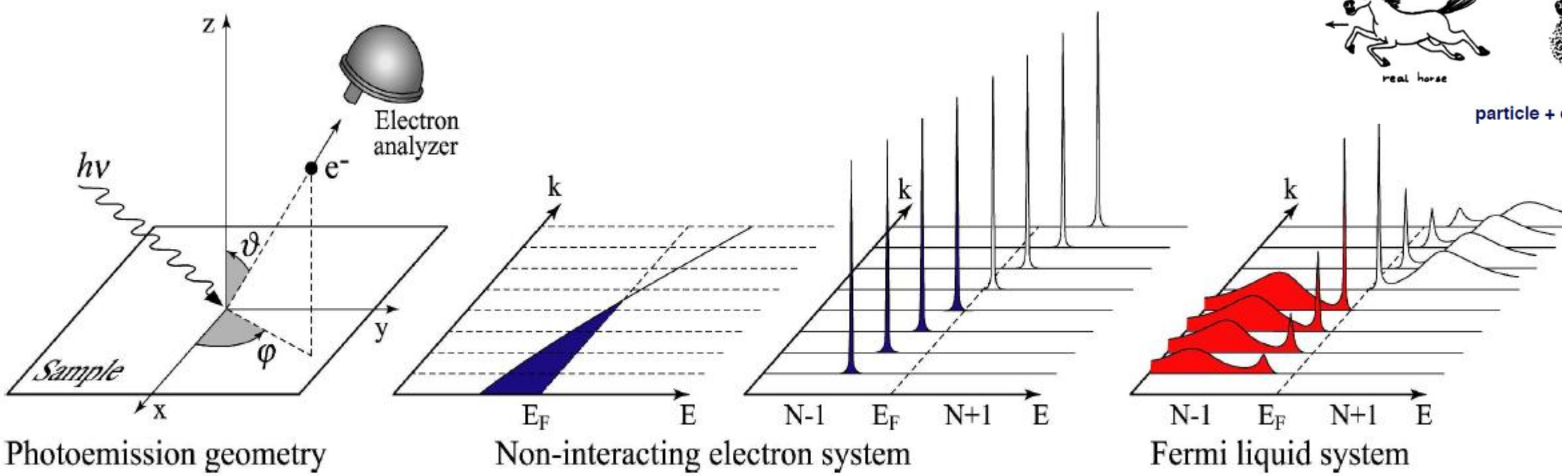


Beyond images– spectral line-shape & electronic correlations

$$I(\vec{k},\omega) \propto \left|\langle f \,|\, \vec{A}\cdot\vec{p} \,|\, i\rangle\right|^2 A(\vec{k},\omega)\, f(\omega)$$

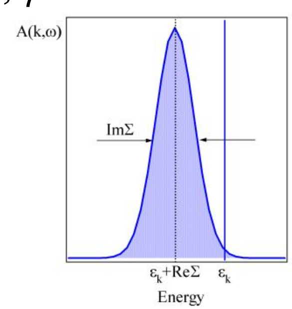
$$f(\omega) = \frac{1}{1+e^{\frac{\omega-\mu}{kT}}}$$





$$G(\vec{k},\omega) = \frac{1}{\omega-\varepsilon_k - i\eta}, \eta \to 0$$

$$A(\vec{k},\omega) = \delta(\omega-\varepsilon_k)$$

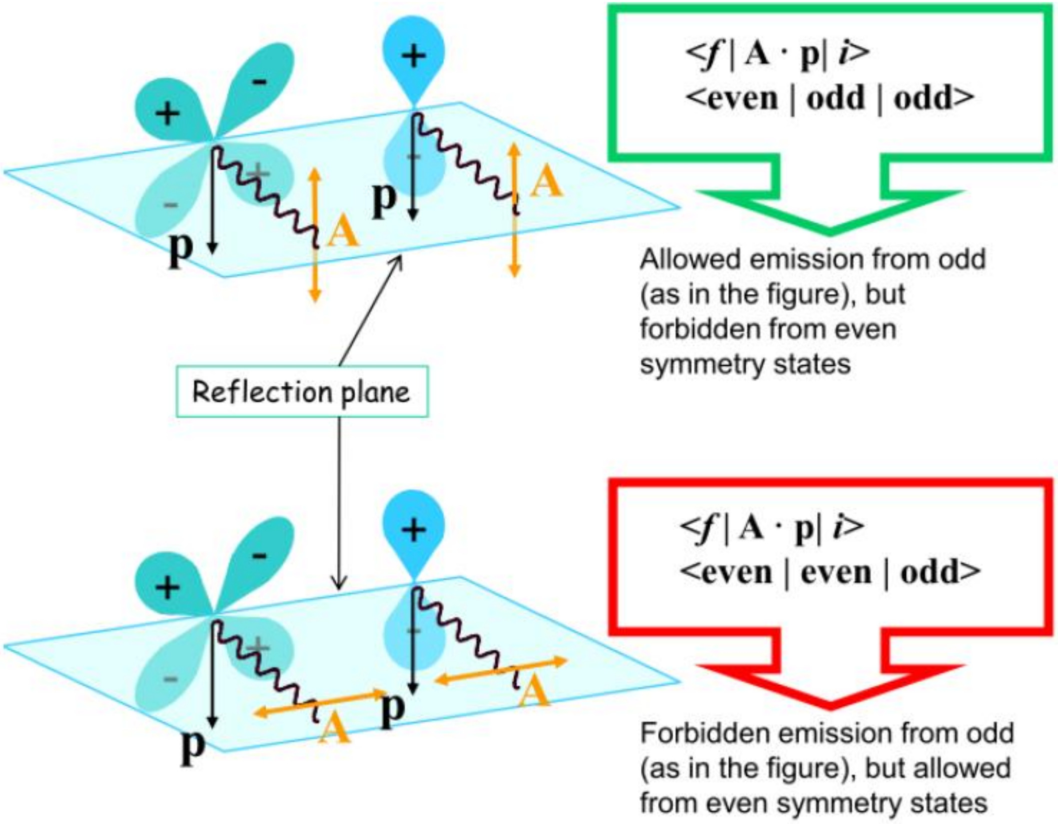


$$G(\vec{k},\omega) = \frac{1}{\omega-\varepsilon_k - \Sigma(\vec{k},\omega)}$$

$$A(\vec{k},\omega) = \frac{1}{\pi}\frac{\left|\mathrm{Im}\Sigma(\vec{k},\omega)\right|}{\left|\omega-\varepsilon_k-\mathrm{Re}\Sigma(\vec{k},\omega)\right|^2+\left|\mathrm{Im}\Sigma(\vec{k},\omega)\right|^2}$$

Matrix elements – orbital character of the bands

$$I(\vec{k},\omega) \propto \left|\langle f|\vec{A}\cdot\vec{p}|i\rangle\right|^2 A(\vec{k},\omega)\,f(\omega)$$



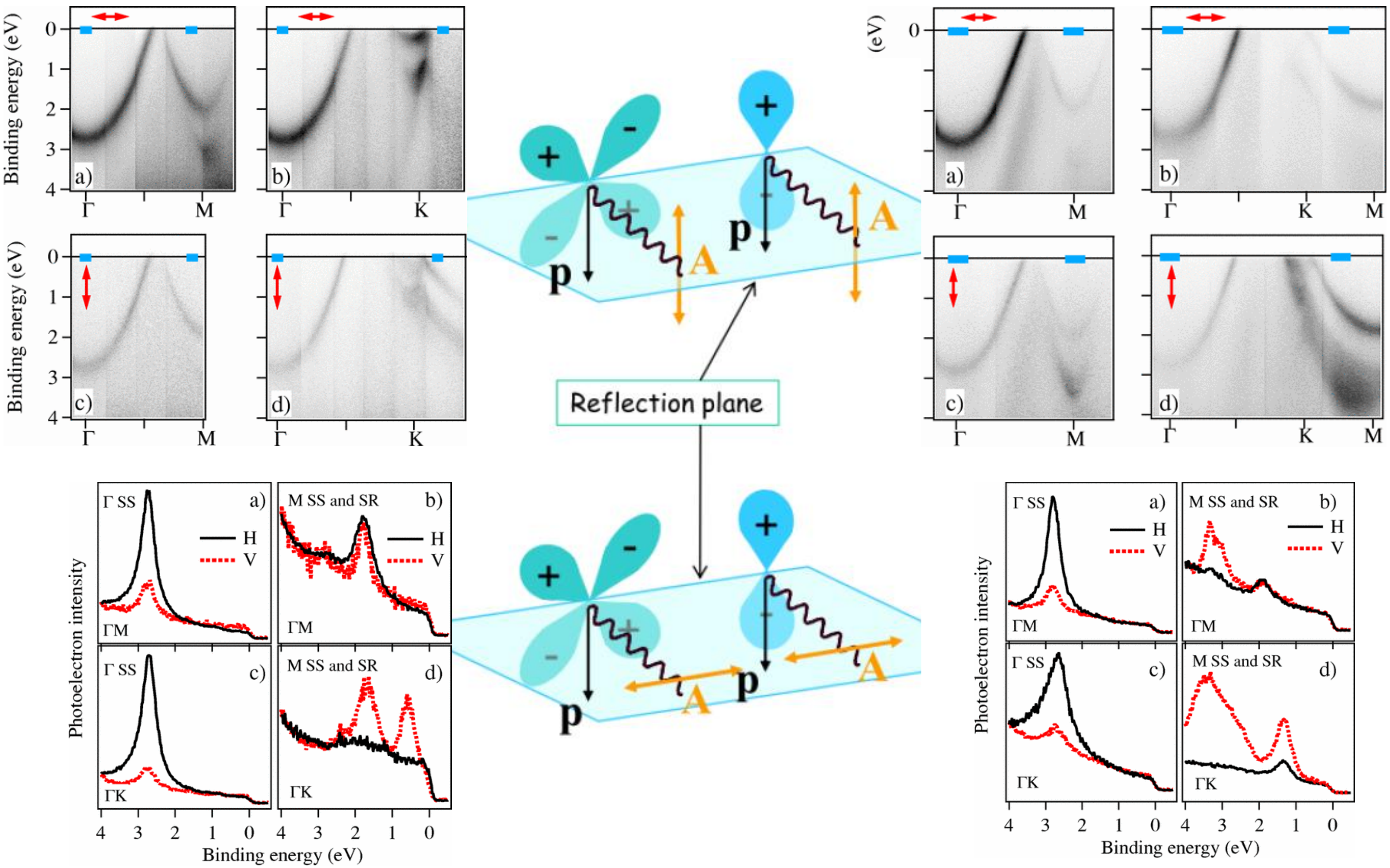
$$H_{int} = \boldsymbol{A}\cdot\boldsymbol{p}$$

The light beam and the analyser define the **scattering plane.**

If to be detected, the photoelectron final state **has to be even** under reflection in the scattering plane.

