

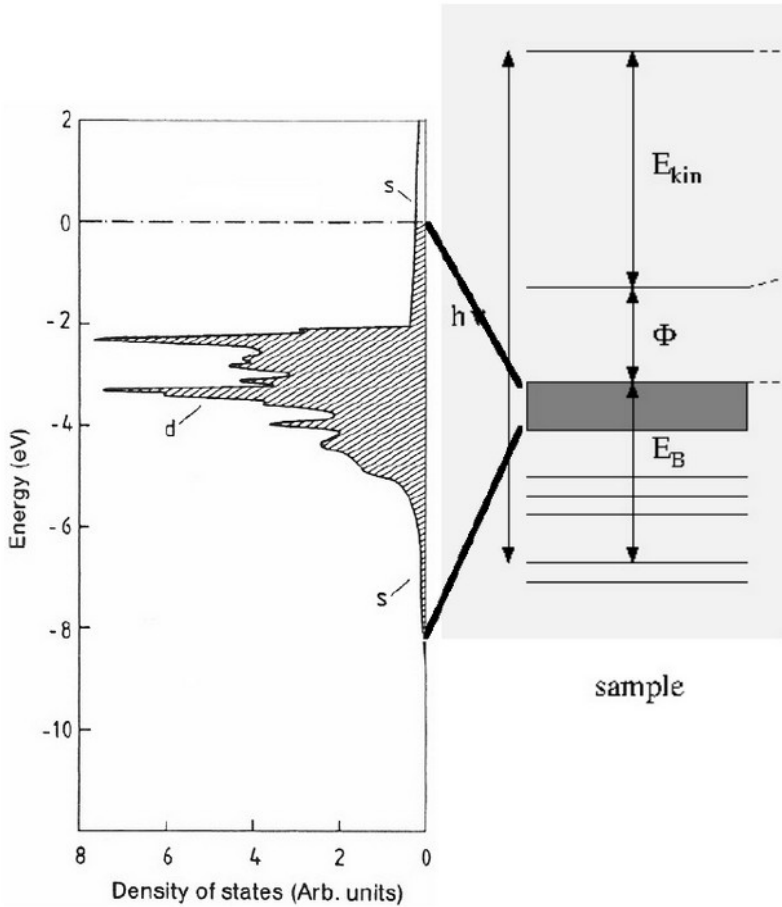
# M<sup>3</sup>ETA

An extensible *Meta*data scheme for advanced *M*omentum *M*icroscopy in the age of big data

04.04.2023 | CHRISTIAN TUSCHE, CHRISTOPH SCHLUETER, MORITZ HOESCH



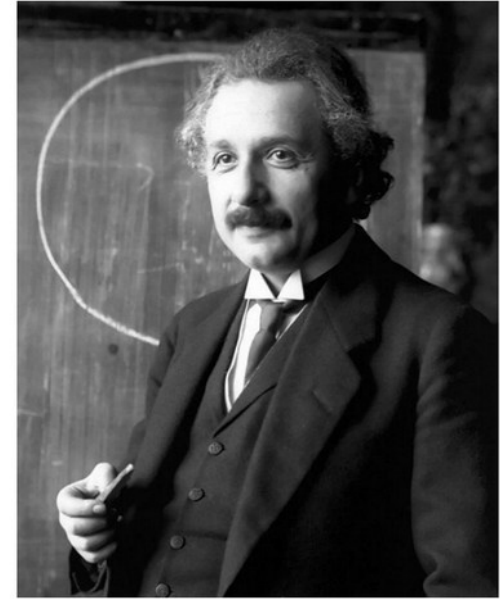
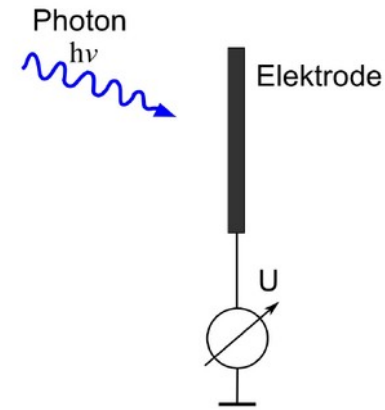
# THE PHOTOEFFECT



6. Über einen  
die Erzeugung und Verwandlung des Lichtes  
betreffenden heuristischen Gesichtspunkt;  
von A. Einstein.

