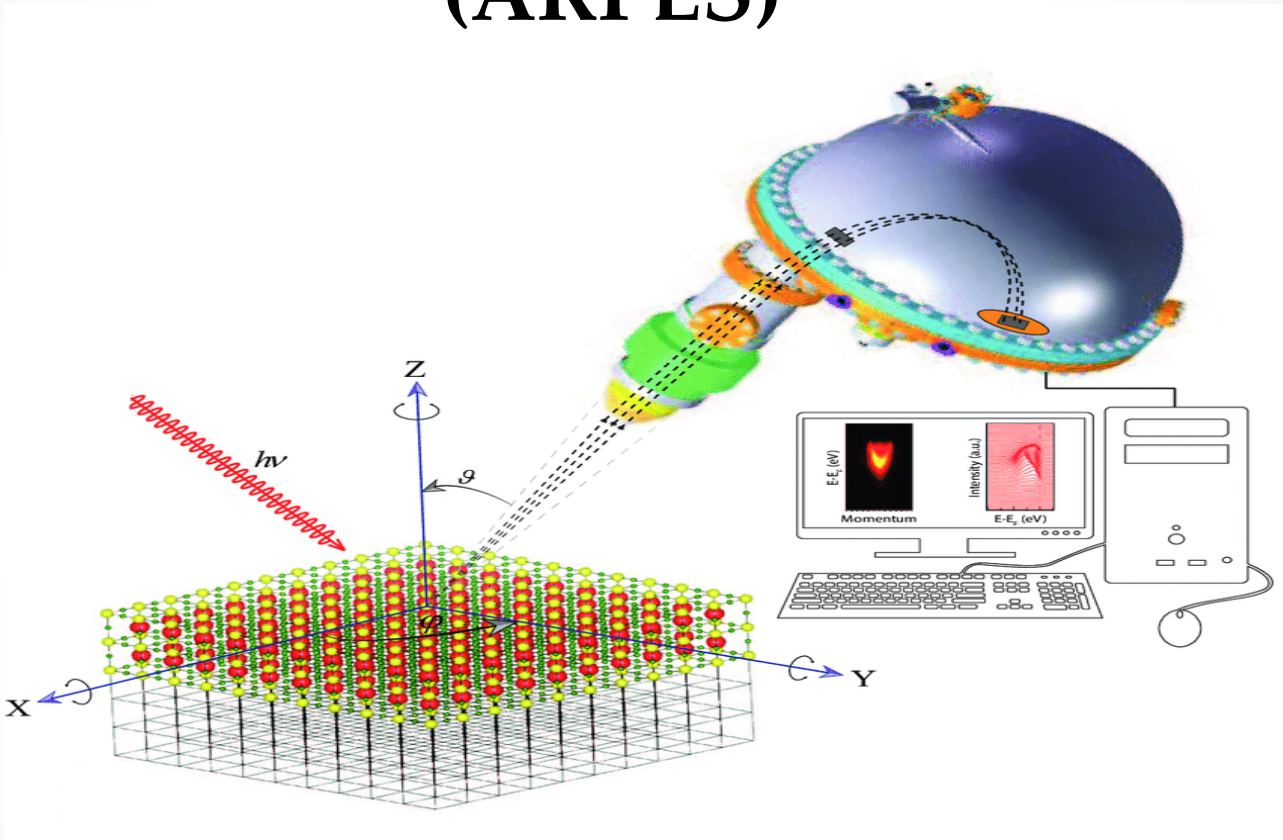
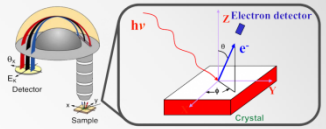
Angle-Resolved Photoemission Spectroscopy (ARPES)

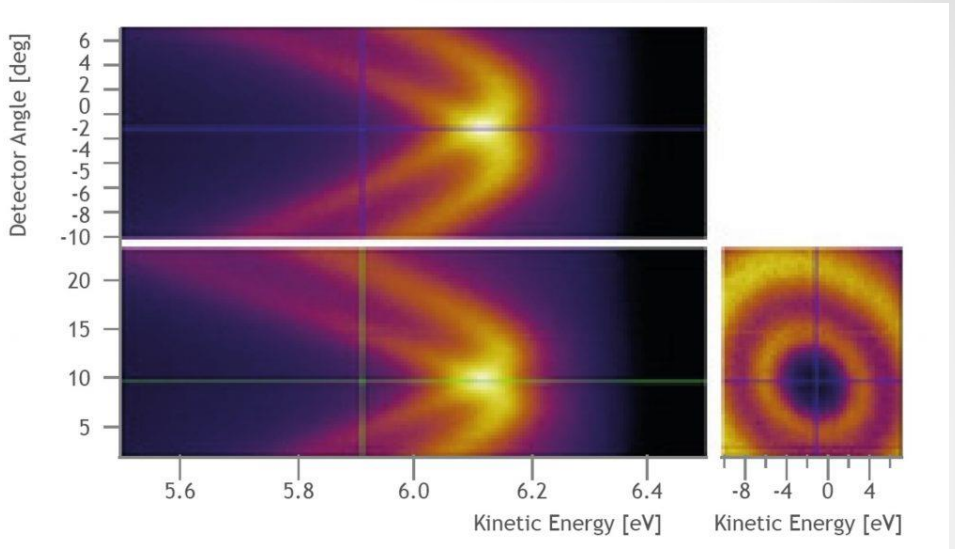


Parnian Lali and Rasta M.Ebrahimi

Dr.Sahebsara

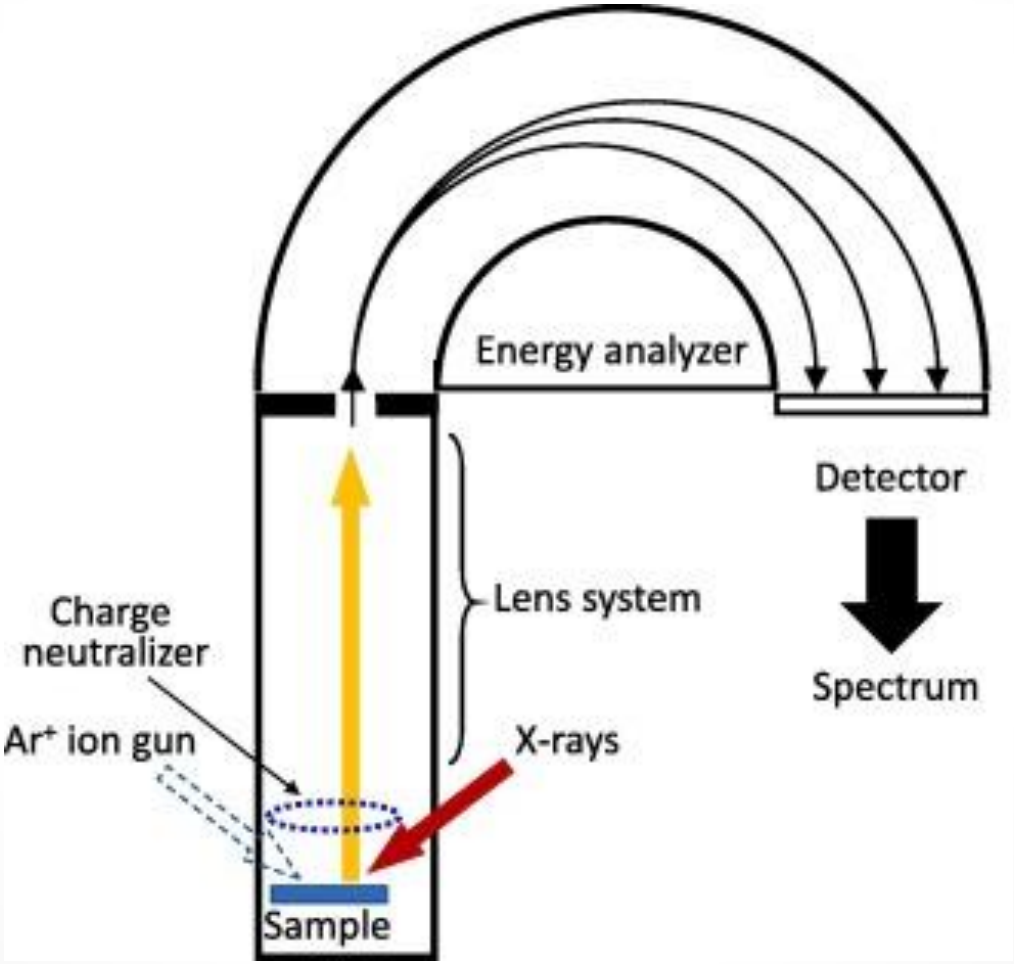
Contents



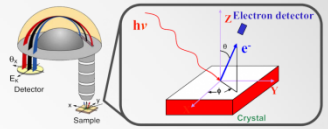


- *Introduction to ARPES*
- *Theory section*
- *Examples of ARPES*
- *ARPES as an experimental method*
- *Conclusion*

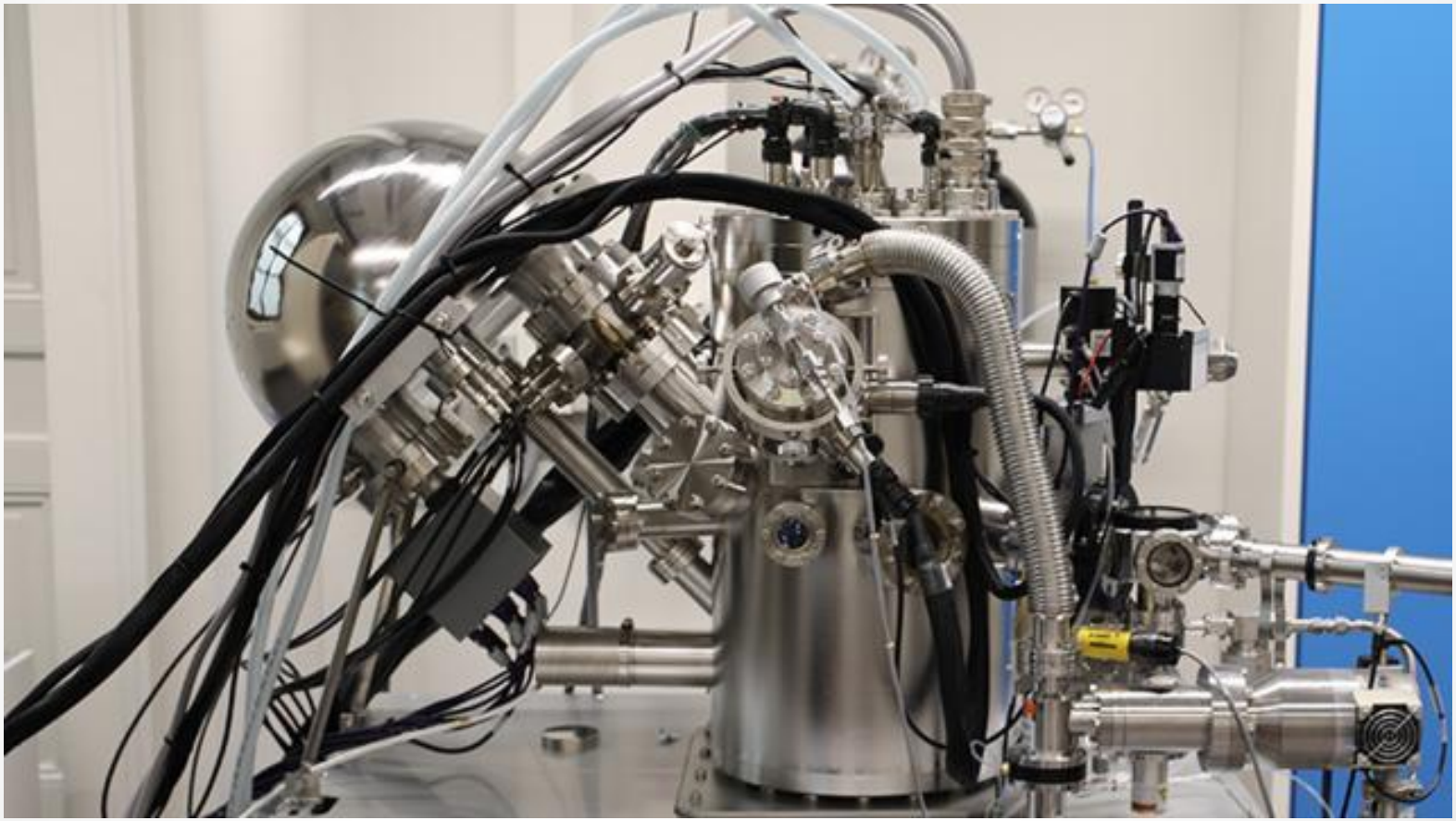
Photoemission Spectroscopy (PES)



Photoemission Spectroscopy (PES)