Access to the **symmetries** (i.e. Orbital character) of the initial state in the solid

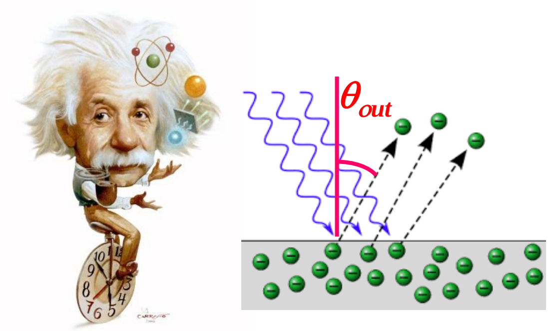
Prevalent s- or p- character of the Be(0001) surface states

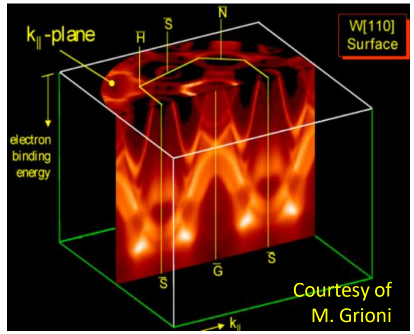


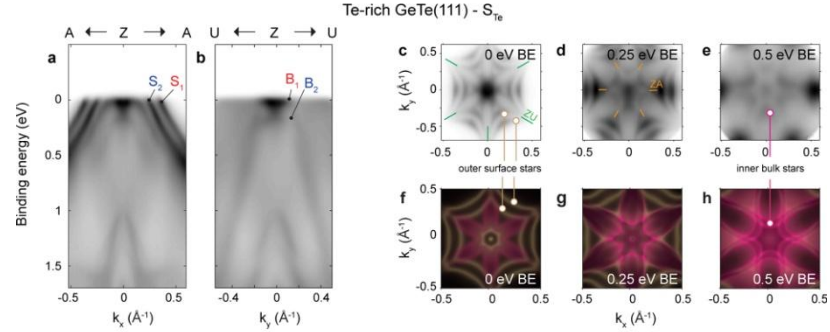
I. Vobornik et al., PRB 2005, PRL 2007

ARPES w/ synchrotron radiation: powerful tool in investigation of electronic properties of materials

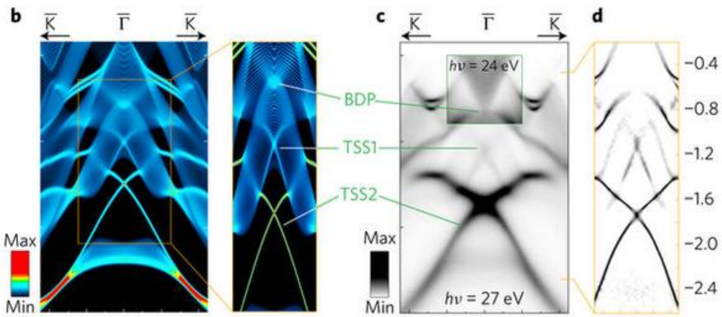
– electronic band structure, orbital character, correlations



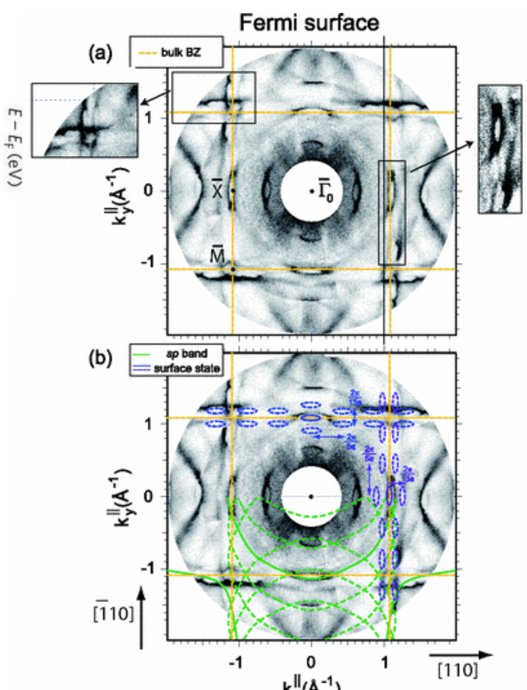




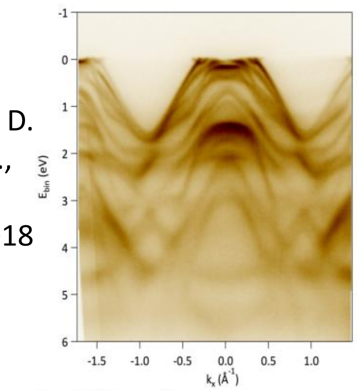
GeTe, C. Rinaldi et al., Nano Letters 2018

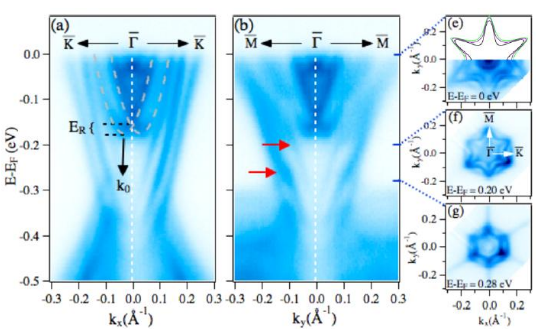


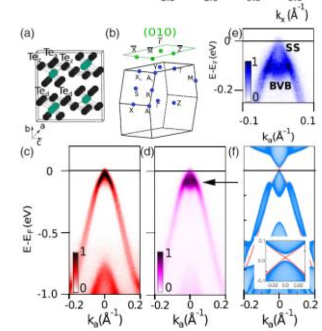
PdTe$_2$, M.S. Bahramy, Nature Materials 2018



WTe$_2$, P. Das, D. DiSante et al., Nat. Comm. 2016; PRL 2018







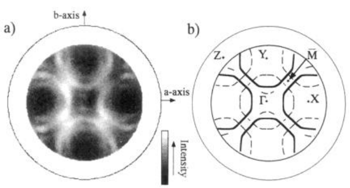
Dirac dispersion and Fermi surface in PbBi$_6$Te$_{10}$
M. Papagno et al., ACS Nano 2016

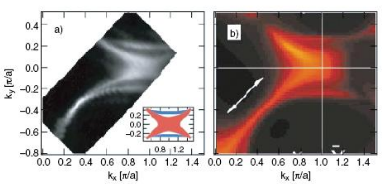
Au(001) surface states
S. Bengio et al. PRB 2012

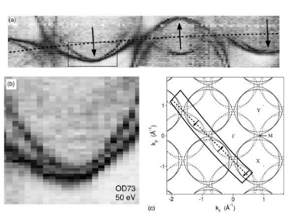
ZrTe$_5$ band structure
G. Manzoni et al., PRL 2016

ARPES and 21st century materials

1994







2004

PHYSICS
GOLD RUSH 2010S

Electronic materials

Spintronic materials

Functional materials

QUANTUM materials!

2004: graphene came into scene

✓ ***The thinnest possible material*** - only one atom thick

✓ ***Ballistic conduction*** - charge carriers travel for μm w/o scattering

✓ ***The material with the largest surface area per unit weight*** – 1 gram of graphene can cover several football stadiums

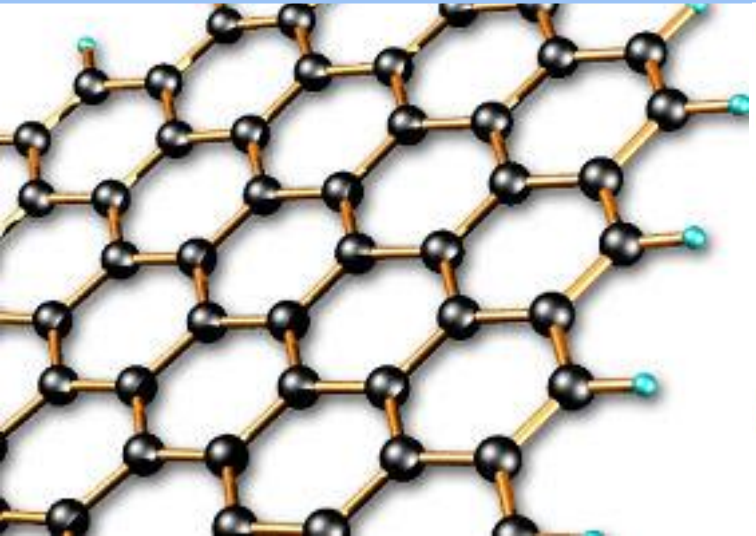
✓ ***The strongest material*** – 40 N/m, theoretical limit

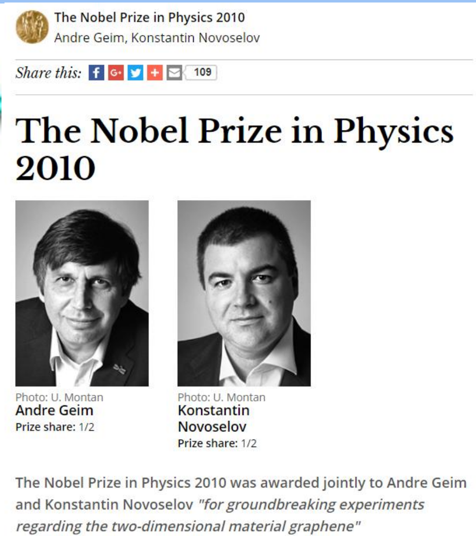
✓ ***The stiffest known material*** - stiffer than diamond

✓ ***The most stretchable crystal*** – can be stretched as much as 20%

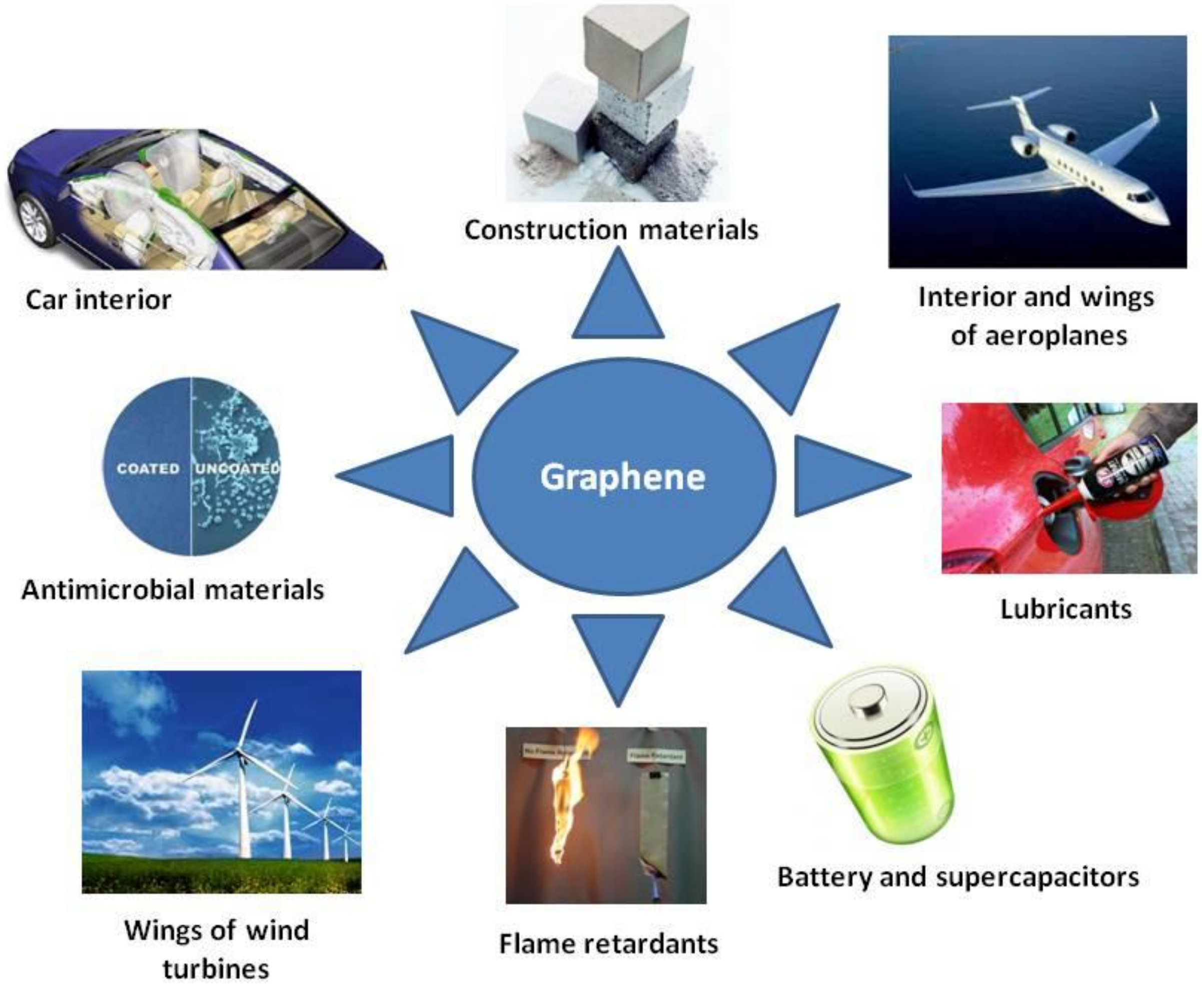
✓ ***The most thermal conductive material*** - ~5000 $Wm^{-1}K^{-1}$ at room temperature