Ann. Phys. 322: 132–148 (1905)

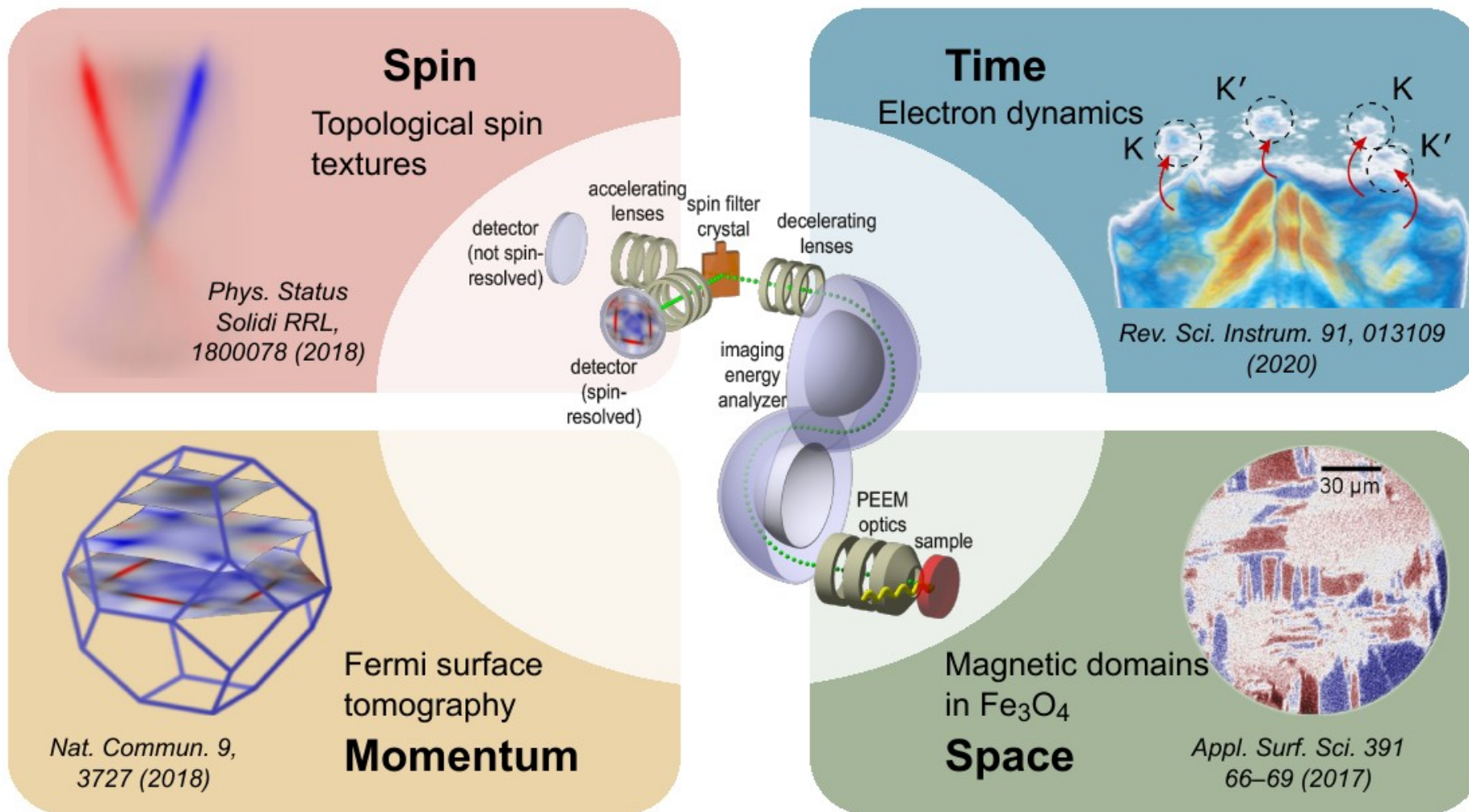
$$e \cdot U = h \cdot \nu - \Phi$$



**Albert Einstein**

- Nobelprize in physics 1921
- Explanation of the photoeffect