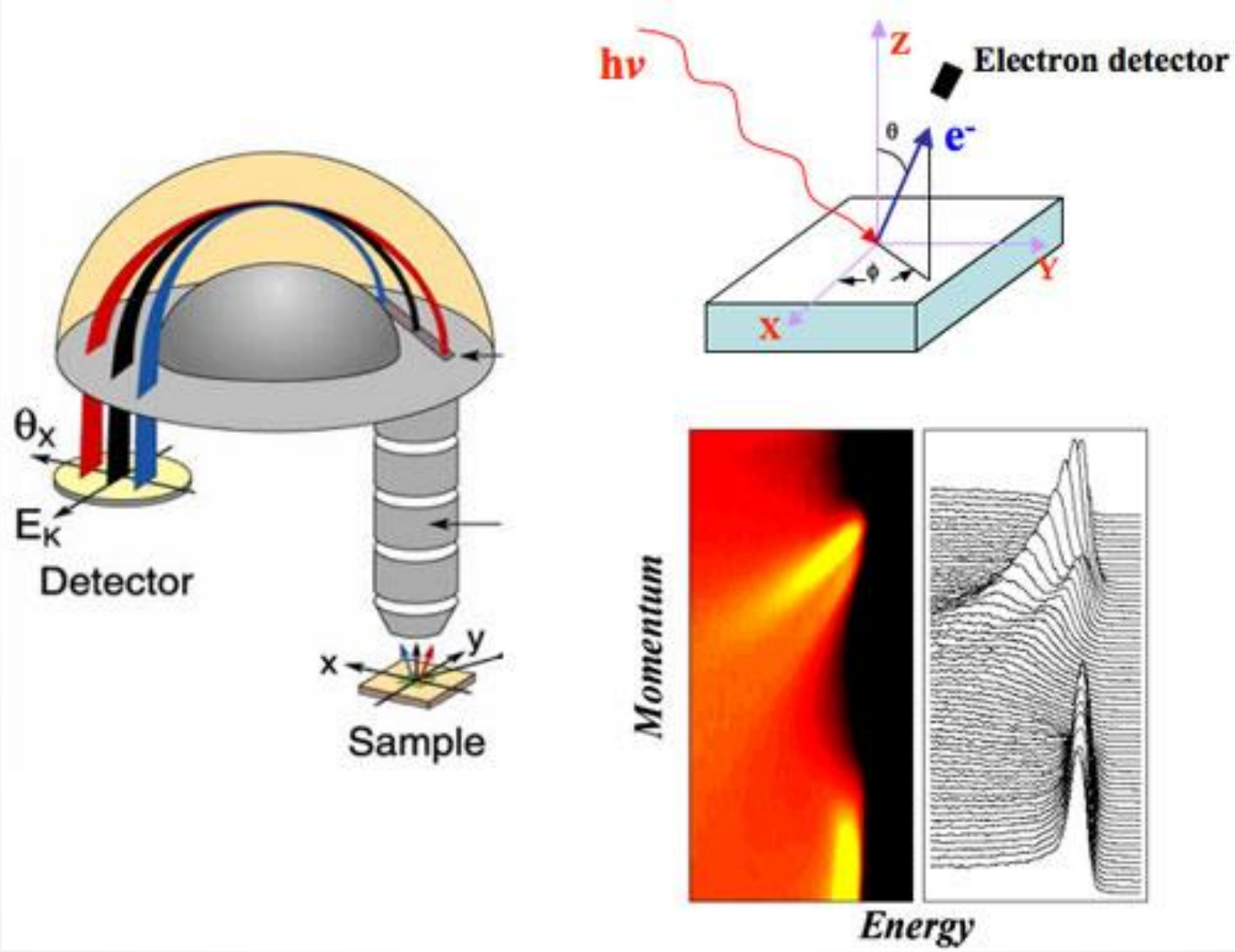


UPS & XPS

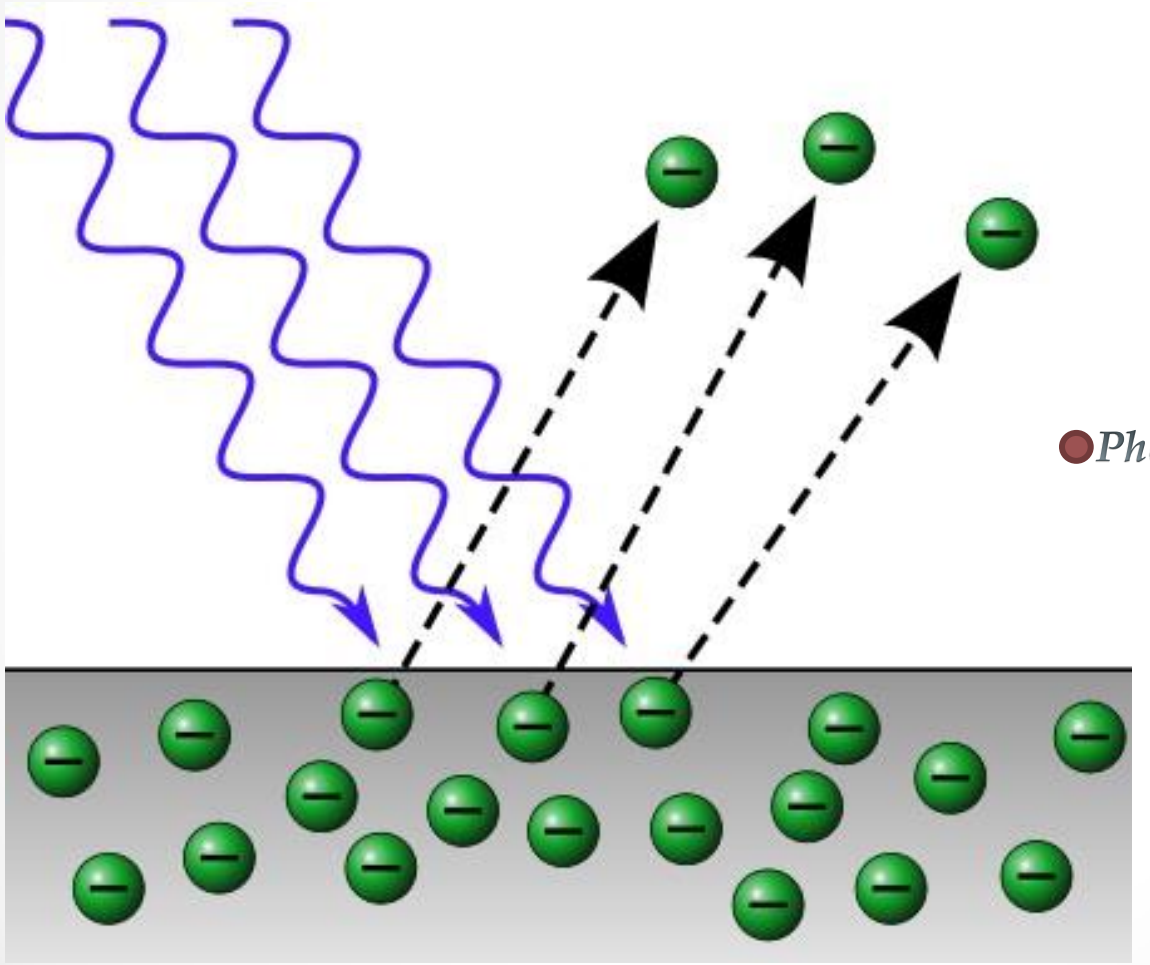


X-ray photoemission spectroscopy (XPS) ,
University of Geneva, Switzerland

ARPES & PES


θx
EK
Detector
x
y
Sample
hν
z
Electron detector
θ
e-
ϕ
Y
X
Momentum
Energy

Photoelectric effect and photoelectrons -**Theory section**



- *Conservation of energy*

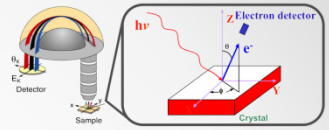
$$h\nu = E_B + \varphi + E_k$$

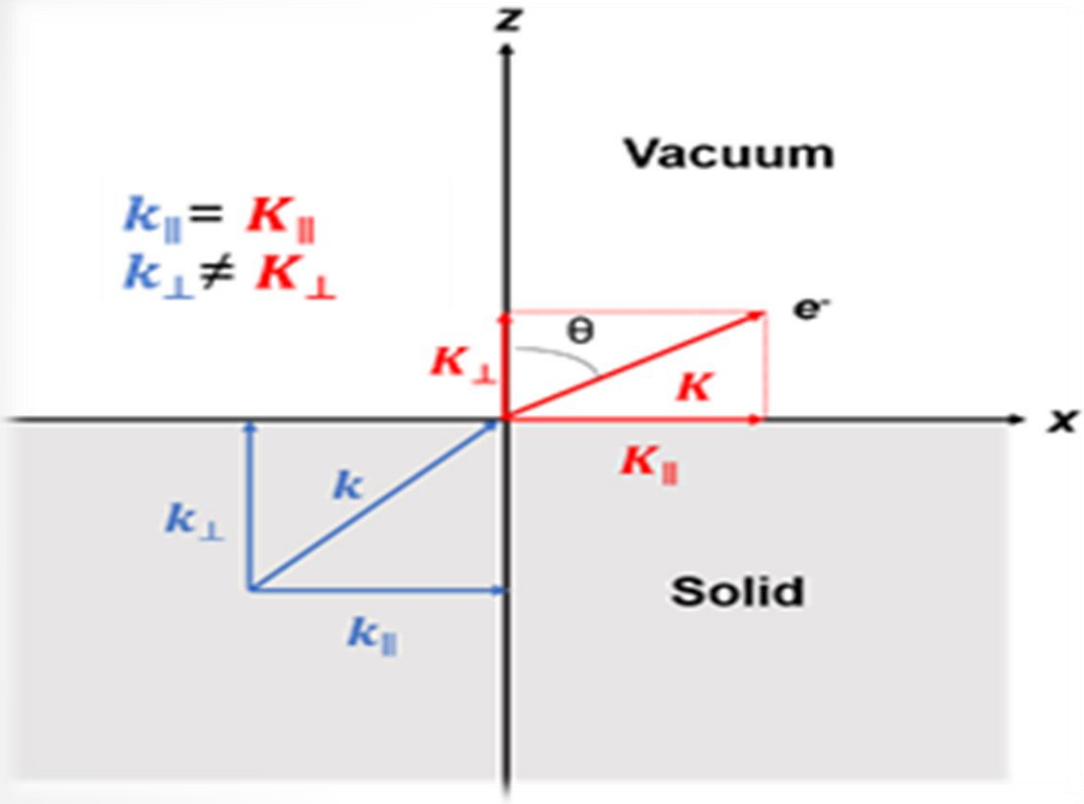
$$E_k = h\nu - E_B - \varphi$$

- *Photoelectron kinetic energy*

$$E_k = \frac{\hbar^2 K^2}{2m_0}$$

Theory section – 2D





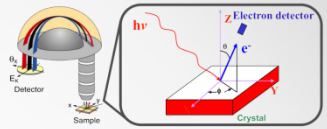
$$E_k = \frac{\hbar^2 K^2}{2m_0}$$

$K_\parallel$ and $K_\perp$ are the surface normal and parallel components of the wave vector $\boldsymbol{K}$ in vacuum :

$$\rightarrow E_k = \frac{\hbar^2 (K_\parallel{}^2 + K_\perp{}^2)}{2m_0}$$

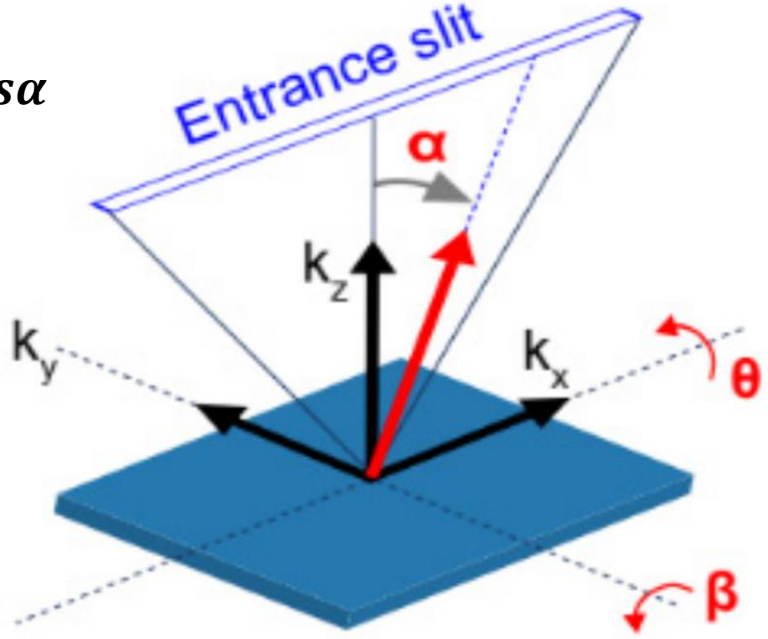
$$\begin{cases} K_\parallel = K\sin\theta \\ K_\perp = K\cos\theta \end{cases} \longrightarrow \begin{cases} \hbar K_\parallel = p = \sqrt{2mE_k}\sin\theta & (K_\parallel = k_\parallel) \\ \hbar K_\perp = \sqrt{(2m(E_k\cos^2\theta - V_0))} & (K_\perp \neq k_\perp) \end{cases}$$

Theory section – 3D

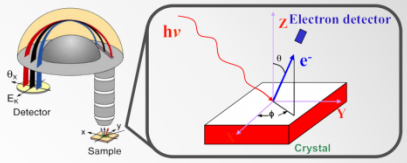


Angle-resolved Photoemission Spectroscopy, Hongyun Zhang, Tommaso Pincelli and etc

$$\begin{cases} k_{x,in} = k_{x,out} = \dfrac{\sqrt{2m_e E_k}}{\hbar}(cos\beta sin\alpha + sin\beta cos\theta cos\alpha) \\ k_{y,in} = k_{y,out} = \dfrac{\sqrt{2m_e E_k}}{\hbar} sin\theta cos\alpha \\ k_{z,in} = \sqrt{k_{z,out}{}^2 + V_0(\dfrac{\sqrt{2m_e}}{\hbar})^2} \end{cases}$$



What are the Measured Quantities and the Desired Quantities?!