✓ ***Impermeable to gases*** – even for helium



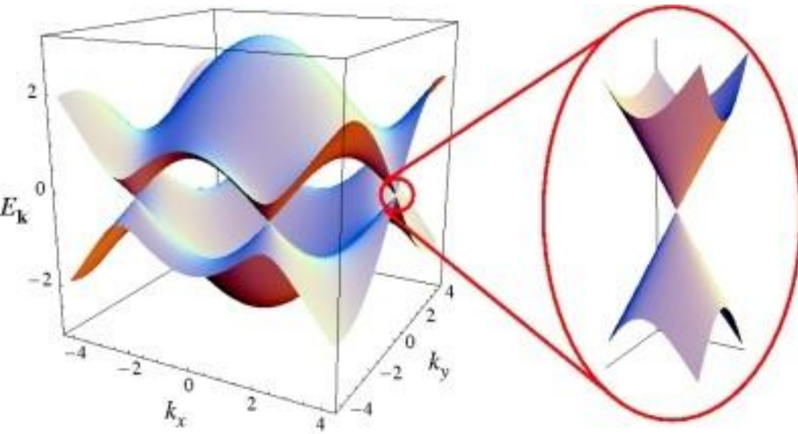


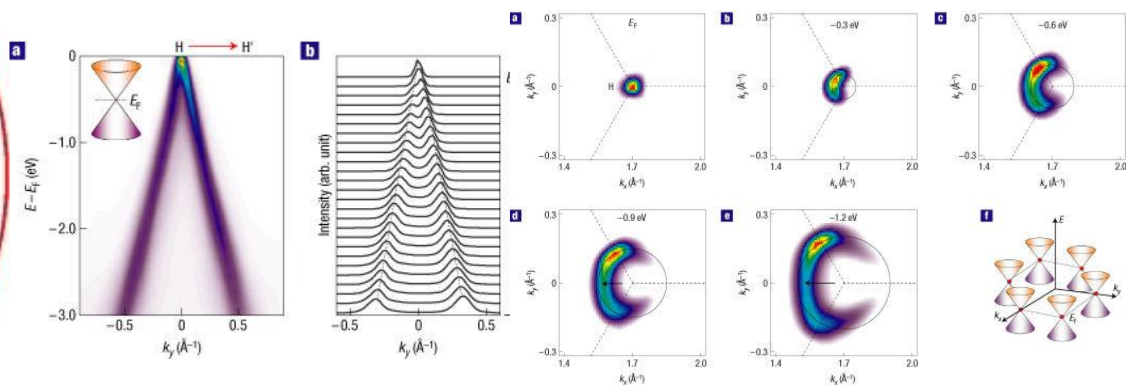
Application areas of Graphene



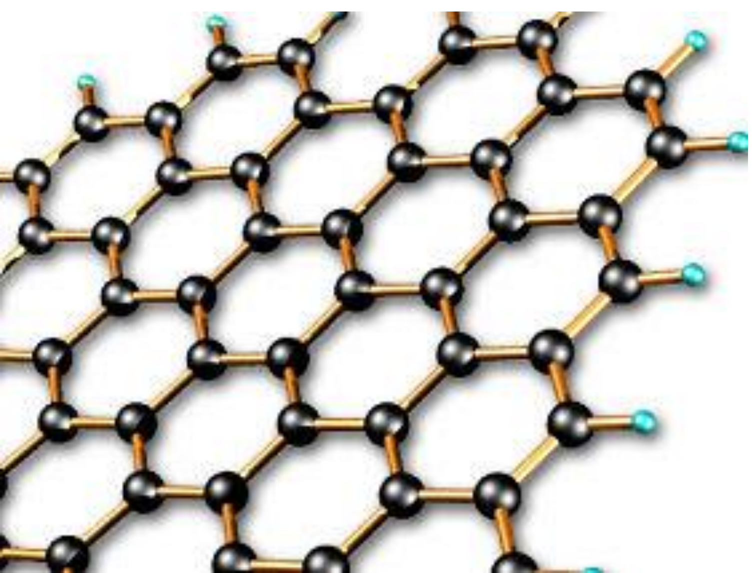
Dirac electrons enter the condensed matter physics…

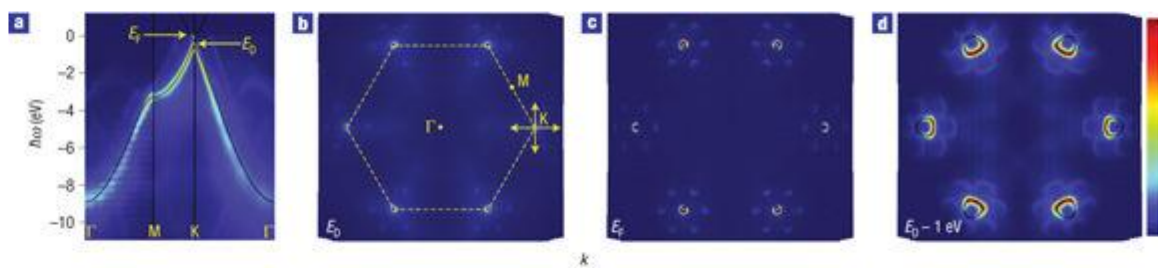
Conical (linear) Dirac dispersion and point-like Fermi surface measured by ARPES:





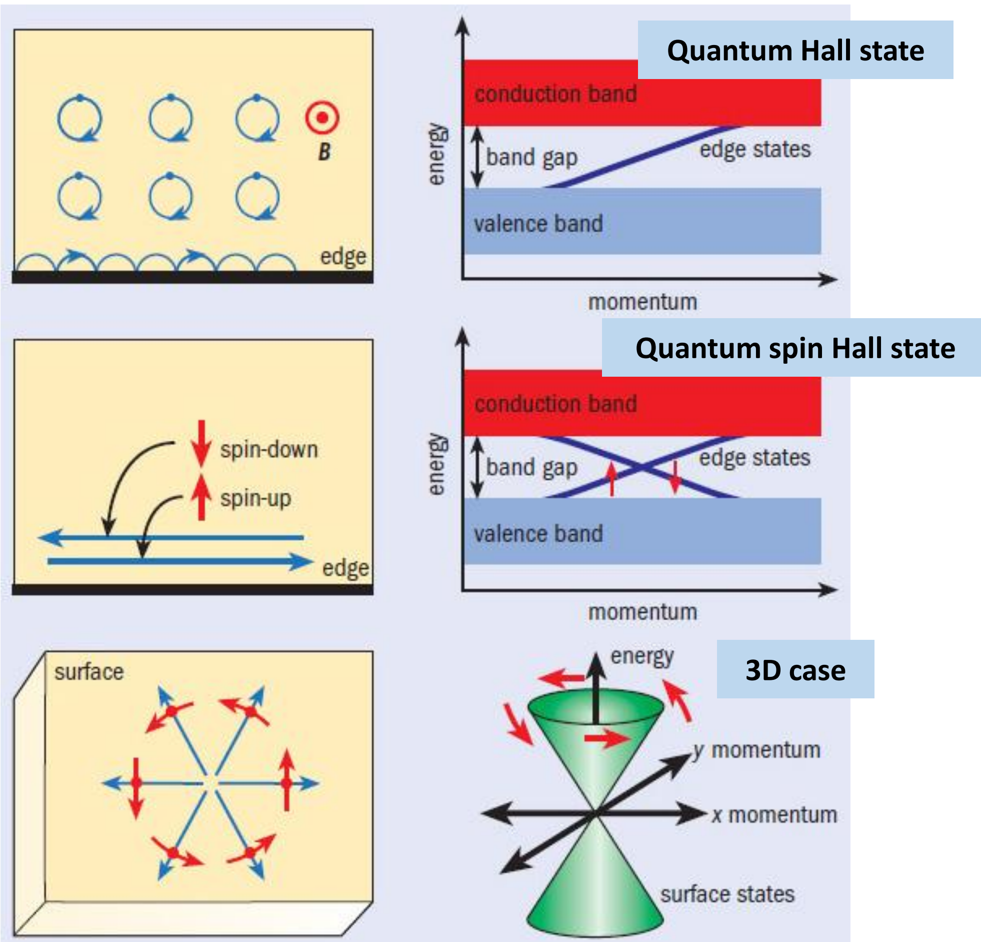
S. Y. Zhou et al., Nature Physics 2, 595 (2006)





A. Bpstwick et al., Nature Physics volume 3, pages 36 (2007)

… and not only in graphene: topological insulators

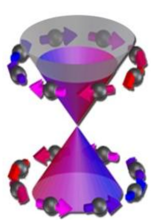


C. Kane & J. Moore, Physics World, Feb.2011, 32

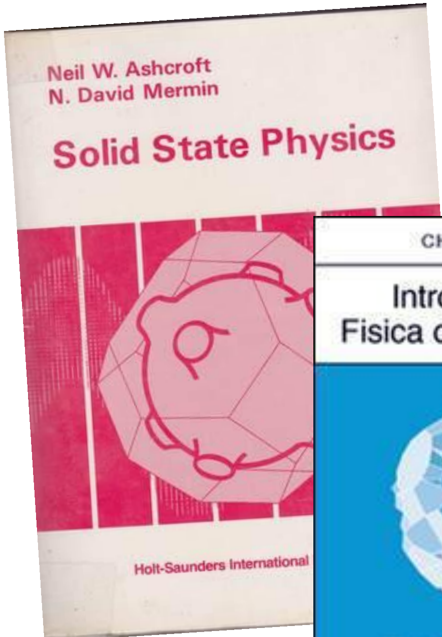
Conical (linear) Dirac dispersion
and
Spin-momentum locking

Characterized with well defined spin texture

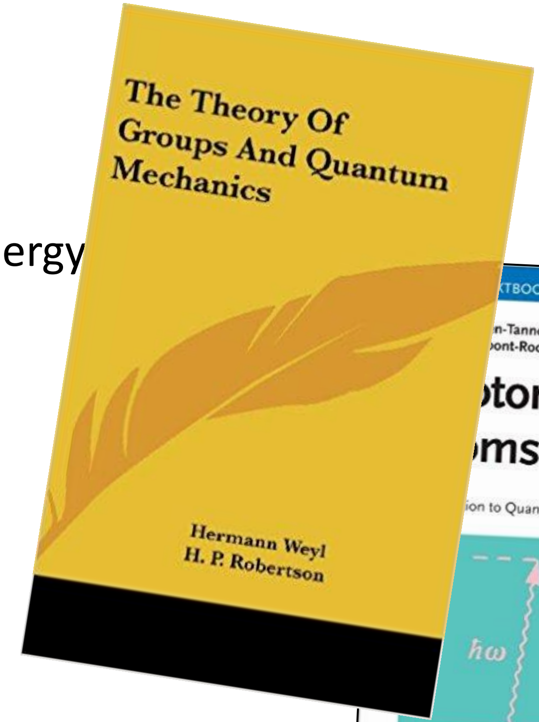
The technique of choice:
Spin-ARPES !

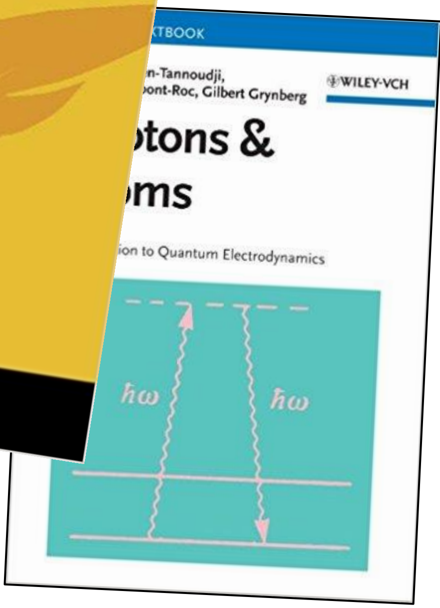


… more textbooks → beyond Ashcroft-Mermin/Kitell



The concepts of high energy physics within condensed matter!