# THE “ALL-IN-ONE” PHOTOEMISSION EXPERIMENT



# TYPICAL REPRESENTATION OF PHOTOEMISSION DATA

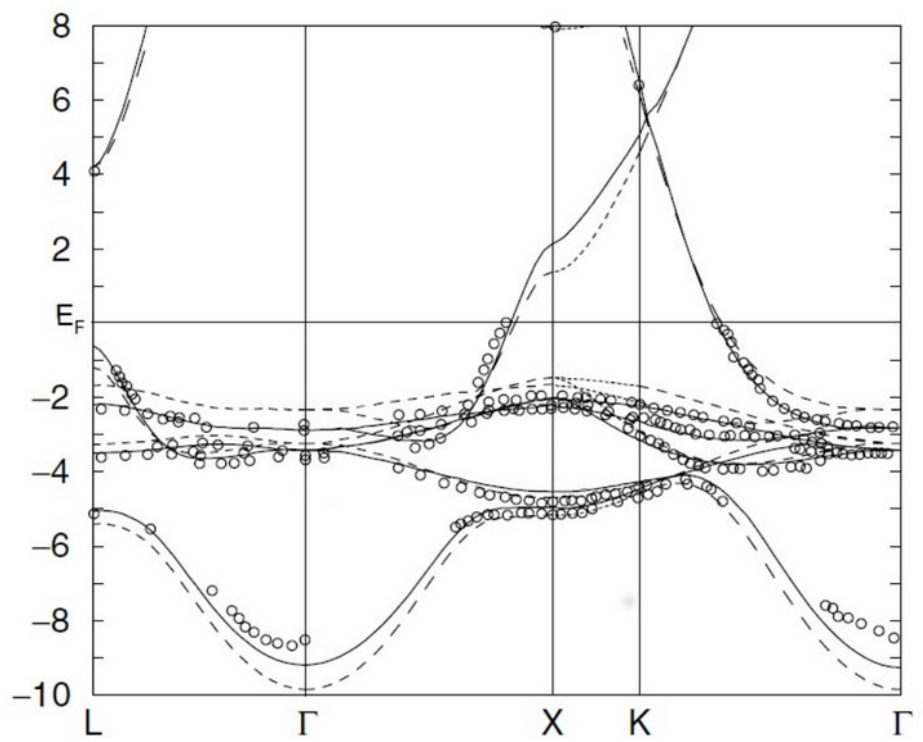
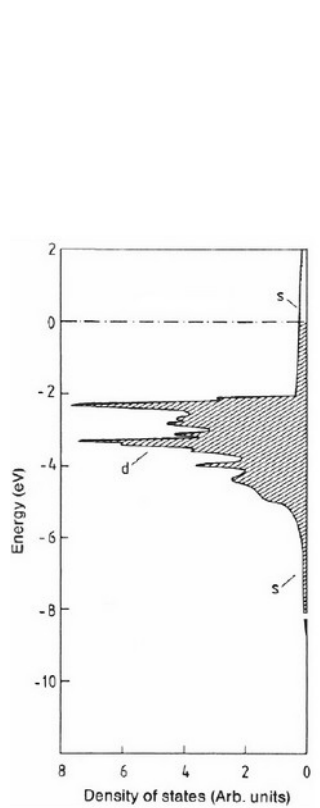
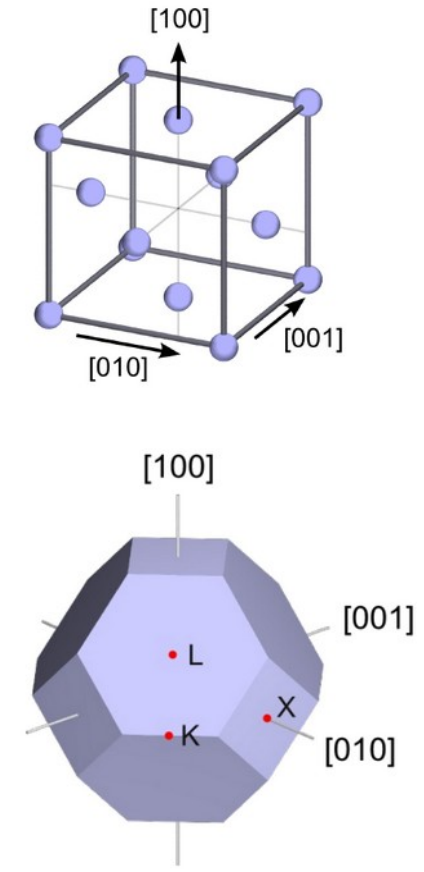
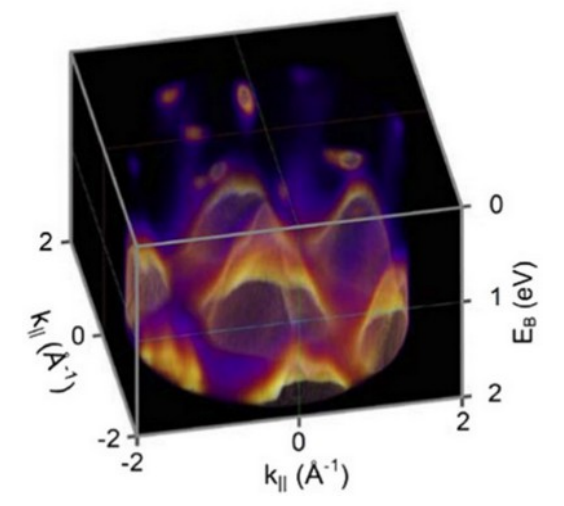