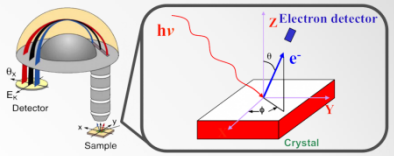
θ

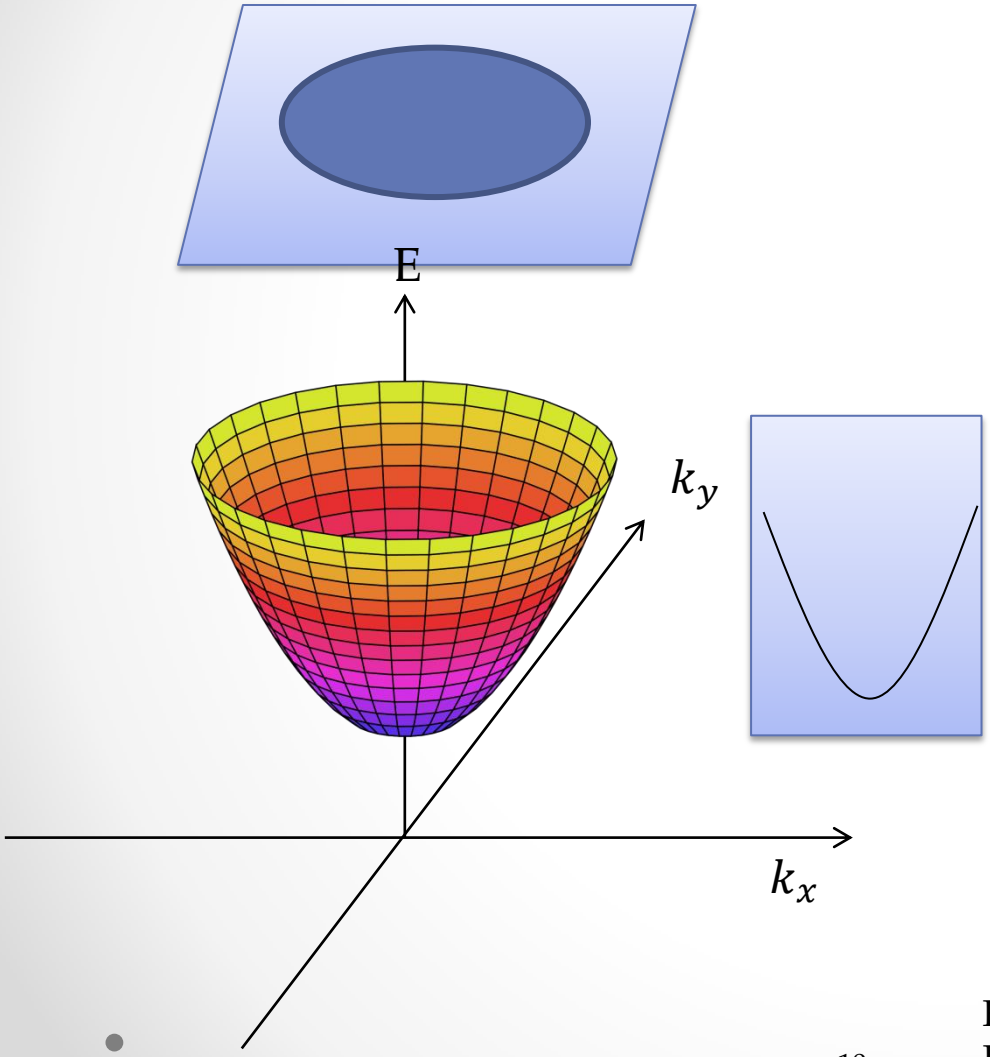
E_k φ

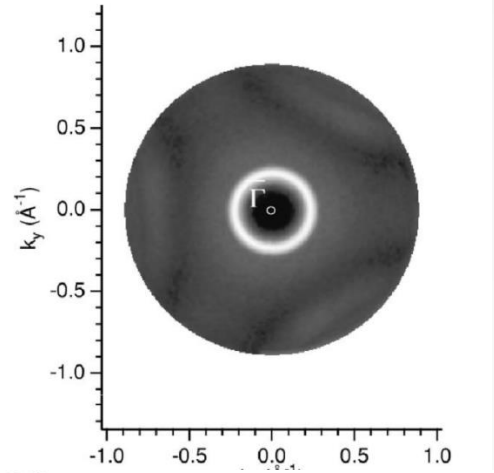
E_B

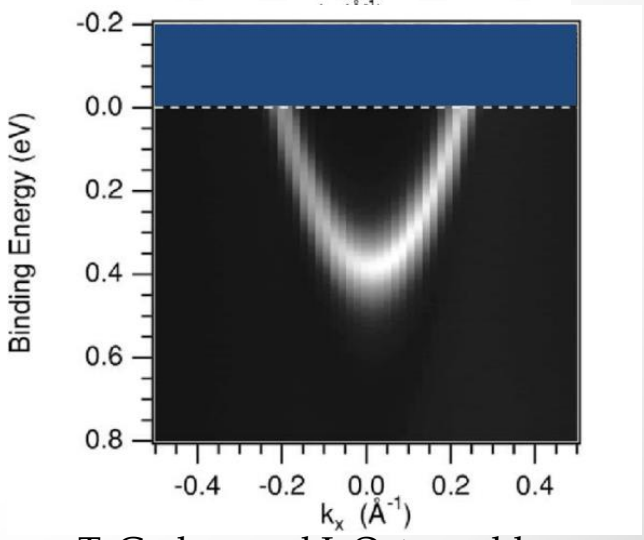
$K_{\parallel}$

a simple example of ARPES : 2D free electron gas on Cu(111)





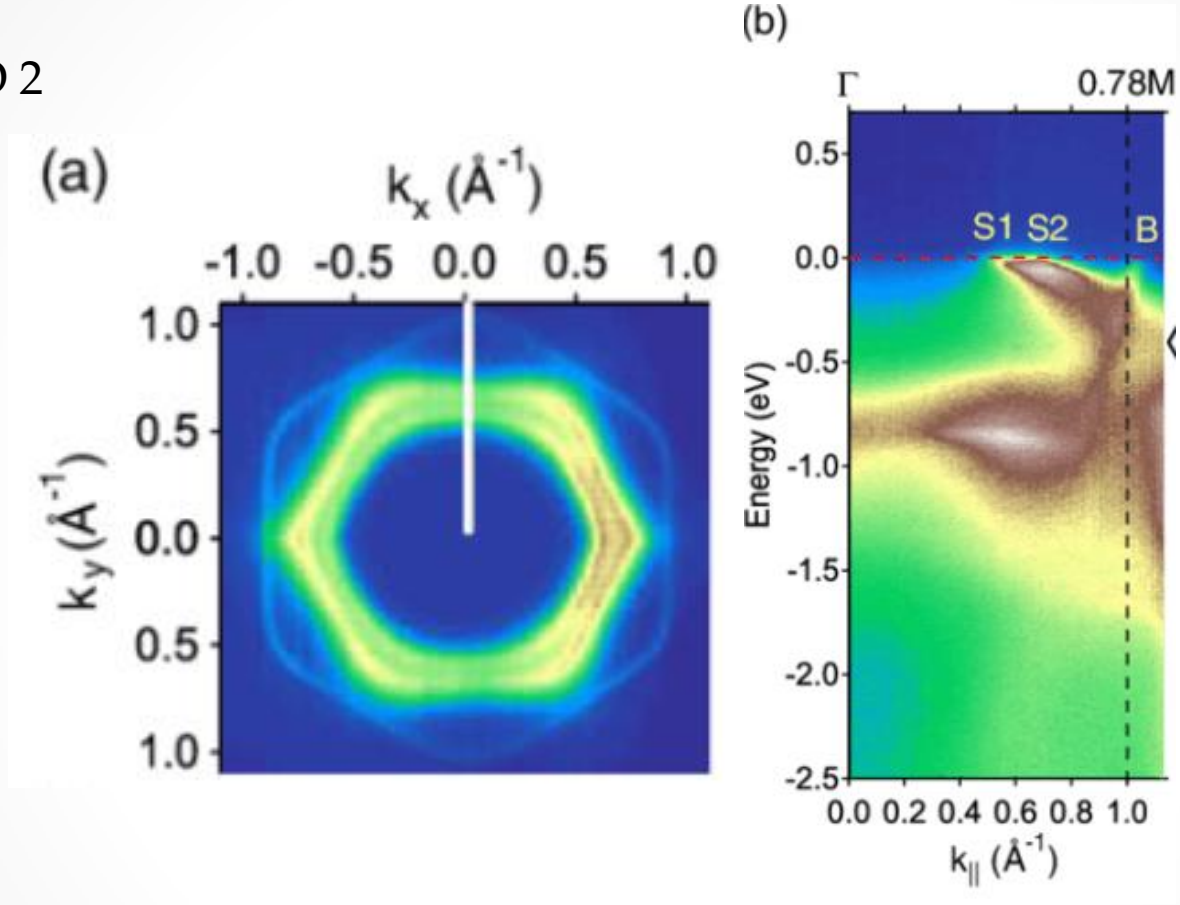




F. Baumberger, T. Greber, and J. Osterwalder Phys. Rev. B **64**, 195411 – Published 26 October 2001

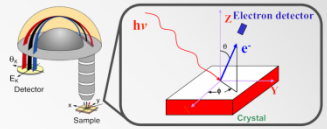
Another examples of ARPES

PdCoO 2

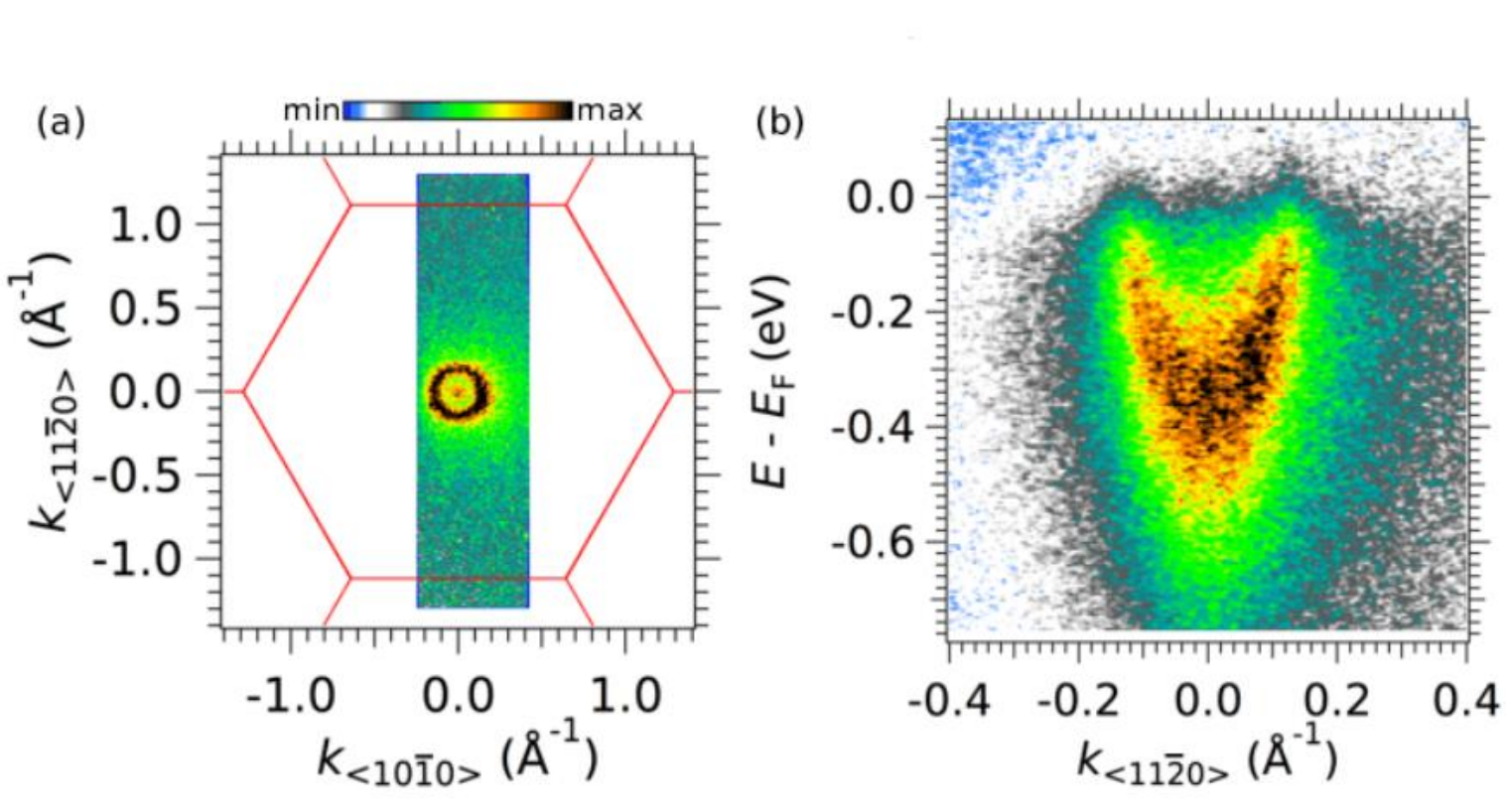


Anisotropic Electric Conductivity of Delafossite PdCoO2 Studied by Angle-Resolved Photoemission Spectroscopy, July 2009