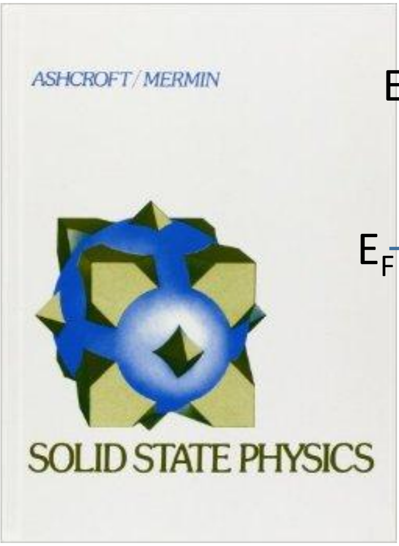
EXOTIC FERMION

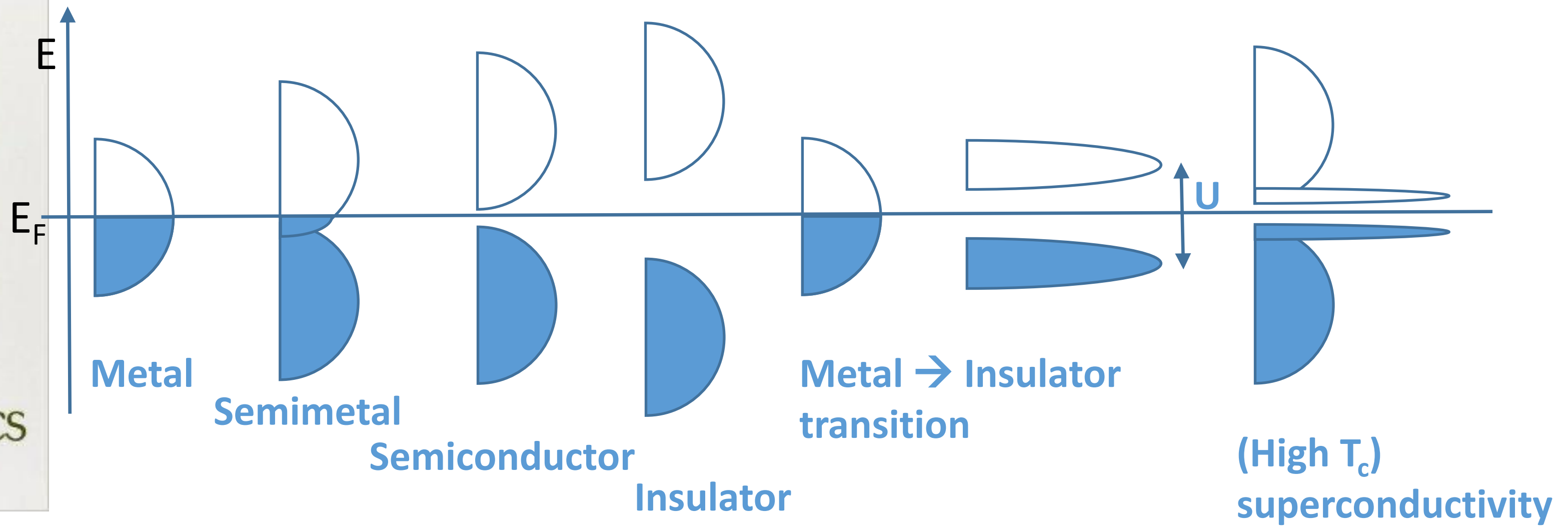
FEVER

PHYSICS

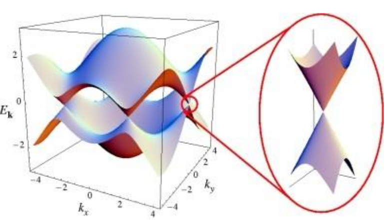
GOLD RUSH 2010S

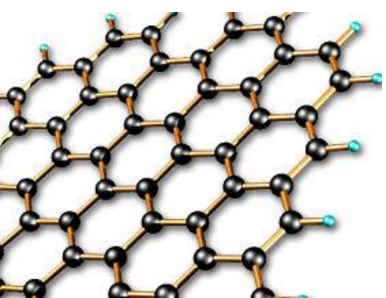
Quantum Materials in 20th century

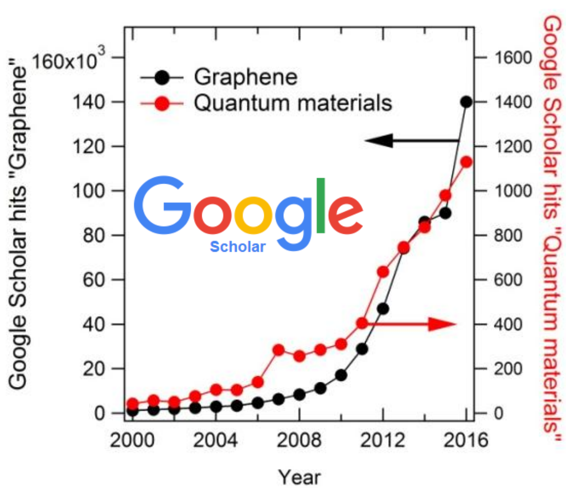


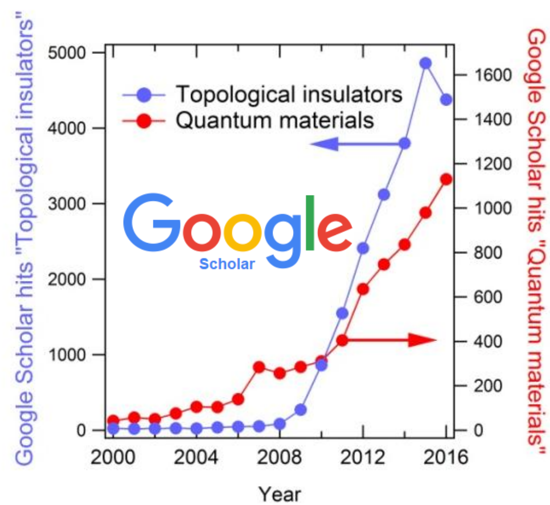


Quantum Materials in 21st century

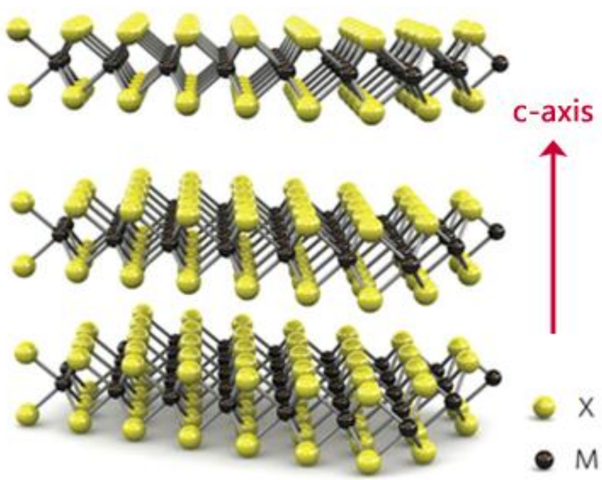






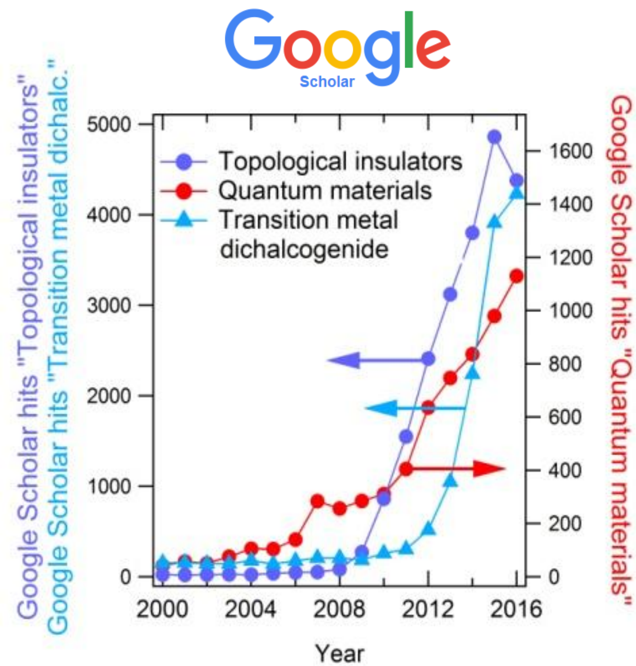


Transition metal dichalcogenides (TMDCs)



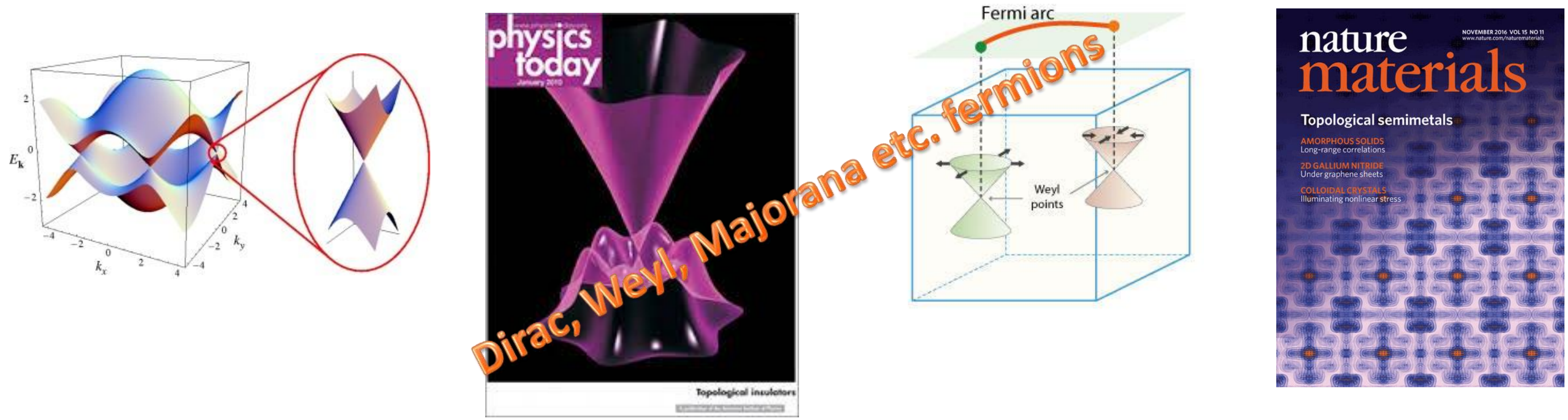
Three dimensional schematic presentation of typical MX_2 structure

M = transition metal
X = S, Se or Te



- **Layered structure** with strong intra-layer covalent bonding and weak (van der Waals type) inter-layer coupling
- Exhibit **wide variety of physical properties** – semimetals (WTe_2, $TiSe_2$), metals (NbS_2, VSe_2), semiconductors (MoS_2, $MoSe_2$), superconductors ($NbSe_2$, TaS_2)
- Properties often conditioned by the **number of layers**
- Host spin polarized electrons and /or Dirac/Weyl fermions

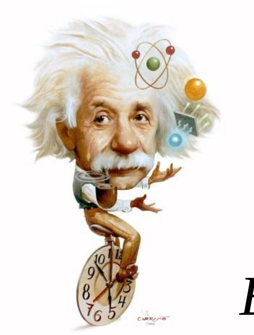
Quantum Materials in 21st century – High energy physics concepts within condensed matter

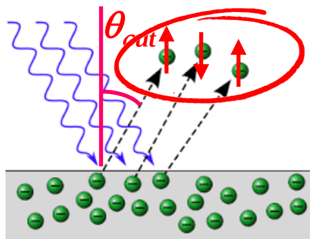


- Low-dimensional materials (2D, surfaces, few atomic layers)
- The Bloch wave functions follow Dirac-like or Weyl-like equations at vicinity of some special points of the Brillouin zone
- Envisioned applications: spintronics, quantum computing, etc.