FIG. 2. Solid line: present GW results for the bulk copper band structure, compared with the DFT-LDA results (dashed line), and with the experimental data reported in Ref. [16] (circles).



More recently:  
Data cubes in three dimensions

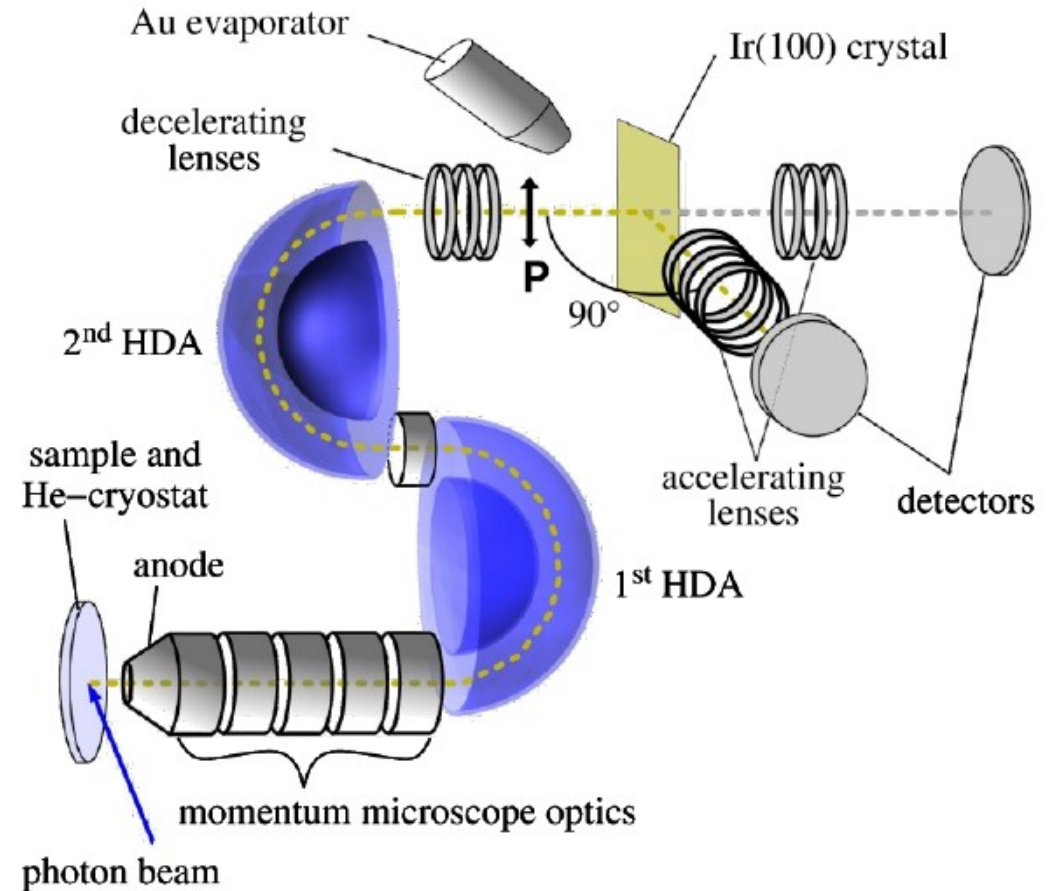
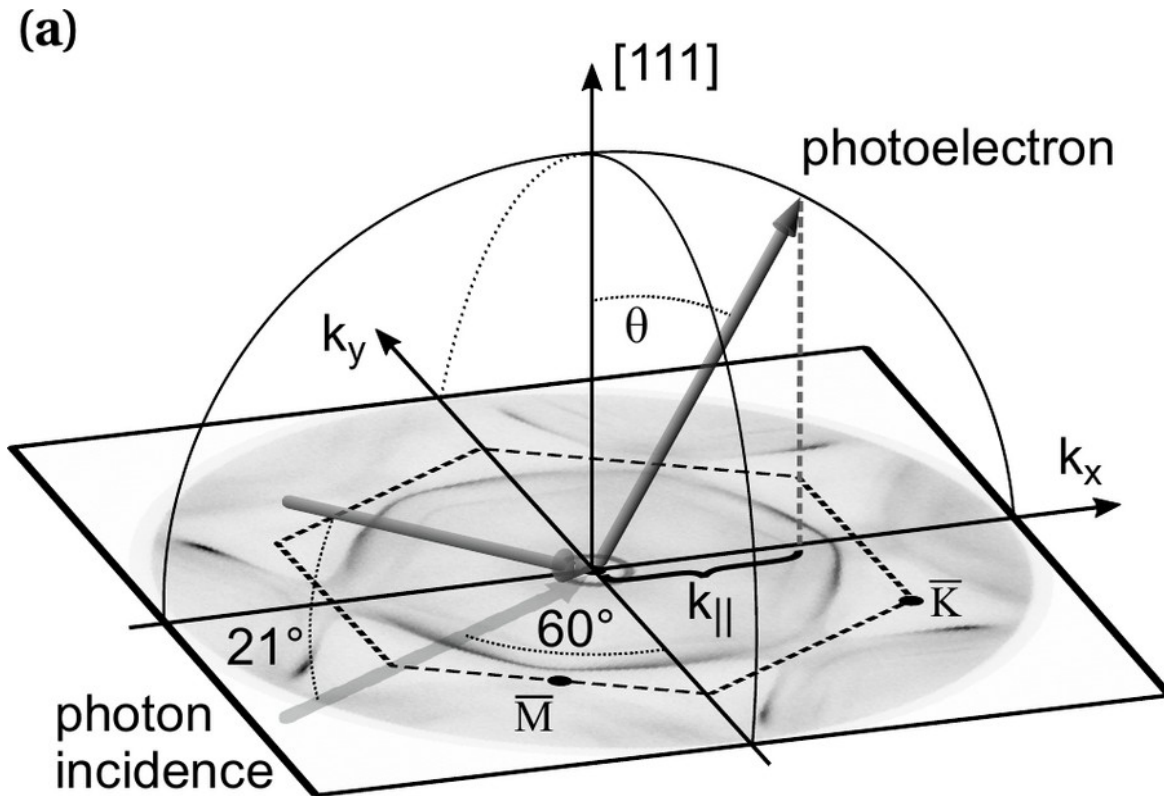