Another examples of ARPES

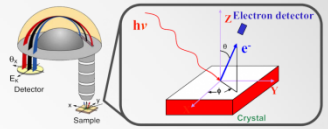


ZnO



High-density two-dimensional electron system induced by oxygen vacancies in ZnO, February 2018

Another examples of ARPES



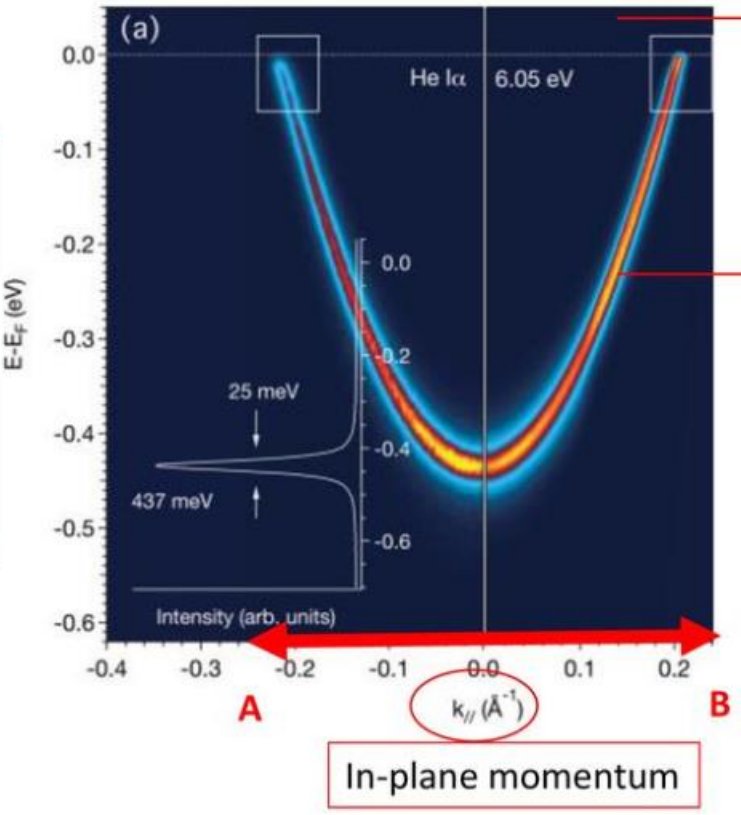
Cu(111 surface)

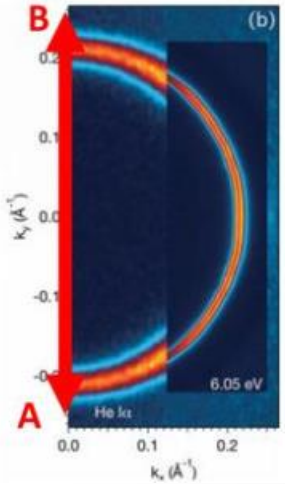
Electron binding energy
$|E_B| = E - E_F$

Fermi-Dirac cutoff

$$F(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1}$$

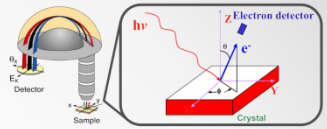
$$\epsilon_k = E(k) = \frac{\hbar^2 k^2}{2m^*}$$



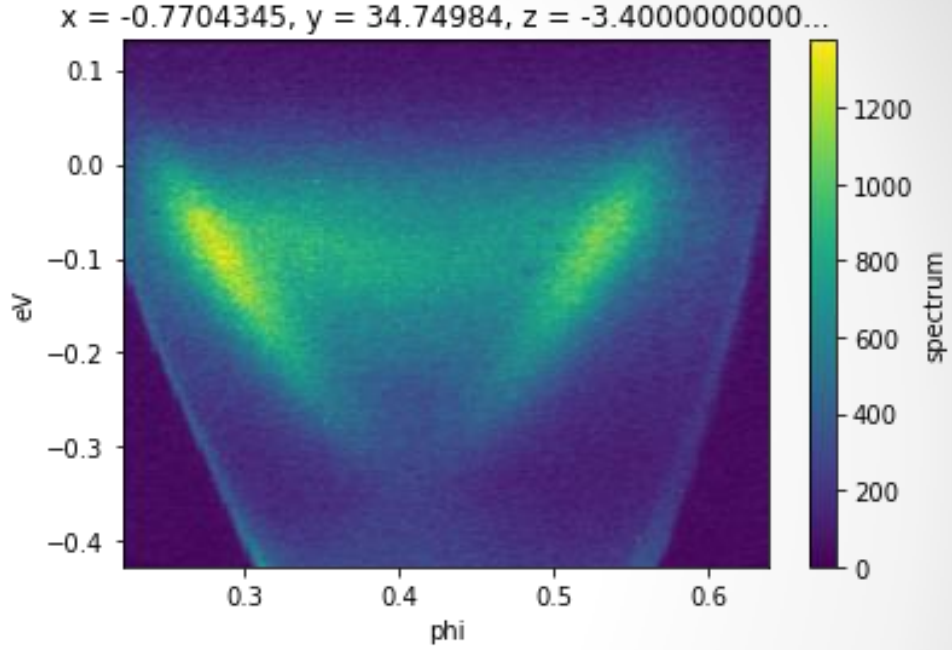


PRB **87**, 075113 (2013)

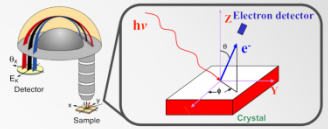
ARPES in Python



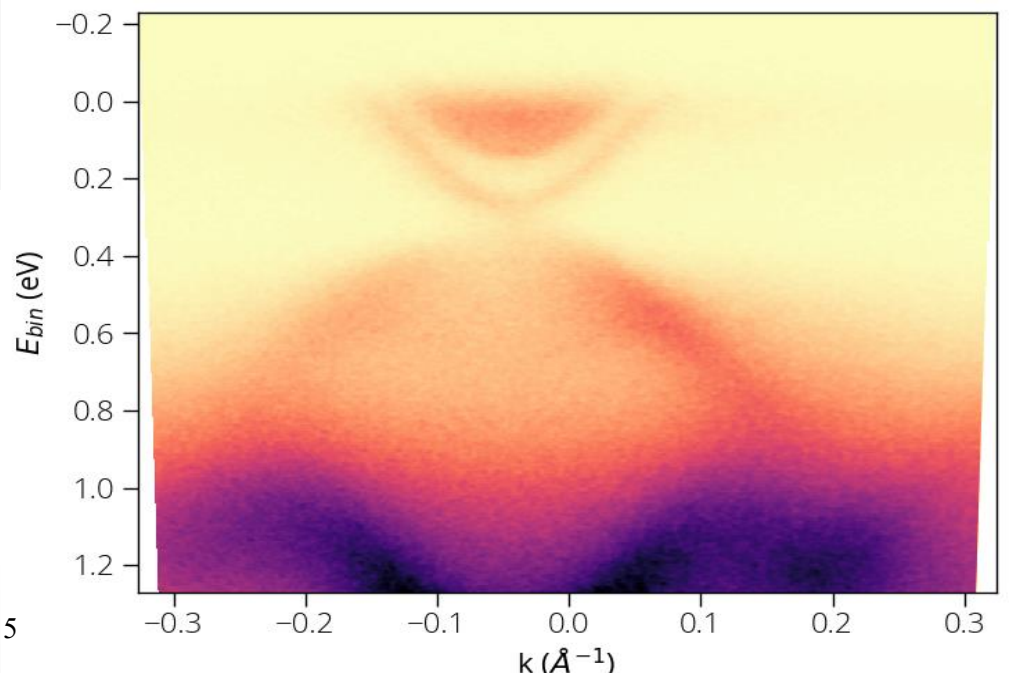
PyARPES



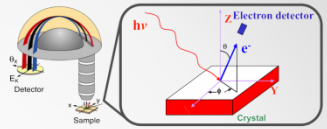
ARPES in Python



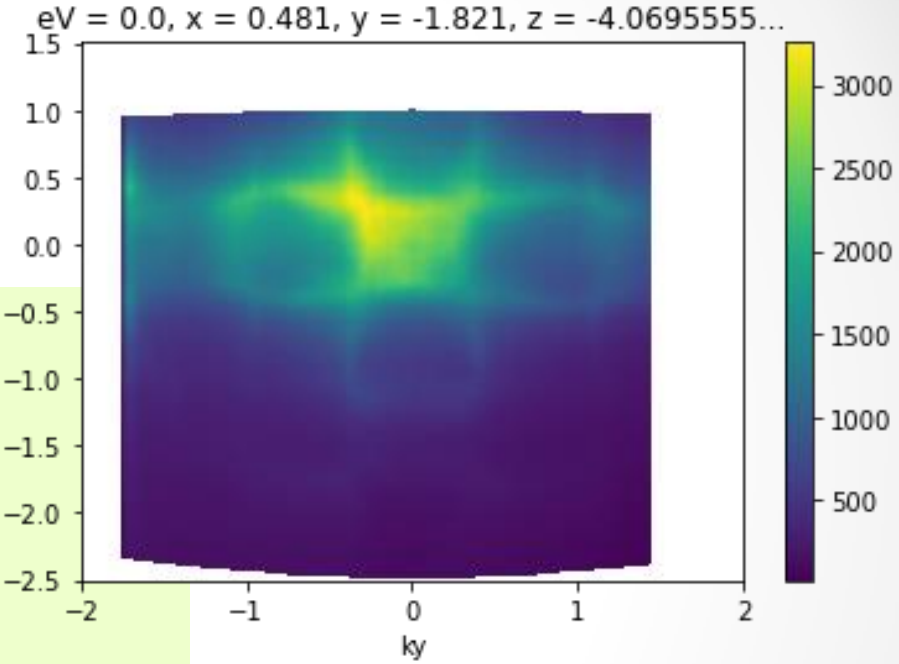

```python
import arpespythontools as arp
data, energy, angle = arp.load_ses_spectra('sample_spectra.txt')
data_k, e_bin, k = arp.k_conv(data, energy, angle, 16.67)
# Fermi energy = 16.67 eV

# Plot image
import matplotlib.pyplot as plt
%matplotlib inline
# Above line is specific to Jupyter Notebook
plt.figure(figsize = (8, 6))
plt.imshow(data_k, origin = 'lower', aspect = 'auto', \
           extent = (k[0], k[-1], e_bin[0], e_bin[-1]))
plt.xlabel("k ($\AA^{-1}$)")
plt.ylabel('$E_{bin}$ (eV)')
plt.set_cmap('magma_r')
plt.show()
```