- The materials characterized by particular **spin texture** → **ARPES Milestone : High-resolution Spin-ARPES**

What else do we learn from photoemitted electrons?





$$E_{kin} = h\nu - E_B - \Phi$$

$$k_{out} = \sqrt{\frac{2m}{\hbar^2} E_{kin}}$$

$$k_{in} = \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$

$$k_{in\parallel} = k_{out\parallel} \equiv k_{\parallel} = \sin \vartheta_{out} \sqrt{\frac{2m}{\hbar^2} E_{kin}} = \sin \vartheta_{in} \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$

Spin:

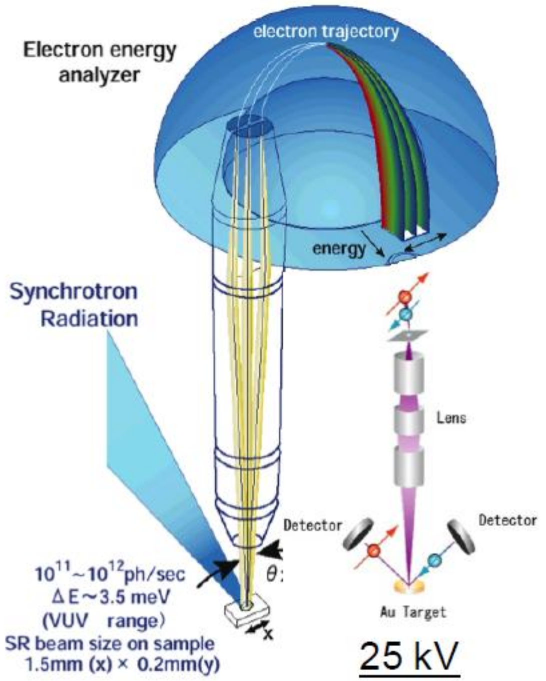
magnetism, spin texture in the systems with strong **spin-orbit** interaction

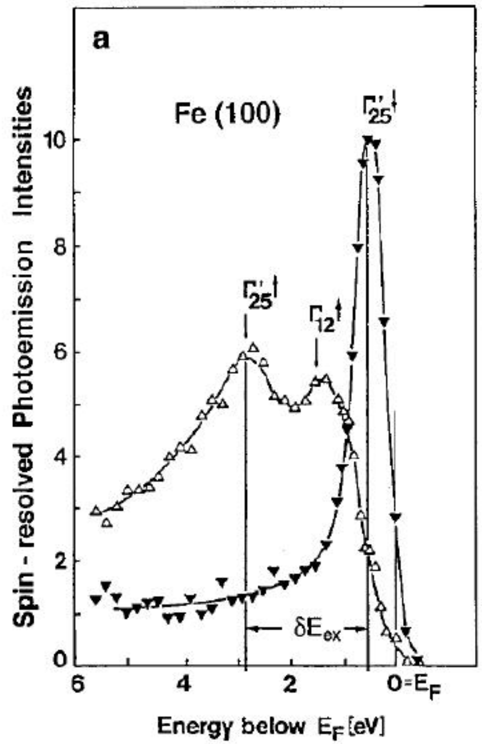
Spin - ARPES: ***E(k), Spin***

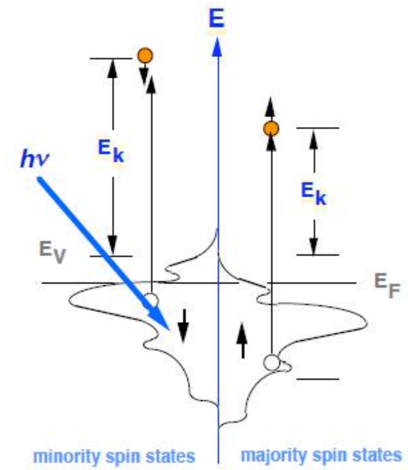
Complete set of quantum numbers of photoemitted electron

Complete photoemission experiment!

Exchange-split spin-polarized bands in ferromagnetic iron



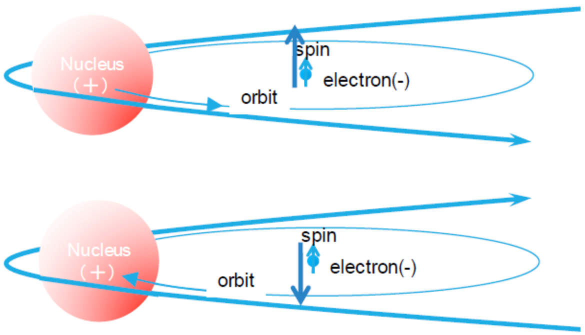




E. Kisker et al. Phys. Rev. B 31, 329 (1985)

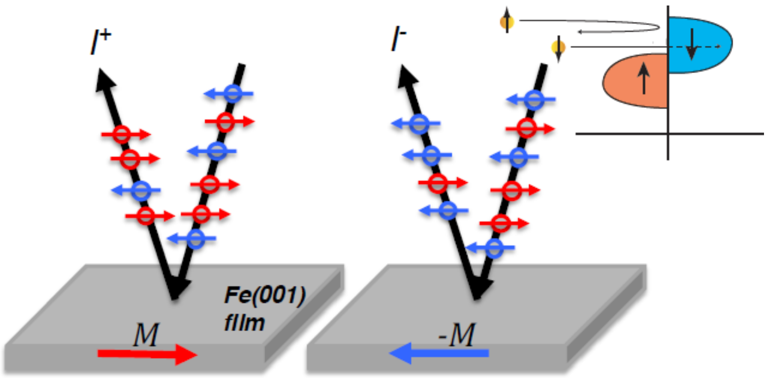
Detecting electron's spin: spin-dependent scattering

MOTT scattering



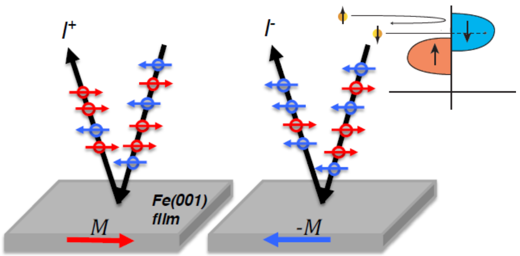
- **spin-orbit interaction**
- left-right asymmetry
- **>25keV**
- **commercial**
- Au target
- **FOM 10^{-4}**

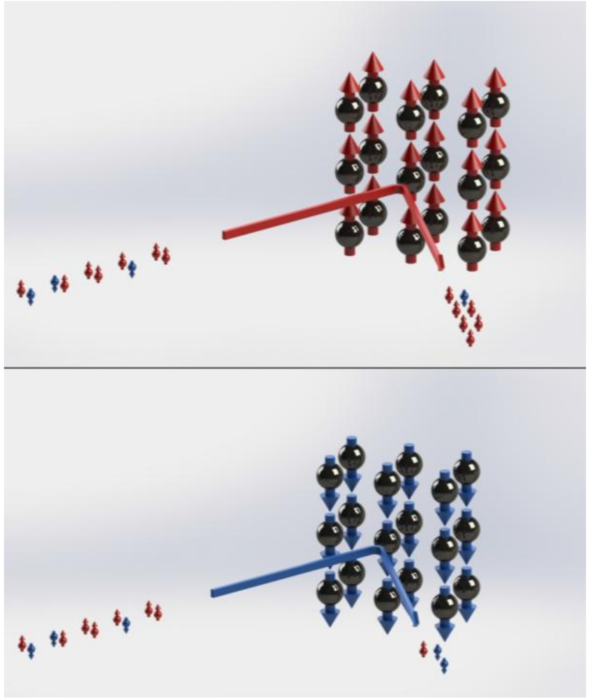
VLEED scattering



- **magnetic exchange interaction**
- parallel-antiparallel asymmetry
- **<15eV**
- **non-commercial**
- FeO target
- **FOM 10^{-2}**

Target magnetization dependent intensity asymmetry between spin up and spin down electrons

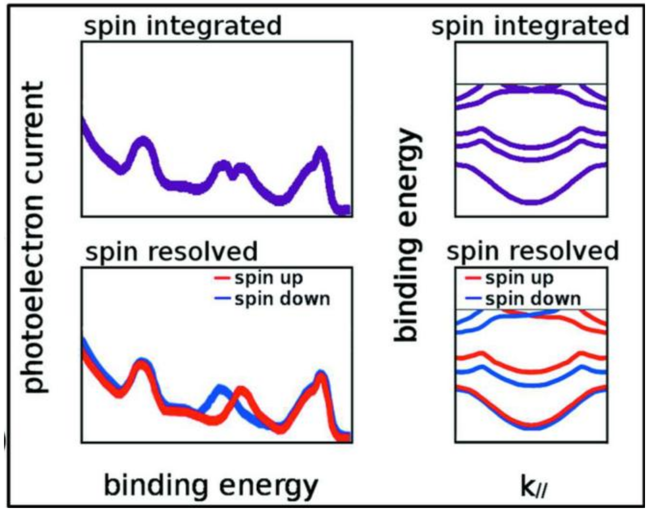




If the target is magnetized Up / Down, the incoming electrons with spin-up/down will be reflected more (top/bottom panel)

If the primary beam is polarized, then non-zero **asymmetry** value will be measure.

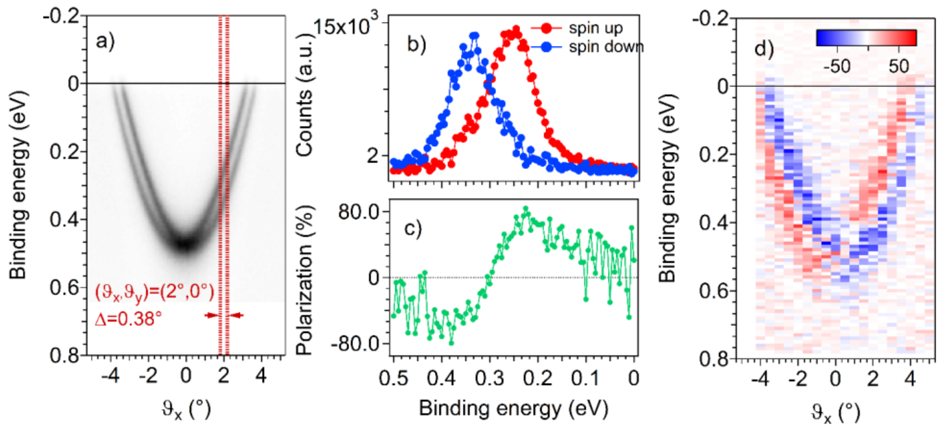
Resulting ARPES spectra →



Spin-integrated vs. spin-resolved ARPES

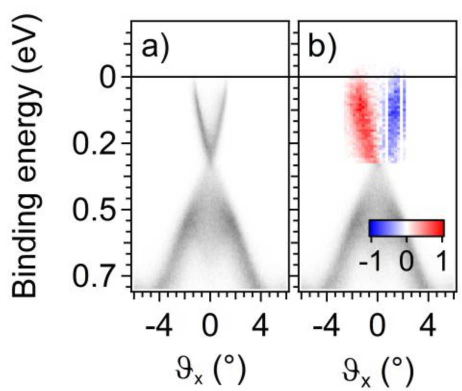
$$P = \frac{1}{S}\frac{EDC_{m\uparrow} - EDC_{m\downarrow}}{EDC_{m\uparrow} + EDC_{m\downarrow}}, \qquad SEDC_{\uparrow\downarrow} = \frac{(1 \pm P)(EDC_{m\uparrow} + EDC_{m\downarrow})}{2}.$$