*New J. Phys.* 17 (2015) 083010

Andrea Marini, Giovanni Onida, and Rodolfo Del Sole: *Phys. Rev. Lett.* 88 (2002)



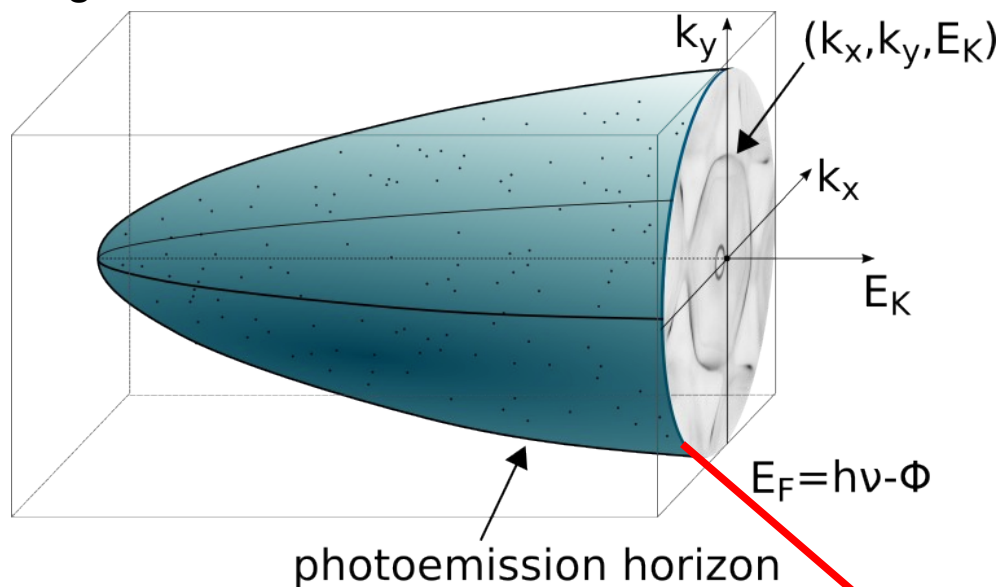
# A SIMPLE MOMENTUM MICROSCOPY EXPERIMENT



Suga / Sekiyama / Tusche, Photoelectron Spectroscopy 2<sup>nd</sup> ed., Springer (2021)