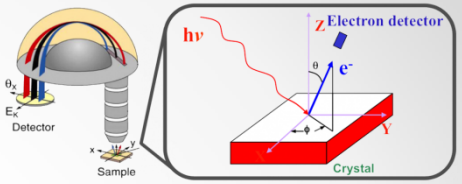
ARPES in Python

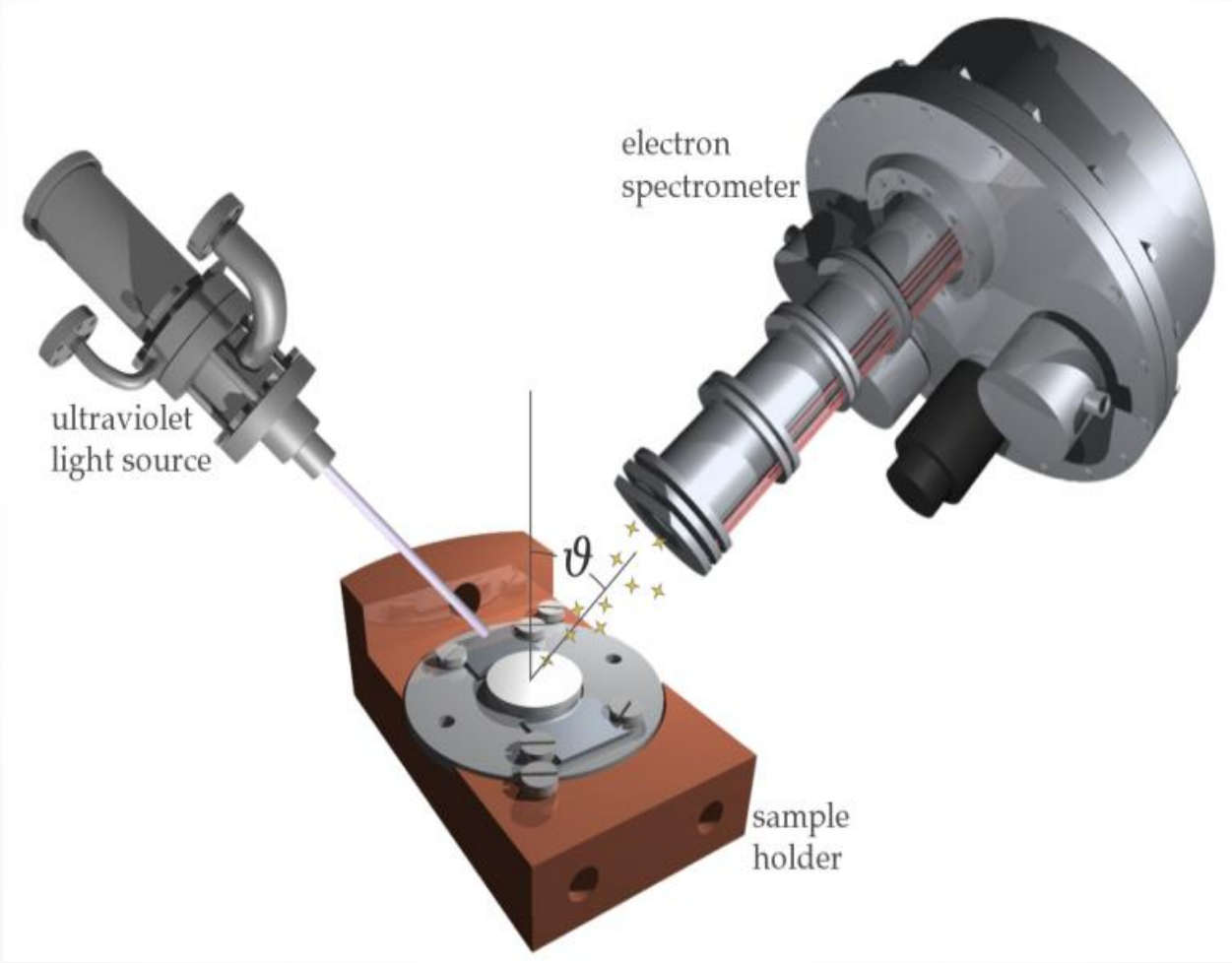



```
from arpes.io import example_data
from arpes.utilities.conversion import convert_to_kspace
from arpes.fits.utilities import broadcast_model
from arpes.fits.fit_models import AffineBroadenedFD, QuadraticModel
import matplotlib.pyplot as plt


def load_energy_corrected():
    fmap = example_data.map.spectrum
    cut = fmap.sum("theta").sel(
        eV=slice(-0.2, 0.1), phi=slice(-0.25, 0.3)
    )

    results = broadcast_model(AffineBroadenedFD, cut, "phi")
    edge = QuadraticModel().guess_fit(results.F.p("fd_center")).eval(x=fmap.phi)
    return fmap.G.shift_by(edge, "eV")

import numpy as np
convert_to_kspace(
    energy_corrected.S.fermi_surface, # just convert the Fermi surface
    kx=np.linspace(-2.5, 1.5, 400),   # along -2.5 <= kx < 1.5 (inv ang.)
                                      #  with 400 steps
    ky=np.linspace(-2, 2, 400),       # as above, with -2 <= ky < 2
).S.plot()
```