Spin integrated
Au(111)
surface
state



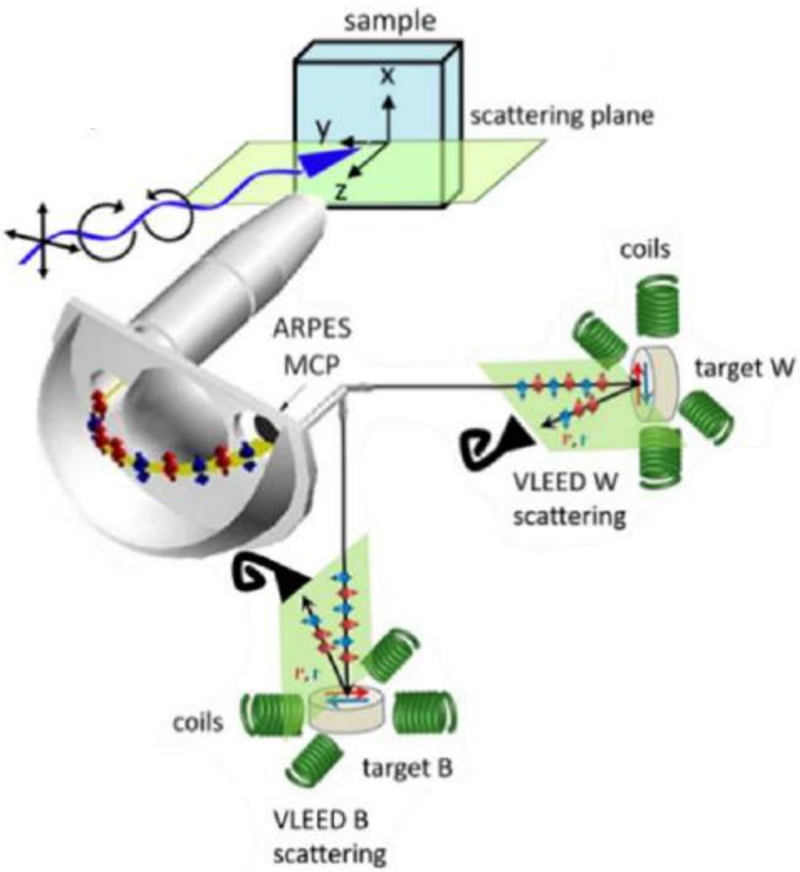
Spin resolved
Au(111)
surface
state

Spin integrated
Bi_2Se_3
topological
surface state



Spin resolved
Bi_2Se_3
topological
surface state

VLEED based spin-ARPES scheme



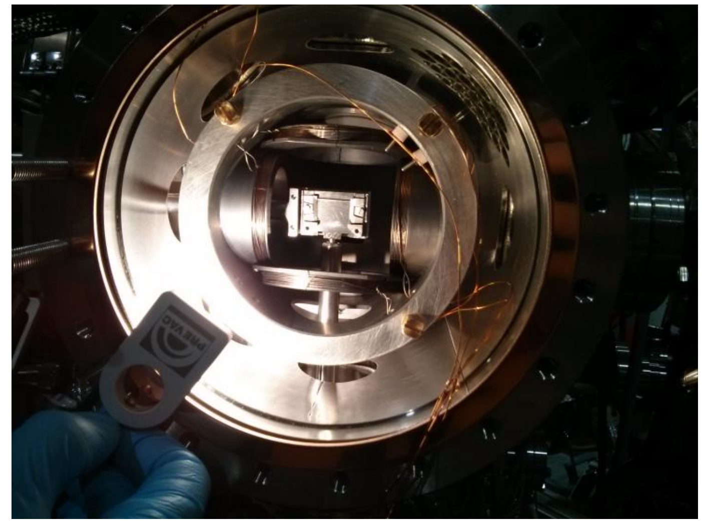
Two scattering chambers

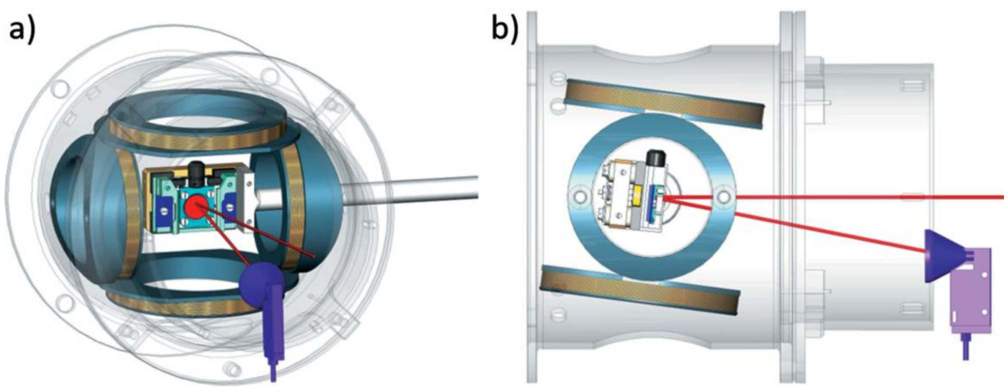
In each two orthogonal directions of spin can be measured

↓

Vectorial (3d) spin analysis

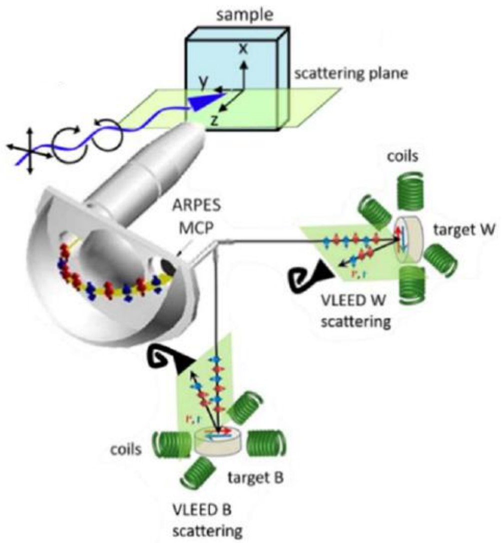
Magnetization coils outside… … and inside the scattering chamber

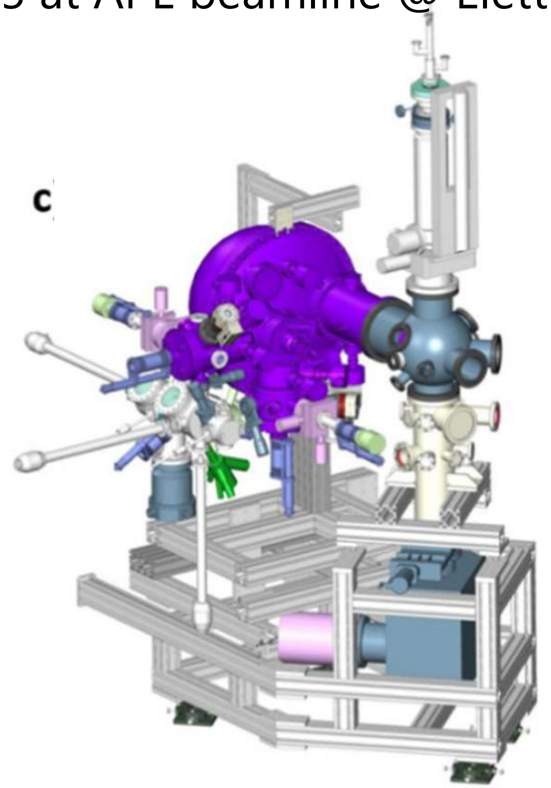


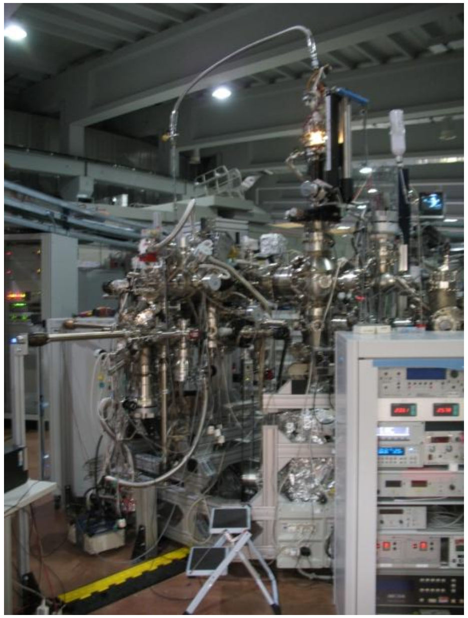


VESPA: spin polarimeter @ APE

- **VESPA**: **V**ery **E**fficient **S**pin **P**olarization **A**nalysis
- Designed, built and commissioned in Trieste (CNR-IOM, NFFA)
- Operates from Dec. 2015 at APE beamline @ Elettra





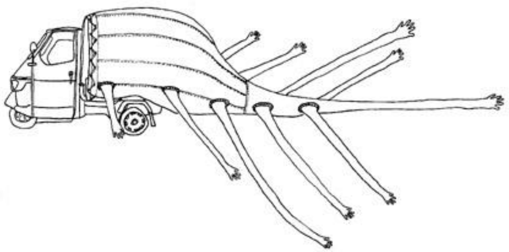


APE: Advanced Photoelectric effect Experiments

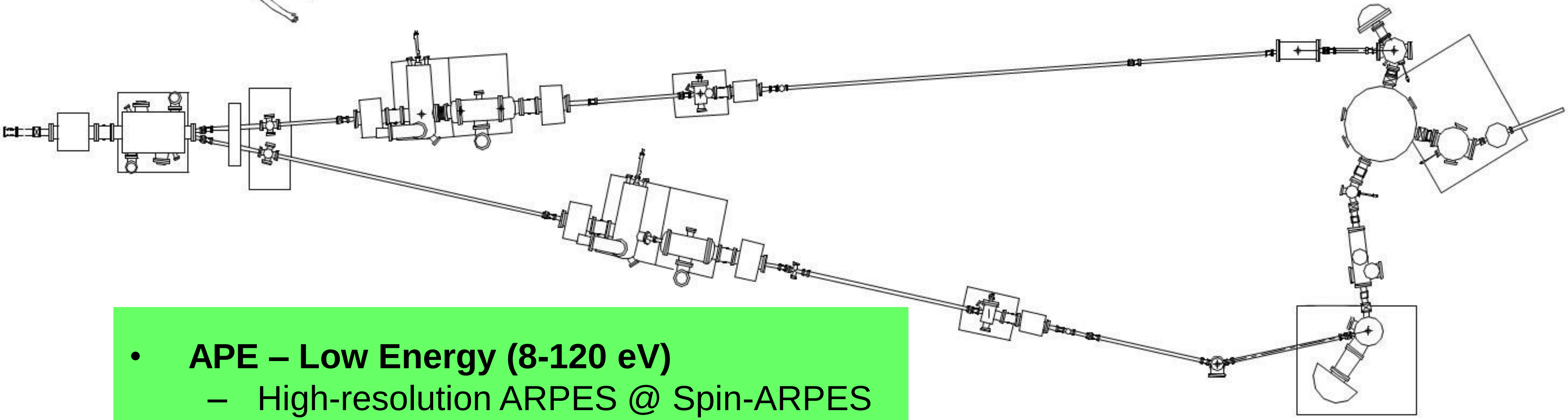
Two independent, off-axis, variable polarization (APPLE type) undulators