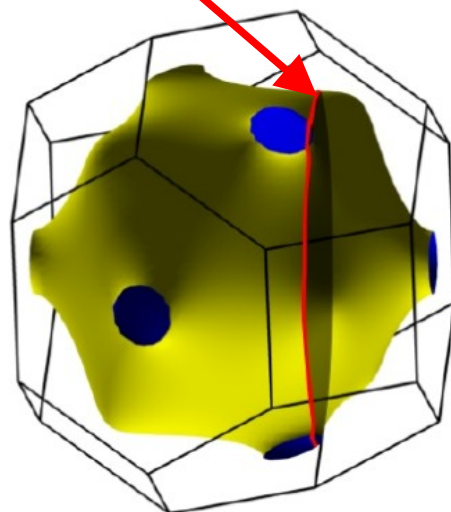
# METADATA IN PHOTOEMISSION

“regular” Photoemission data in a 3D cube

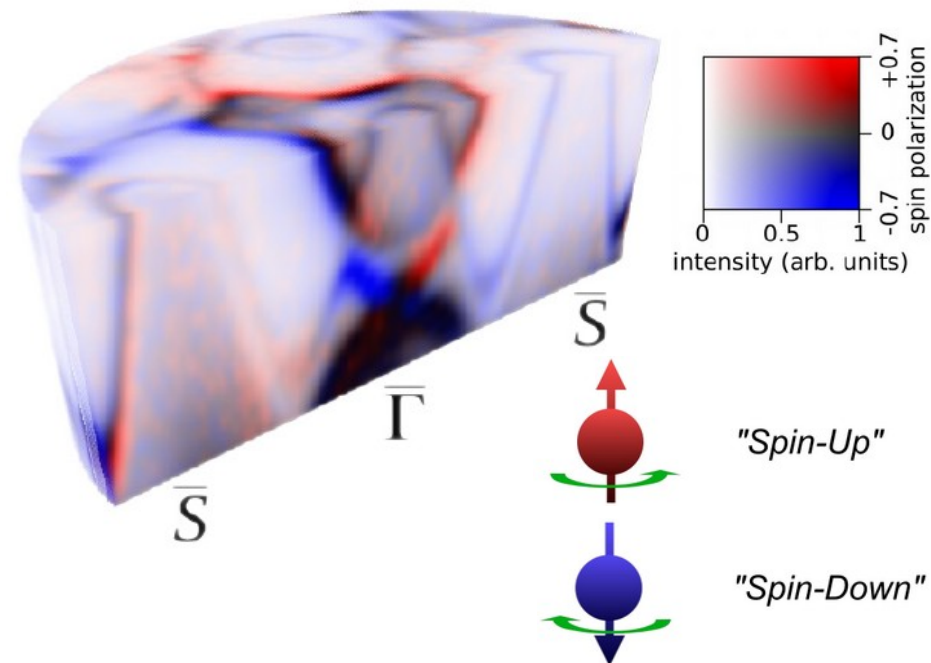


**Fermi surface**

→  $I(k_x, k_y, k_z, E_B)$   
Photoemission  
Intensities in 4D



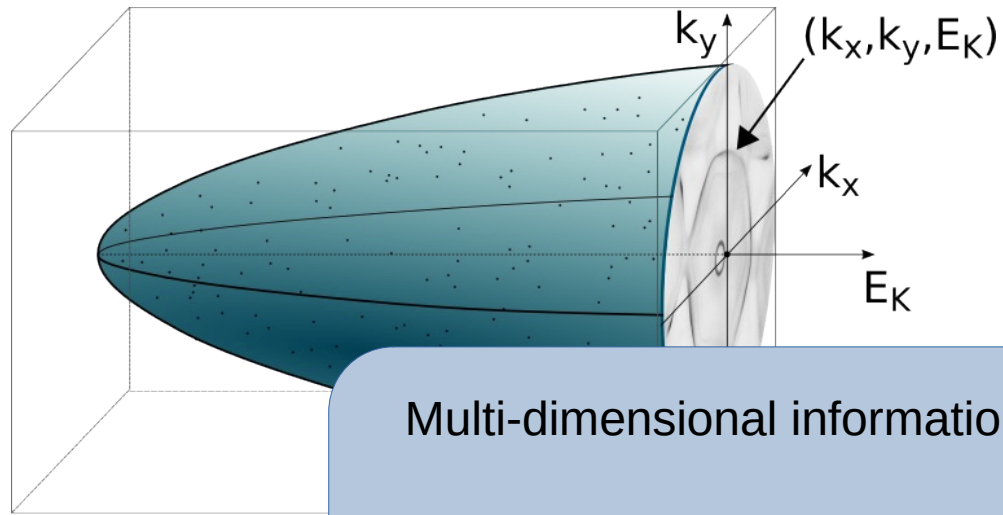
... including the Electron Spin  
→ a 5D data set



Y.-J. Chen, M. Hoffmann, B. Zimmermann, G. Bihlmayer,  
S. Blügel, C. M. Schneider, C. Tusche,  
*Nature Commun. Physics* 4, 179 (2021)

# METADATA IN PHOTOEMISSION

“regular” Photoemission data in a 3D cube



... including the Electron Spin  
→ a 5D data set



Multi-dimensional information  $I(k_x, k_y, k_z, E, S, \hbar\nu, \sigma, \tau)$

*Particular important at large scale facilities  
Synchrotron, free-electron-laser, etc.*

**8D data sets: *Need for a standardized and structured metadata description***

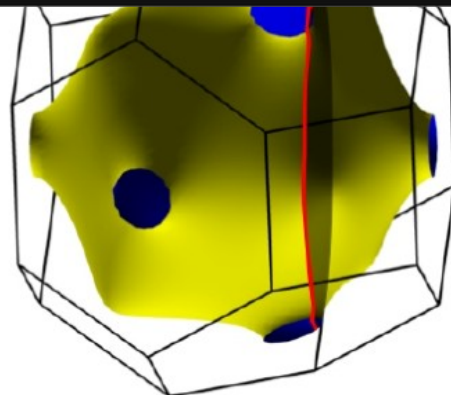
pl

Spin-Up"