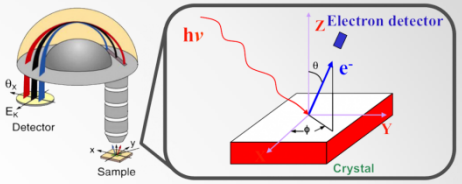


ARPES as an experimental method

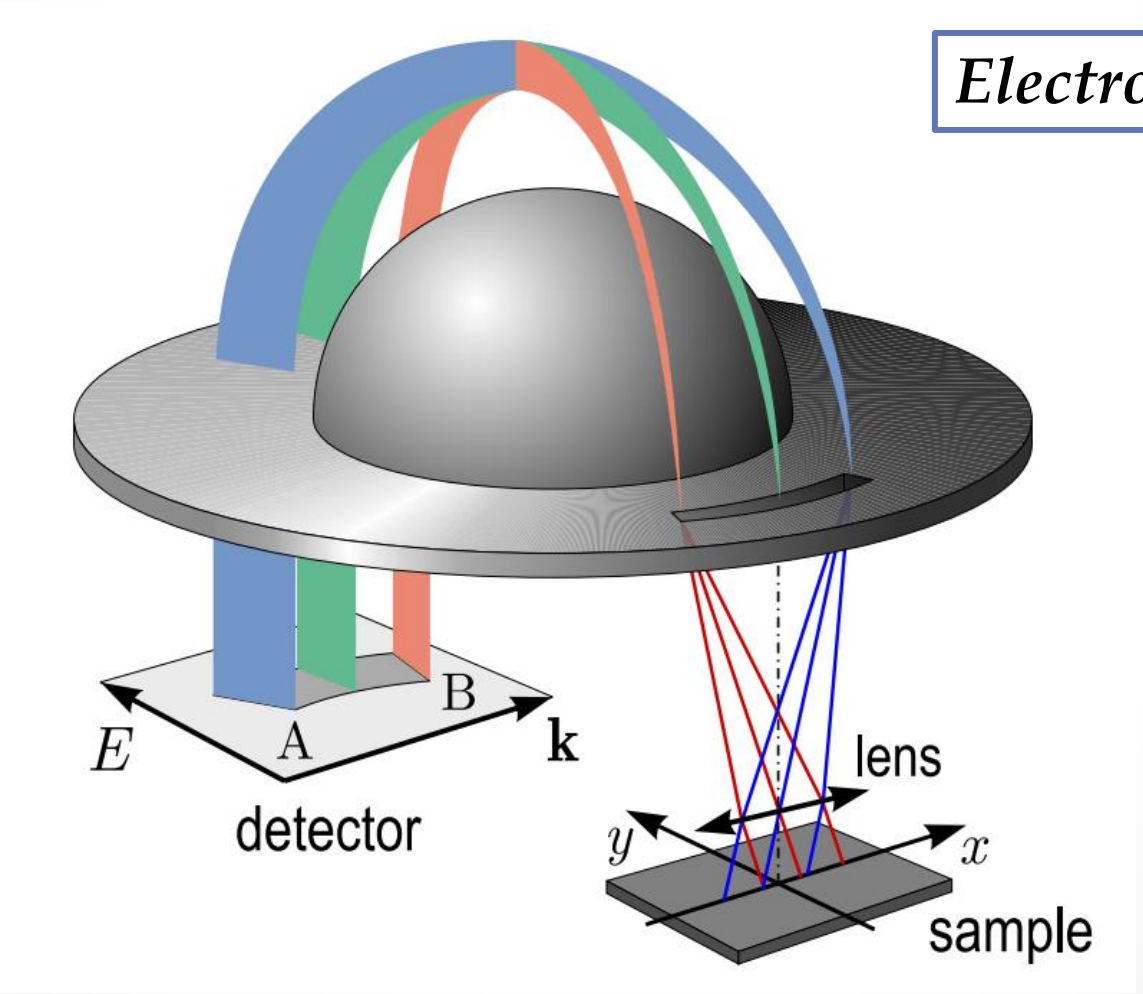




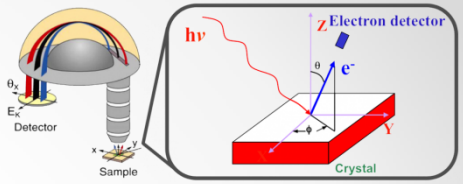
ARPES as an experimental method

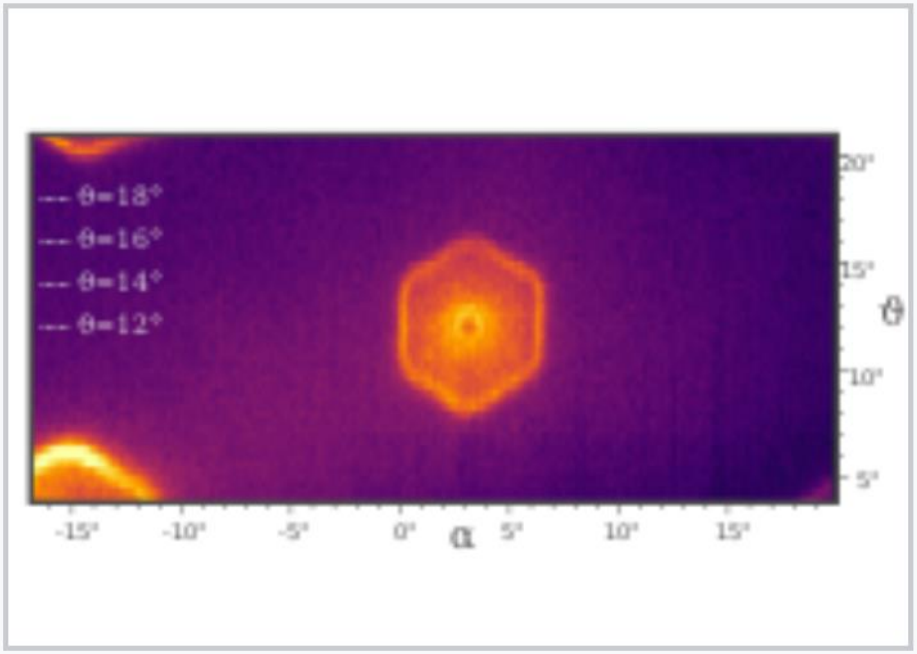


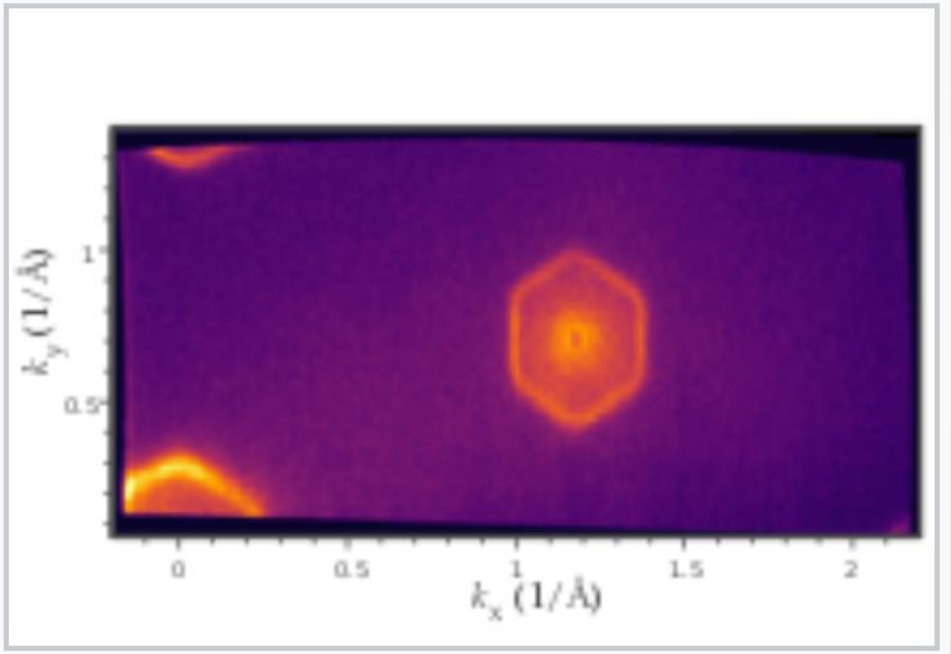
Electron analyzer



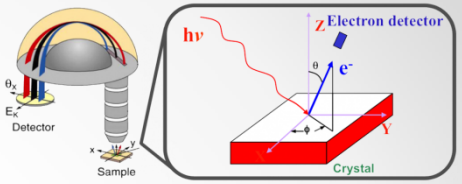
Applications

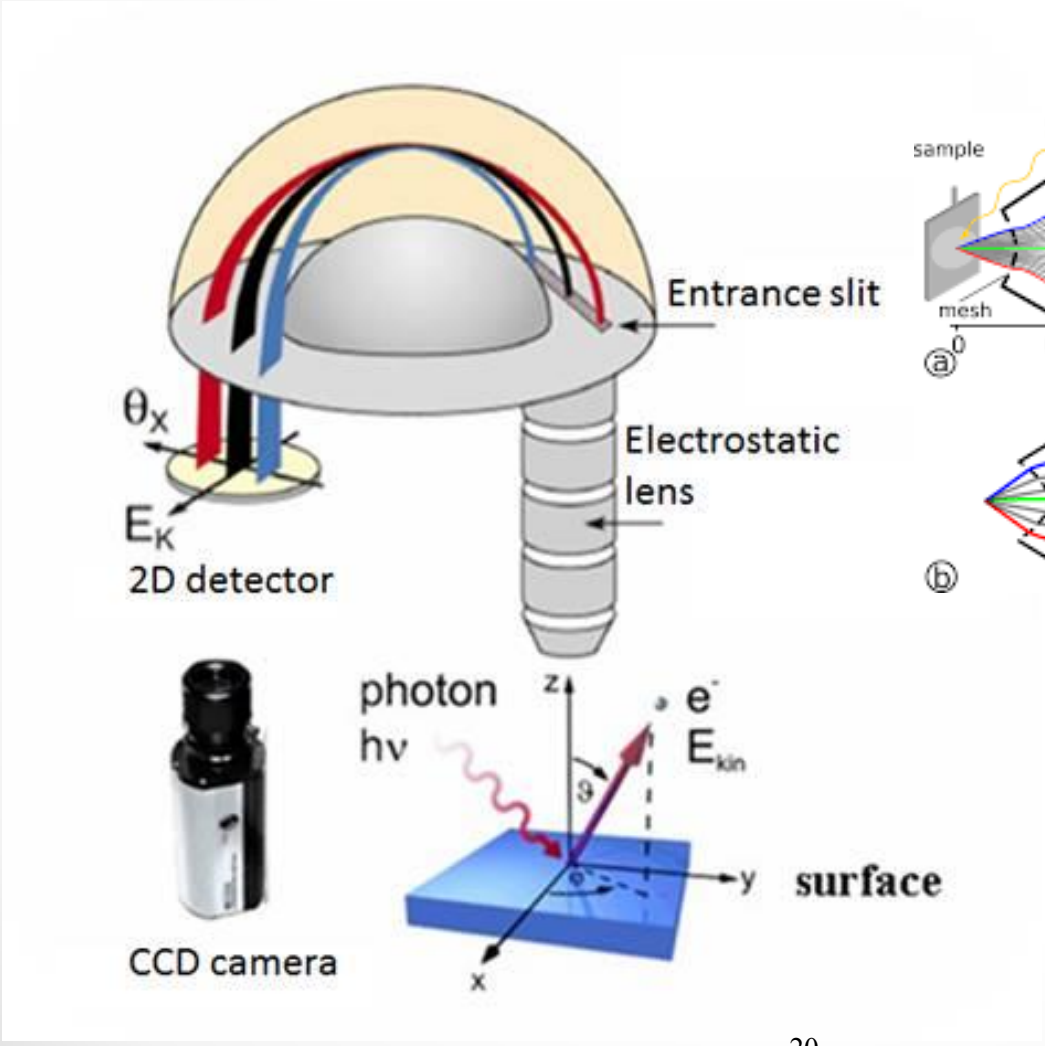


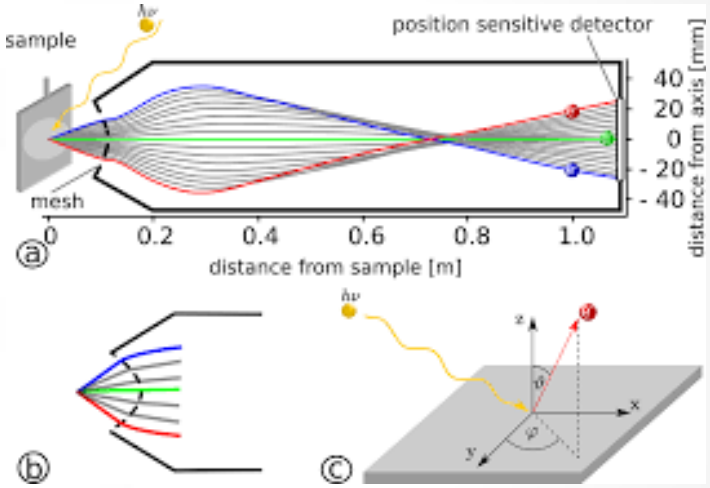




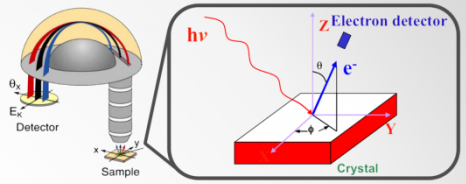
ARPES as an experimental method







ARPES as an experimental method



acceptance angle

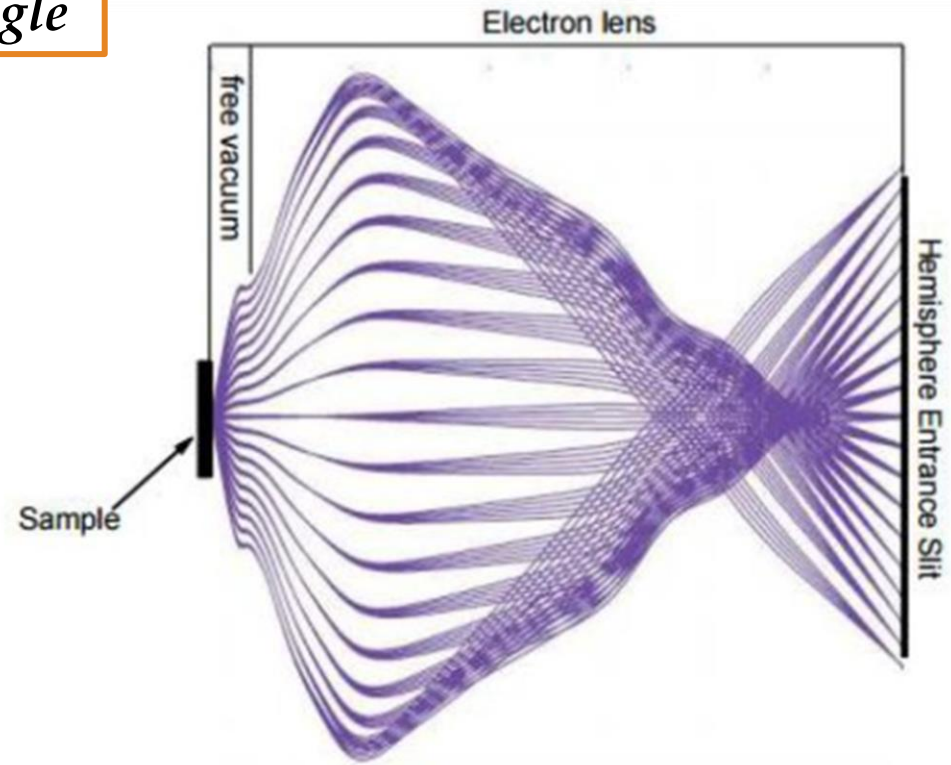
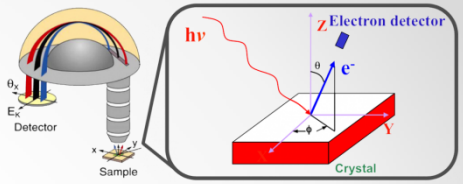
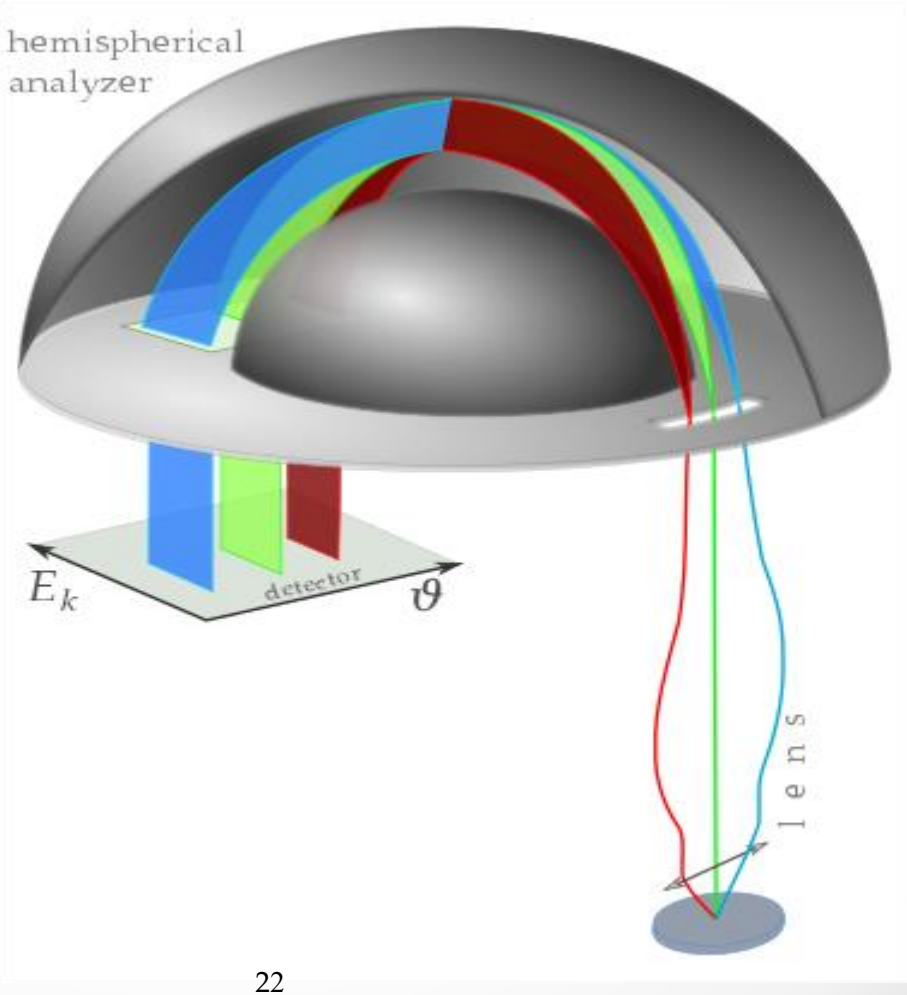


Image from VG Scienta and PhD Thesis of Dr. Ari Deibert Palczewski
(http://lib.dr.iastate.edu/cgi/viewcontent.cgi?article=2629&context=etd)

ARPES as an experimental method



Pass energy-E_p



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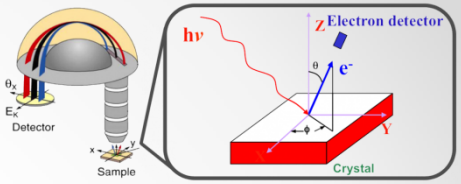
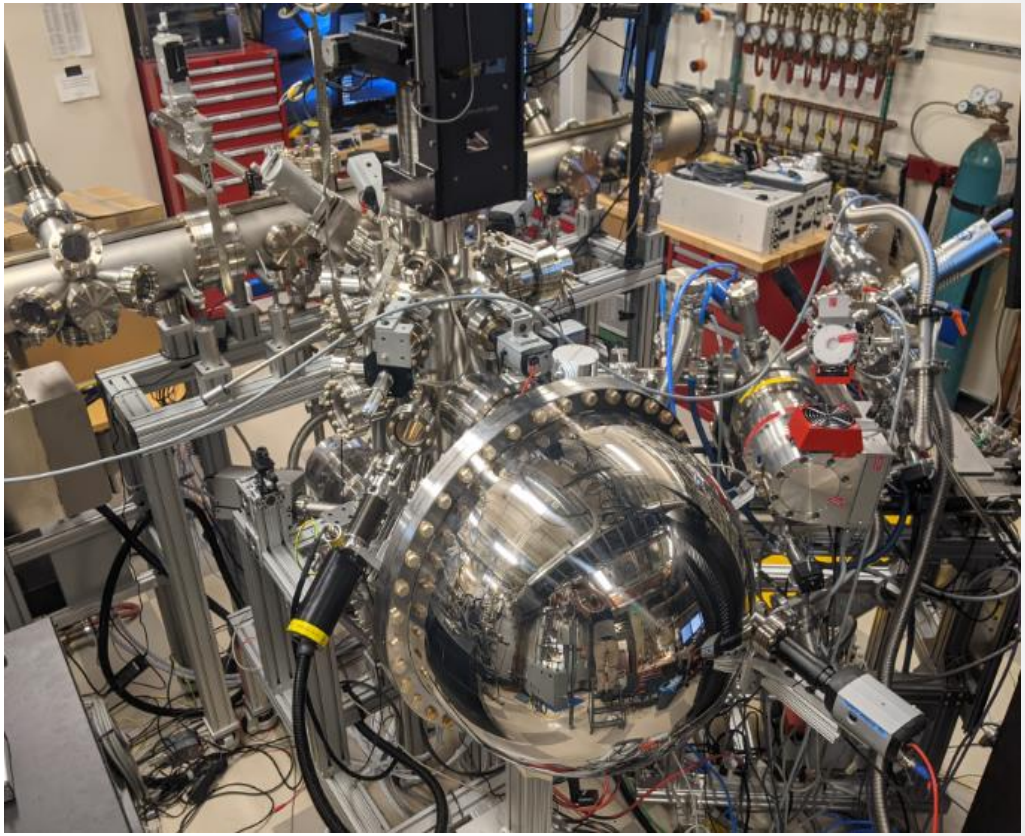