→**two independent canted beamlines operating simultaneously**

→First users: 2003

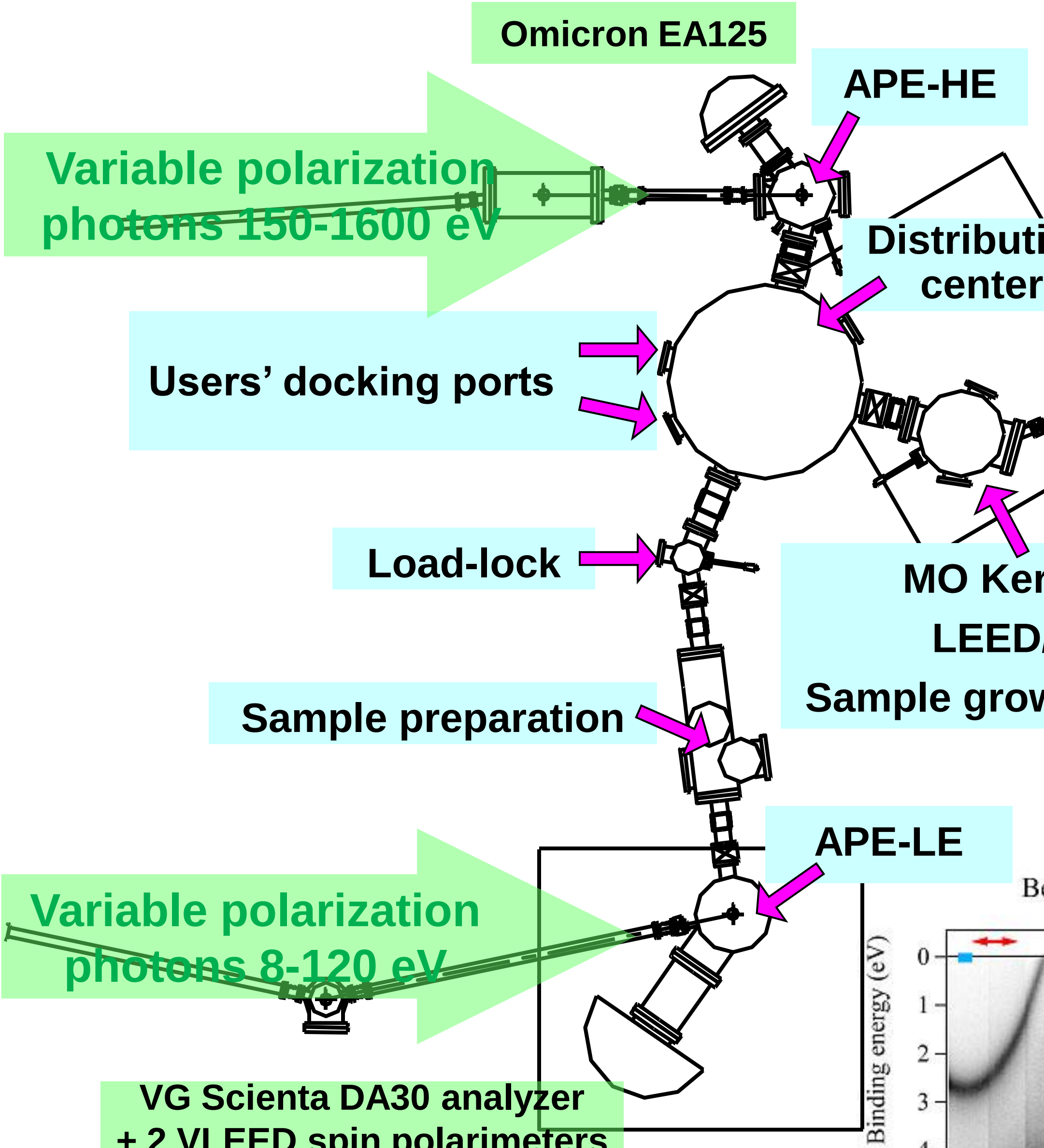


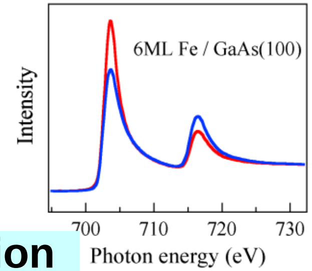
- **APE – High Energy (150-1600 eV)**
  - XPS spectroscopy
  - X-ray absorption (XAS, XMCD, XMLD)

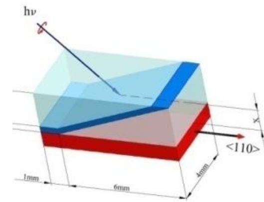


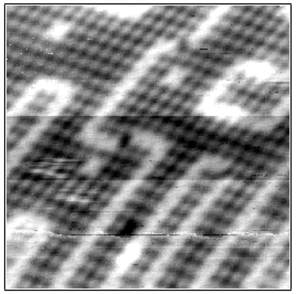
- **APE – Low Energy (8-120 eV)**
  - High-resolution ARPES @ Spin-ARPES
  - Electronic band structure
  - Fermi surface mapping
  - Fermi surface instabilities

APE surface science laboratory

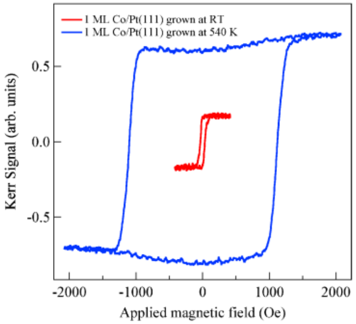


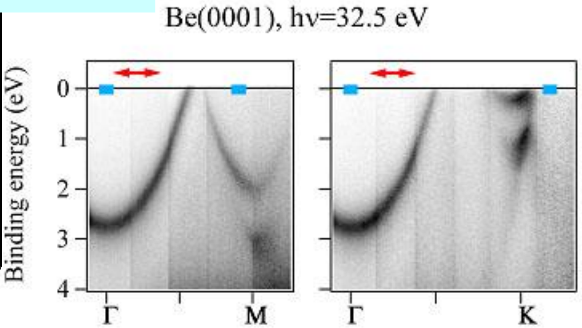


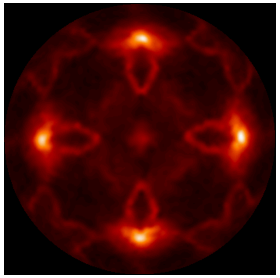




S segregation on Fe(100)





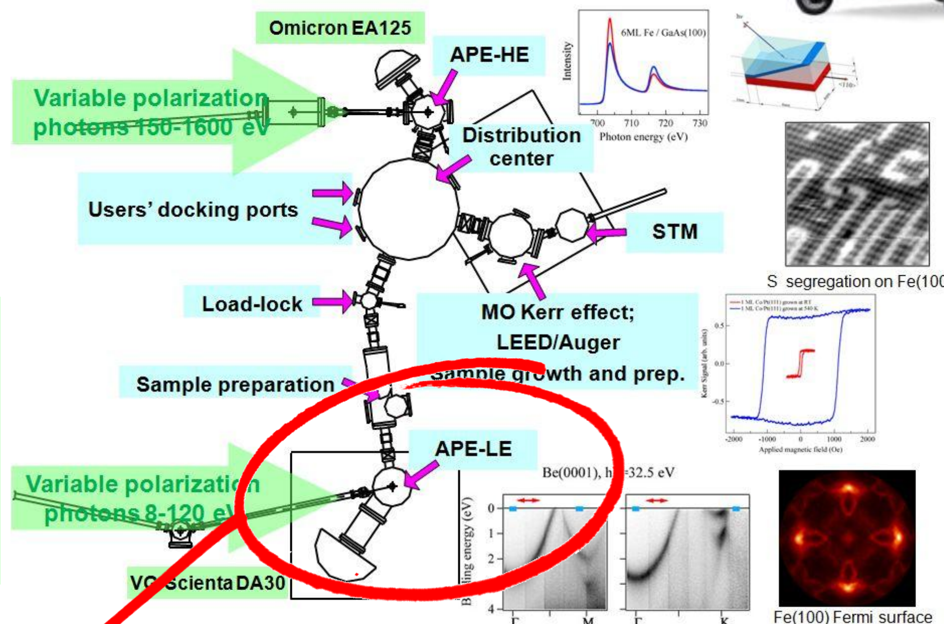


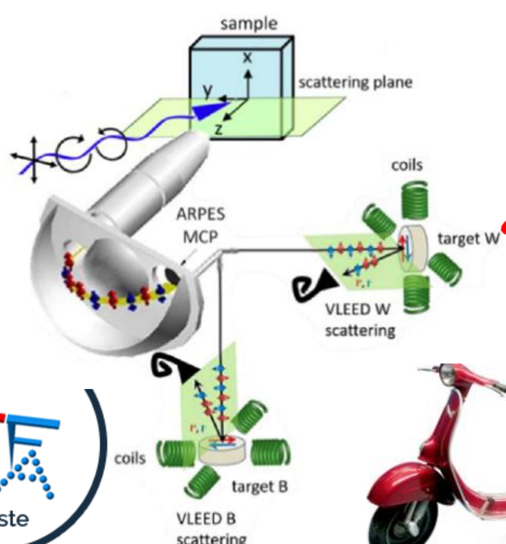
Fe(100) Fermi surface

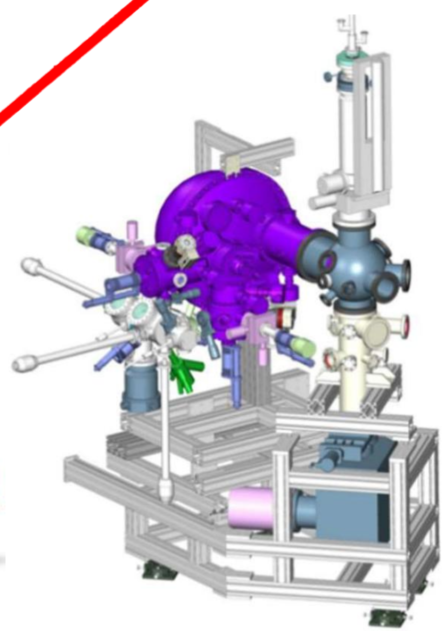
Complete Photoemission Experiment @ beamline APE

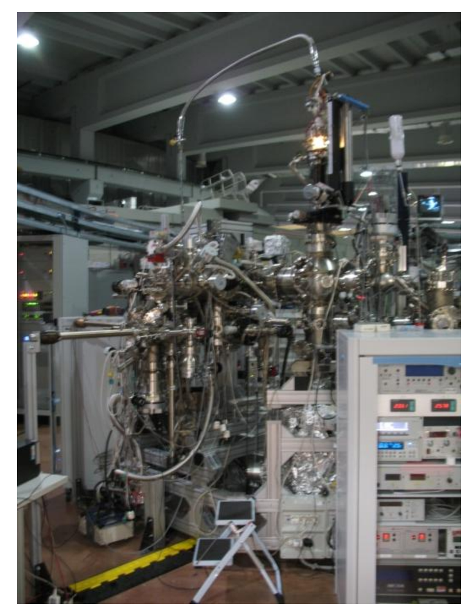
➔ **APE – High Energy (150-1600 eV)**
- XPS spectroscopy
- X-ray absorption (XAS, XMCD, XMLD)
- **NEW: Spectroscopy in-operando and ambient pressure**

➔ **APE – Low Energy (8-120 eV)**
- High-resolution ARPES
- Electronic band structure
- Fermi surface mapping
- Fermi surface instabilities
- **NEW: Spin-resolved ARPES**







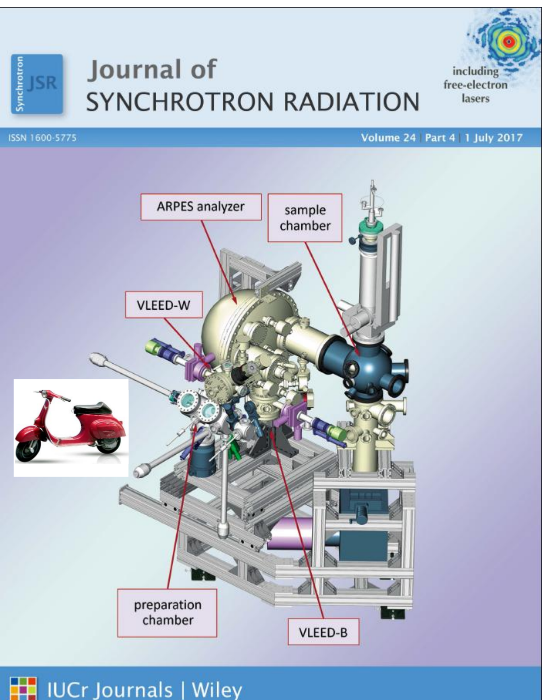


Trieste

Spin-resolved ARPES at beamline APE (CNR-IOM, NFFA)

In search for spin polarized electrons for future spintronic materials

-  **VESPA**: **V**ery **E**fficient **S**pin **P**olarization **A**nalysis
- Designed, built and commissioned in Trieste (CNR-IOM, NFFA)
- Operates from 2015 at APE beamline  @ Elettra
- C. Bigi et al. JSR (2017) 24, 750-756, on the title page of JSR:

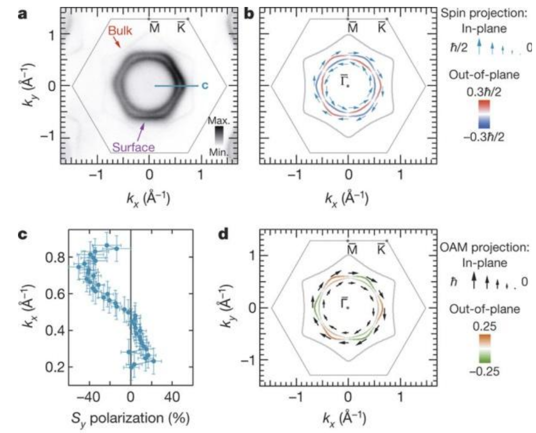


- **Some recent results:**

Maximazing Rashba-like spin splitting in $PtCo_2$

V. Sunko *et al.*, Nature **549**, 492–496 (2017)

Surface induced symmetry breaking enhances spin-orbit interaction and induces spin polarized electrons on the surface of $PtCo_2$.