Spin-Down"

Fermi surface

→  $I(k_x, k_y, k_z, E_B)$   
Photoemission  
Intensities in 4D



Y.-J. Chen, M. Hoffmann, B. Zimmermann, G. Bihlmayer,  
S. Blügel, C. M. Schneider, C. Tusche,  
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# STRUCTURED METADATA FORMAT

## NeXus

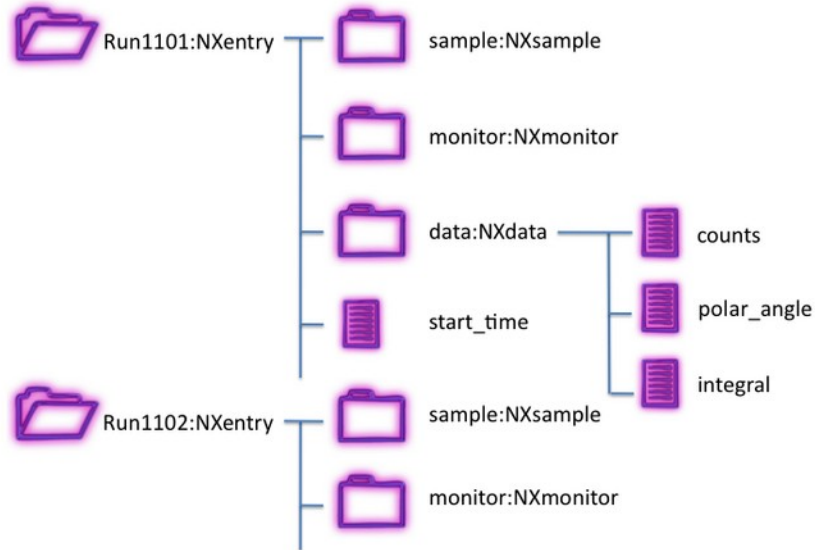


figure from <https://www.nexusformat.org>

NeXus files (hdf5) contain *fields* and *groups*.

Tree structure of hdf5 and the availability of symbolic links in the hdf5 files.

**Design principles of NeXus include structuring data and metadata into one or several NXentry groups.**

## NeXus format as a basis for structured data description

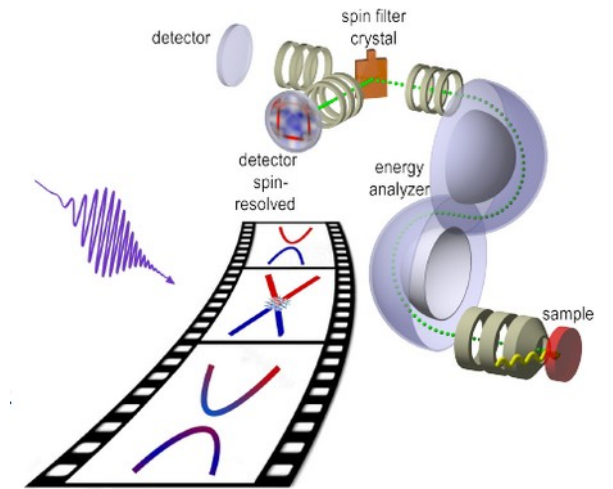
- Example: *Nxarpes*
  - Application definition for angular resolved photoelectron spectroscopy
  - It has been drawn up with hemispherical electron analysers in mind
- **NeXus format for momentum microscopy**
  - Physical description of different dimensions
  - Applicable to different experiments
  - Link to reference data → analysis, procedures



# SUMMARY

## Main Goals of M<sup>3</sup>eta

- Development of a ***unified metadata scheme for all momentum microscopy experiments***
- ***Physical description*** of different experimental dimensions
- Implementation of ***data writers*** and ***validity testers***
- A common meta data description opens the way to ***automated work flows for analysis and visualization***



***Ultrafast time-resolved  
Momentum Microscopy***