Energy resolution

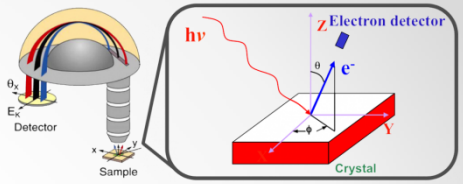
$$\Delta E = \frac{E_p S}{D}$$

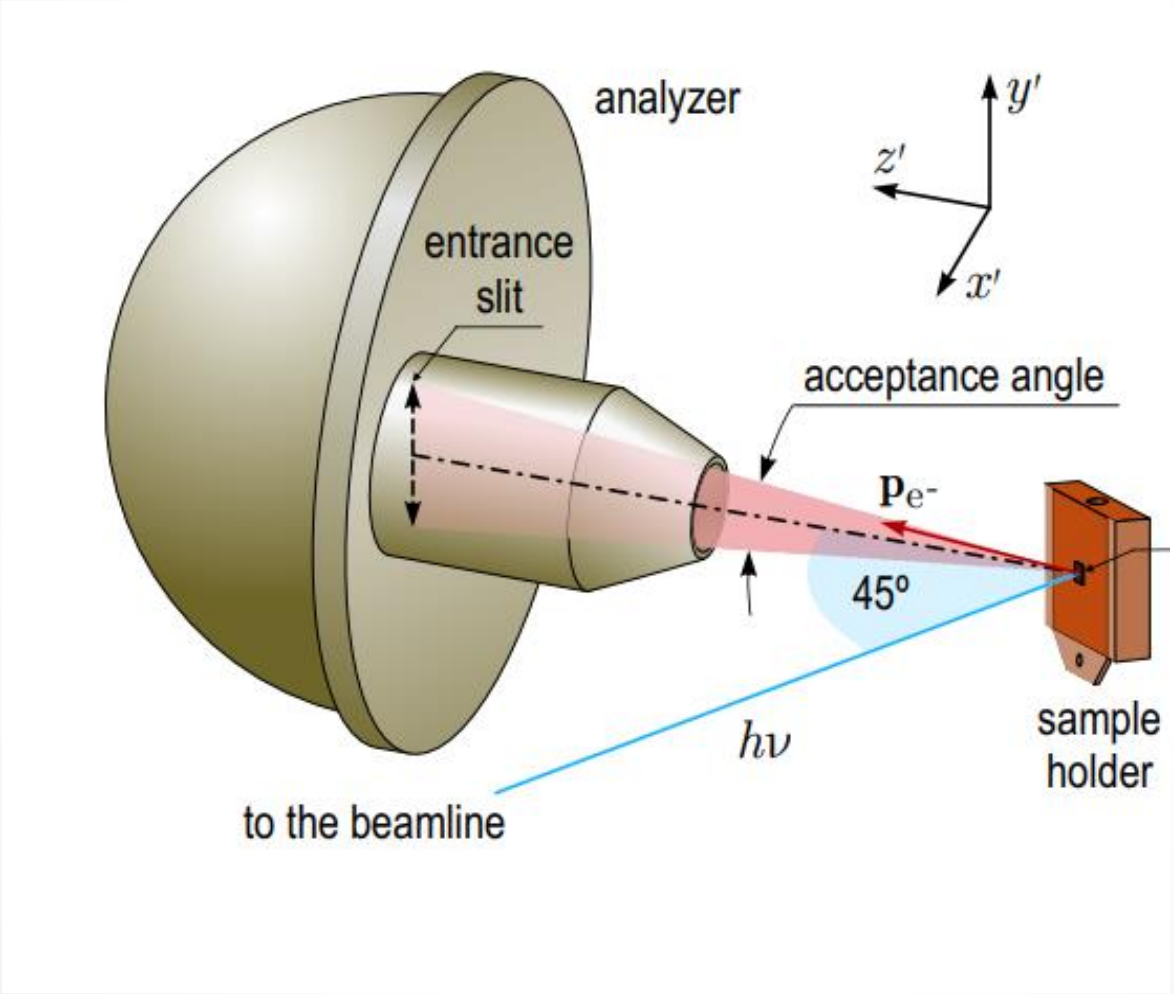
D *: mean diameter of the analyzer*



The resolving power of the analyzer → $R = \frac{E}{\Delta E} = \frac{D}{S}$

ARPES as an experimental method





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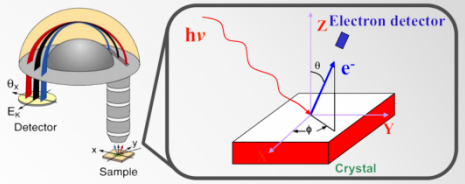
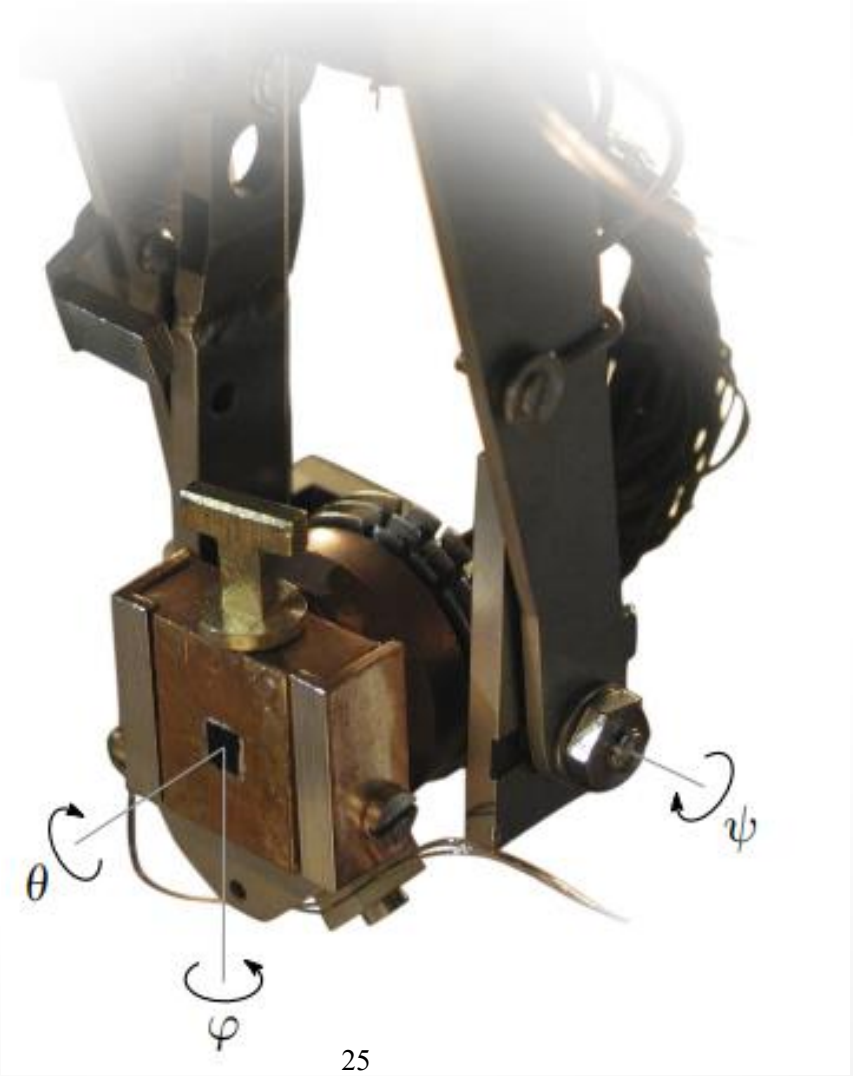
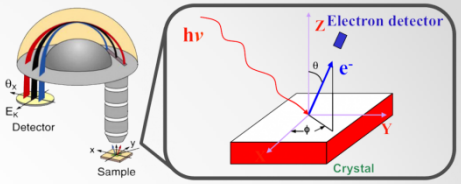