Co-existence of type-I and type-II three dimensional bulk Dirac fermions in $PdTe_2$

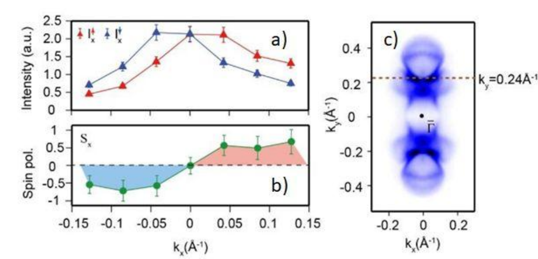
M.S. Bahramy *et al.*, Nature Materials, 2018

Spin-resolved ARPES data confirm the helical spin texture of the two surface states in $PdTe_2$ and therefore their topological nature.

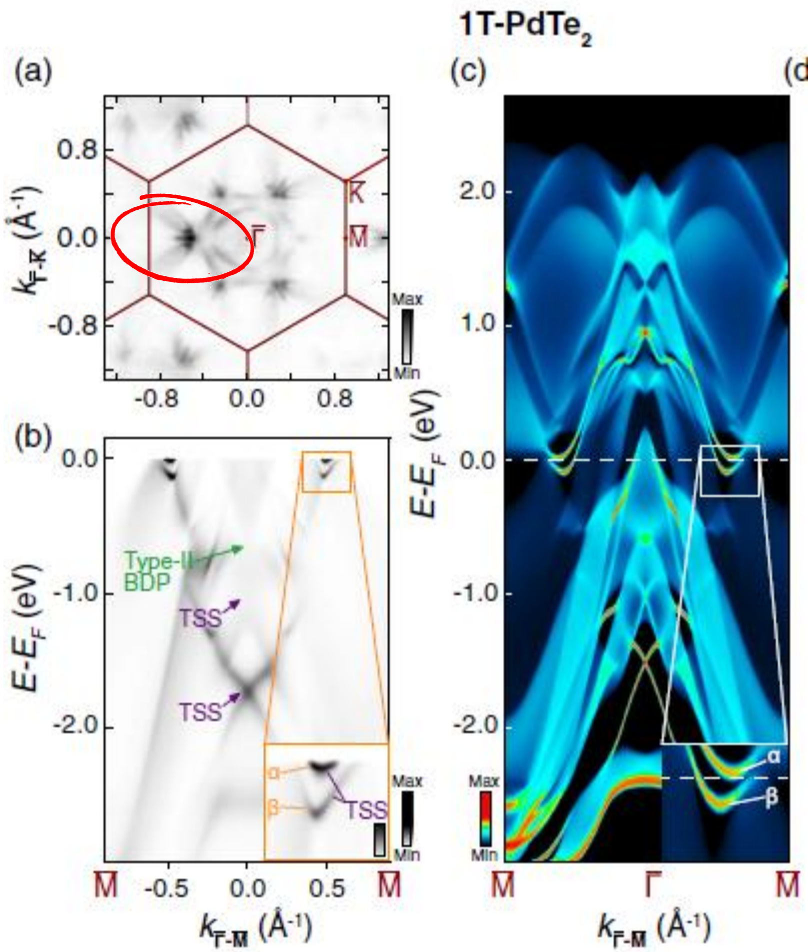
Weyl electrons on the surface of $MoTe_2$

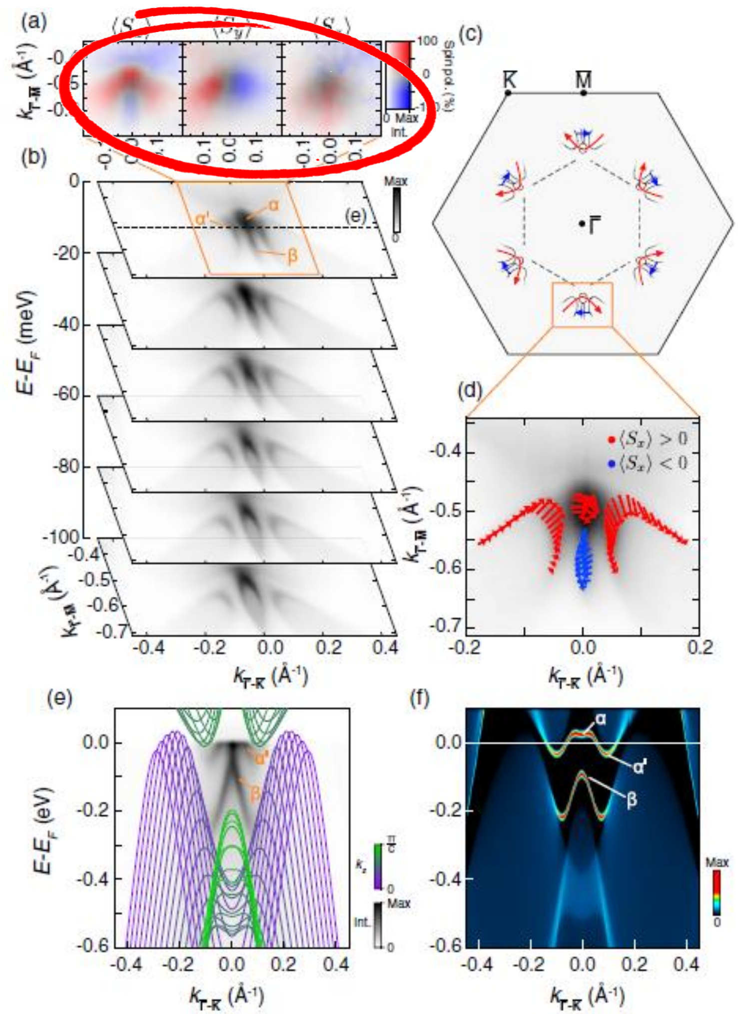
J. Jiang *et al.,* Nature Communications 8, 13973 (2017)

Measured spin polarization provides evidence of the presence of Weyl electrons in $MoTe_2$.



Latest result: Spin- Fermi surface mapping





O.J. Clark et al., PRL 2018

After this lecture…

→ **feeling of what ARPES and Spin-ARPES can do for you**

→ If interested in quantum properties of materials - electronic band structures, Fermi surfaces, electronic correlations, spin polarization:

http://www.elettra.trieste.it/elettra-beamlines/ape.html

http://www.trieste.nffa.eu/

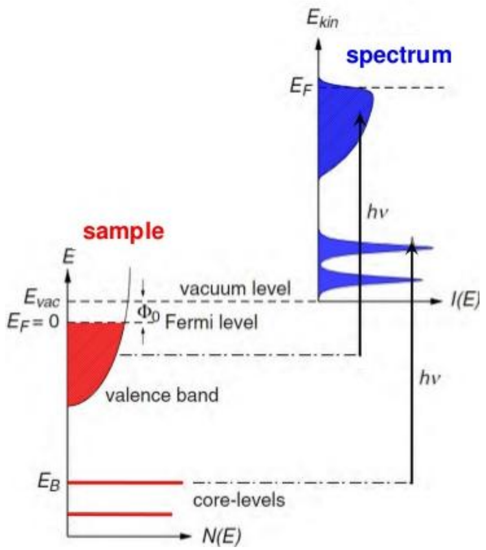
Interested in learning more?

- **ARPES:**
  - S. Hüfner, Photoelectron Spectroscopy – Principles and Applications, 3rd ed. (Berlin, Springer, 2003)
  - S. Suga, A. Sekiyama, Photoelectron Spectroscopy – Bulk and Surface Electronic Structures (Berlin, Springer, 2014)

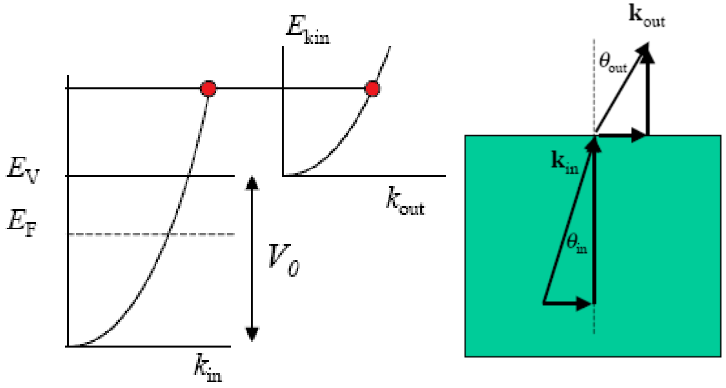
  - F. Reinert and S. Hüfner, New Journal of Physics 7, 97 (2005)
  - A. Damascelli, Physica Scripta T109, 61 (2004)
  - S. Hüfner et al., J. Electron Spectrosc. Rel. Phen. 100, 191 (1999)

- **Spin-ARPES:**
  - Taichi Okuda, J. Phys.: Condens. Matter 29 483001 (2017)
  - Chiara Bigi et al., J. Synchrotron Rad. 24, 750-756 (2017)

Photoemission relations



$$E_{kin} = h\nu - E_B - \Phi$$



$$w_{fi} = \frac{2\pi}{\hbar} \left| \langle f | H_{\text{int}} | i \rangle \right|^2 \delta(E_f - E_i - h\nu)$$

$$H_{\text{int}} = \frac{e}{mc} \vec{A} \bullet \vec{p}$$

$$I(\vec{k},\omega) \propto \left| \langle f | \vec{A} \cdot \vec{p} | i \rangle \right|^2 A(\vec{k},\omega) f(\omega)$$

$$A(\vec{k},\omega) = \frac{1}{\pi} \frac{\left| \operatorname{Im} \Sigma(\vec{k},\omega) \right|}{\left| \omega - \varepsilon_k - \operatorname{Re} \Sigma(\vec{k},\omega) \right|^2 + \left| \operatorname{Im} \Sigma(\vec{k},\omega) \right|^2}$$

$$f(\omega) = \frac{1}{1 + e^{\frac{\omega - \mu}{kT}}}$$

$$k_{out} = \sqrt{\frac{2m}{\hbar^2} E_{kin}}$$

$$k_{in} = \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$

$$k_{out\|} = k_{in\|} \equiv k_{\|} = \sin \vartheta_{out} \sqrt{\frac{2m}{\hbar^2} E_{kin}} = \sin \vartheta_{in} \sqrt{\frac{2m}{\hbar^2} (E_{kin} + V_0)}$$