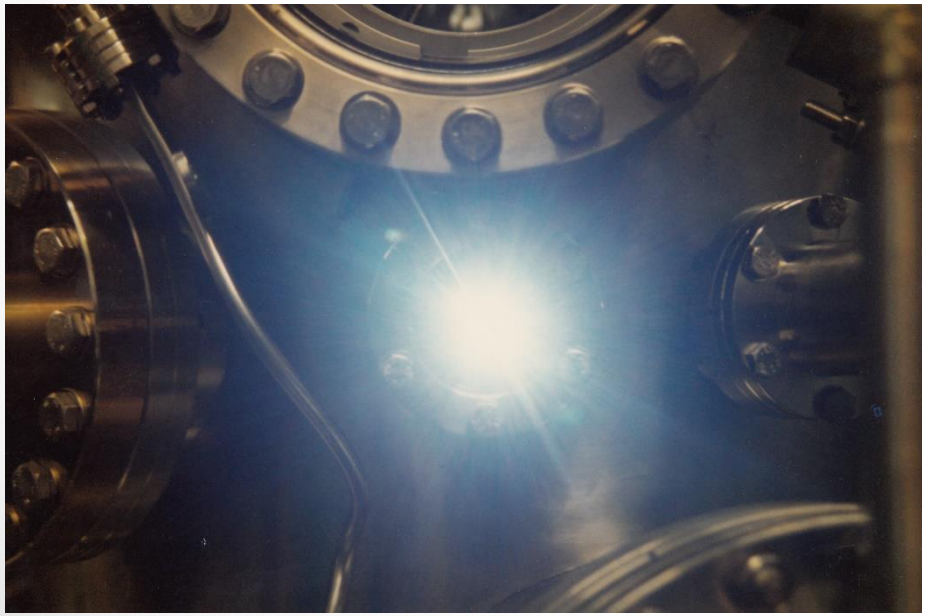
sample holder



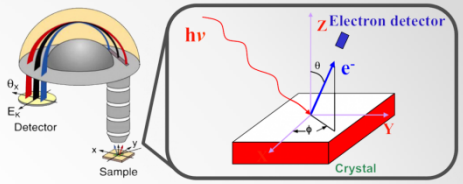
ARPES as an experimental method



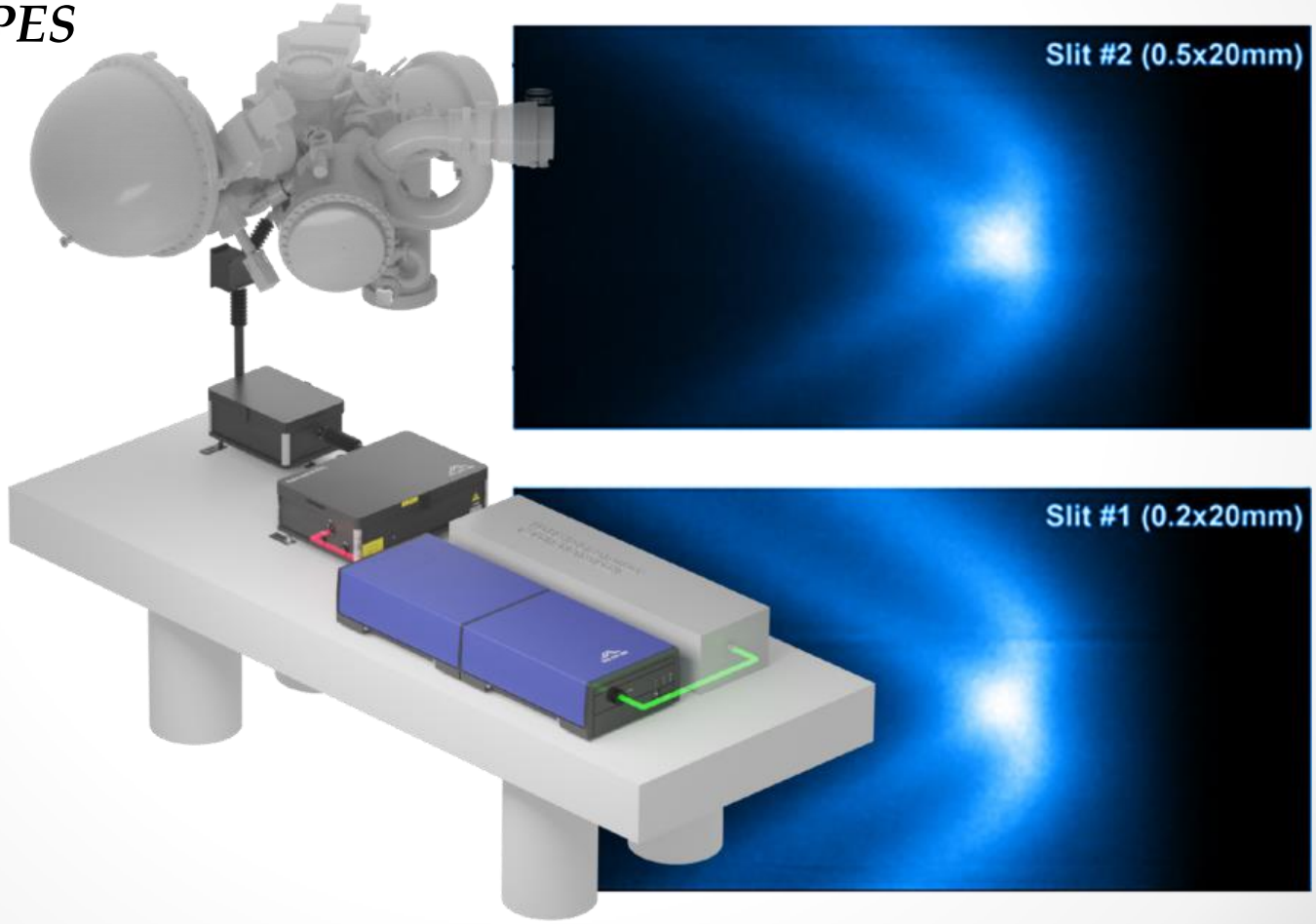
Synchrotron light sources



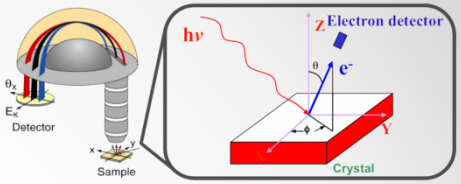
ARPES as an experimental method



- *Laser-ARPES*



ARPES as an experimental method



- ***Laser-ARPES***
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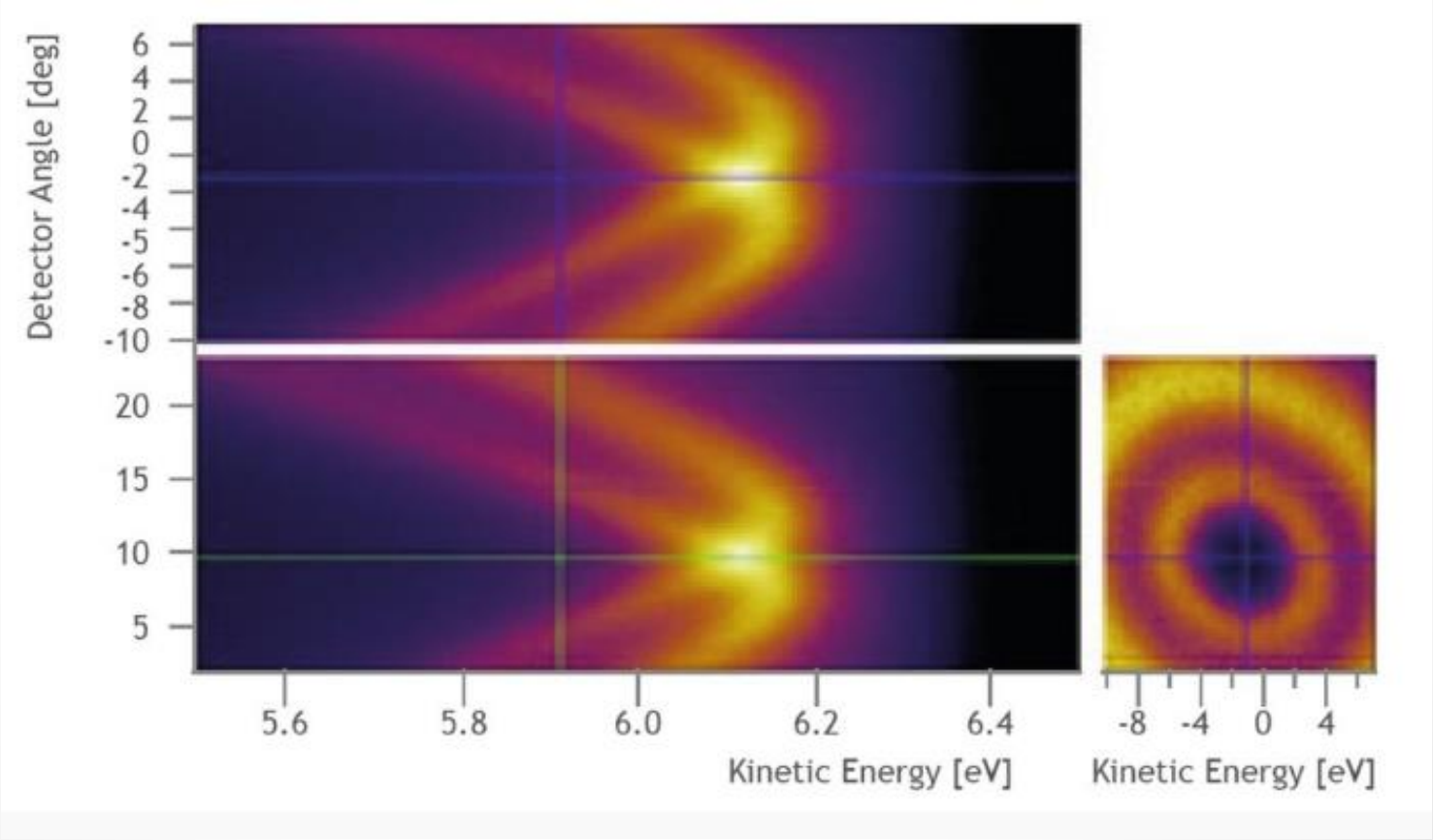
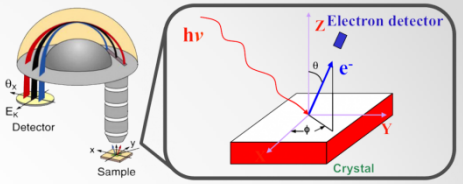


ARPES as an experimental method



ARPES برای نقشه برداری در موارد زیر استفاده میشود:

ساختار پیوند های اشغال شده بسیاری فلزات و نیمه رسانا ها.

حالت های آشکار شده در گپ های پیوندی تصویر شده .

حالت های چاه پتانسیل که در سیستم با کاهش ابعاد برانگیخته میشوند.

مواد با قطر یک اتم مانند گرافن.

ساختار های پیوندی زیرساخت.

گپ ها.

دینامیک شبه ذرات بسیار همبسته مانند ابررسانا های دمای بالا.

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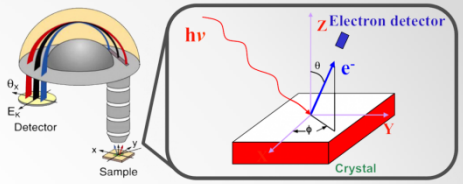

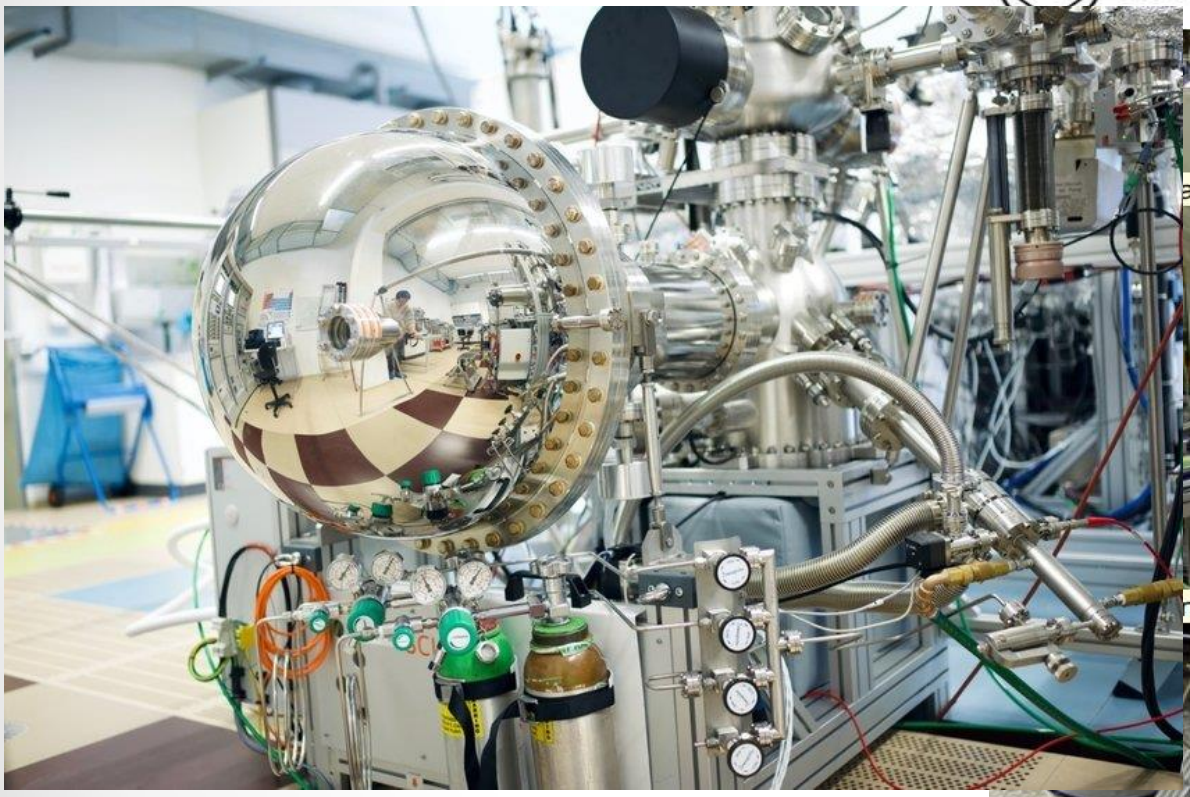

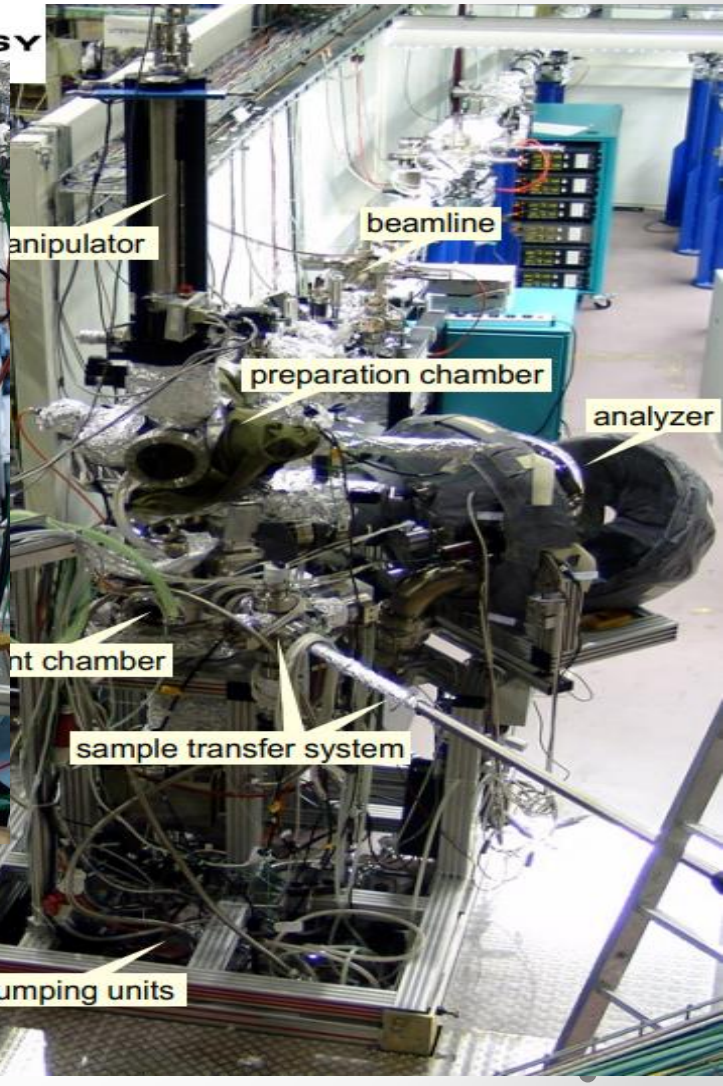

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