



# Data processing: a concrete example from NanoESCA endstation @ ELI-ALPS

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# NanoESCA - Google

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**Nanoesca** Musical artist

<https://scientaomicron.com/electron-spectroscopy/NanoESCA>

**NanoESCA - Scienta Omicron**

NanoESCA is an energy-filtering photoemission microscope that can easily switch between the imaging of the momentum space and the real space of ...

[Key Facts](#) · [More Information](#) · [Specifications](#) · [Results](#)



<http://www.bristol.ac.uk/physics/facilities/nanoesca>

**Bristol NanoESCA Laboratory | School of Physics**

The Bristol NanoESCA Facility is the newest and one of the most advanced surface analysis instruments in UK. The NanoESCA II offers extraordinary surface ...



<https://www.fkf.mpg.de/Techniques/Equipment>

**NanoESCA (Electron Spectroscopy for Chemical Analysis)**

Determines quantitatively the chemical composition, the atomic structure, and the electronic structure of surfaces and interfaces on  $\mu\text{m}$  and nm scales.



<https://www.focus-gmbh.com/PEEM%20%2f%20NanoESCA>

**NanoESCA - FOCUS GmbH**

The NanoESCA is a sophisticated analytical instrument designed for imaging and small spot photoemission spectroscopy as well as  $\mu$ -ARUPS.

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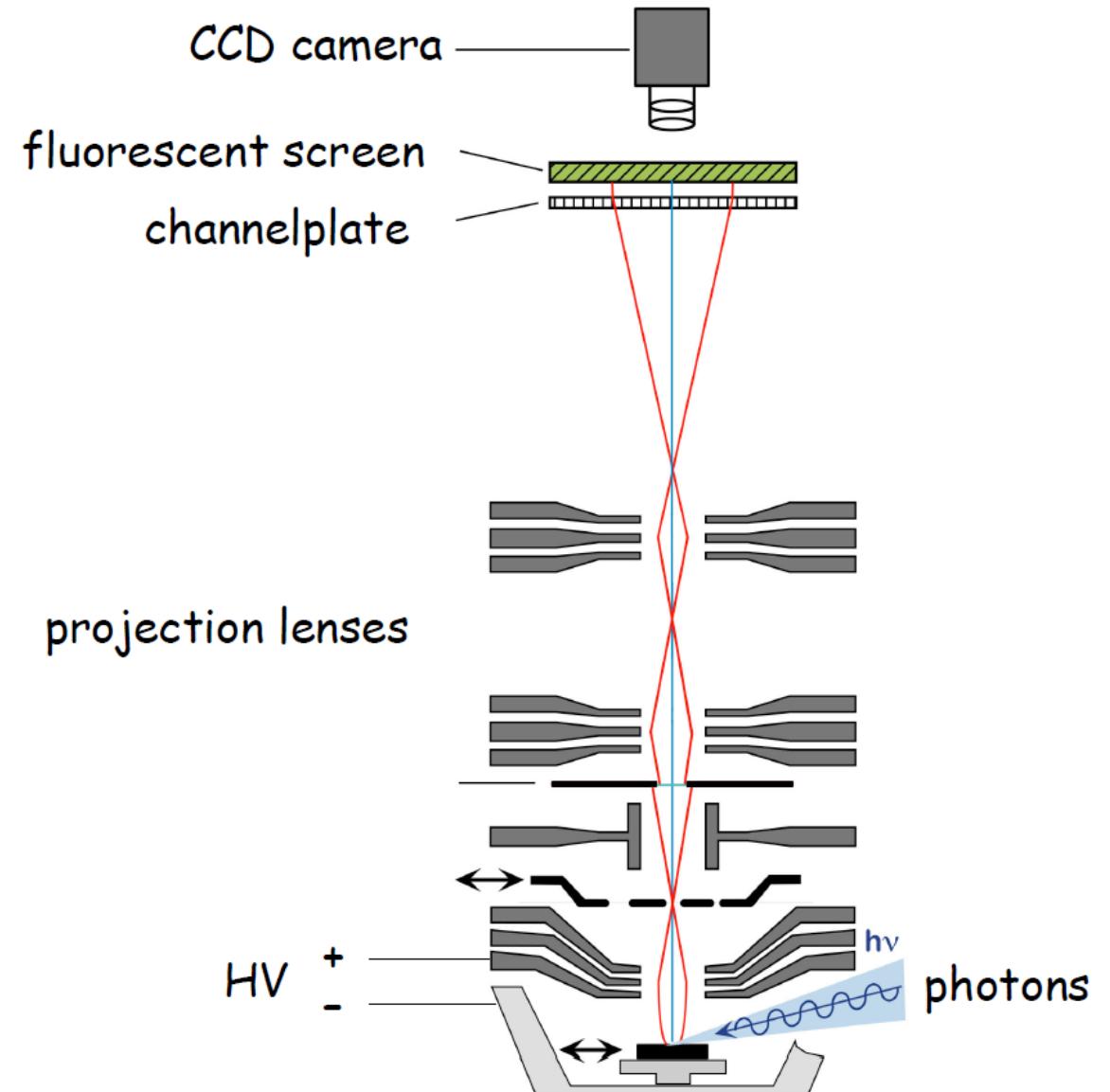
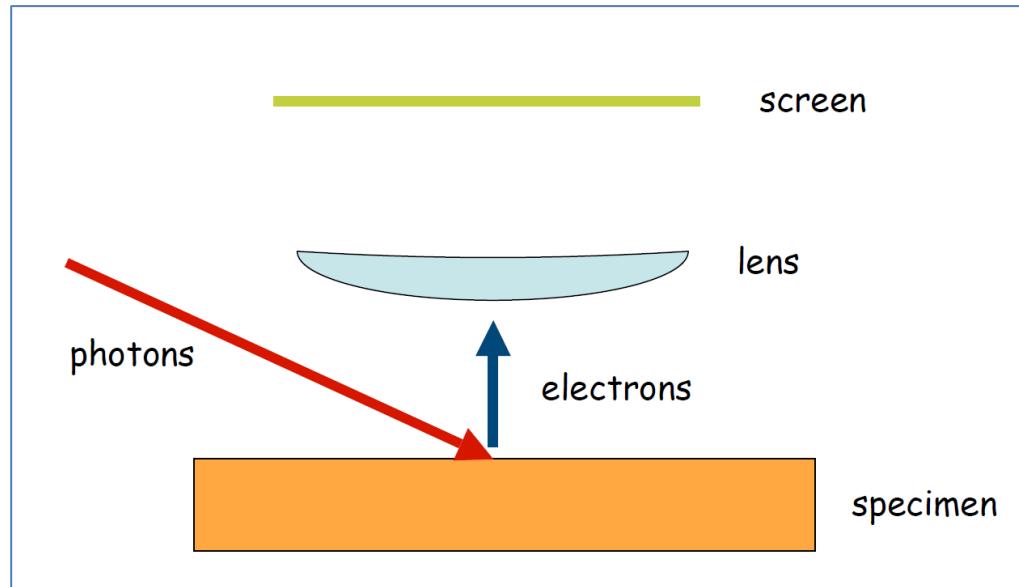
Last Time That I Checked  
Dedication · 2022

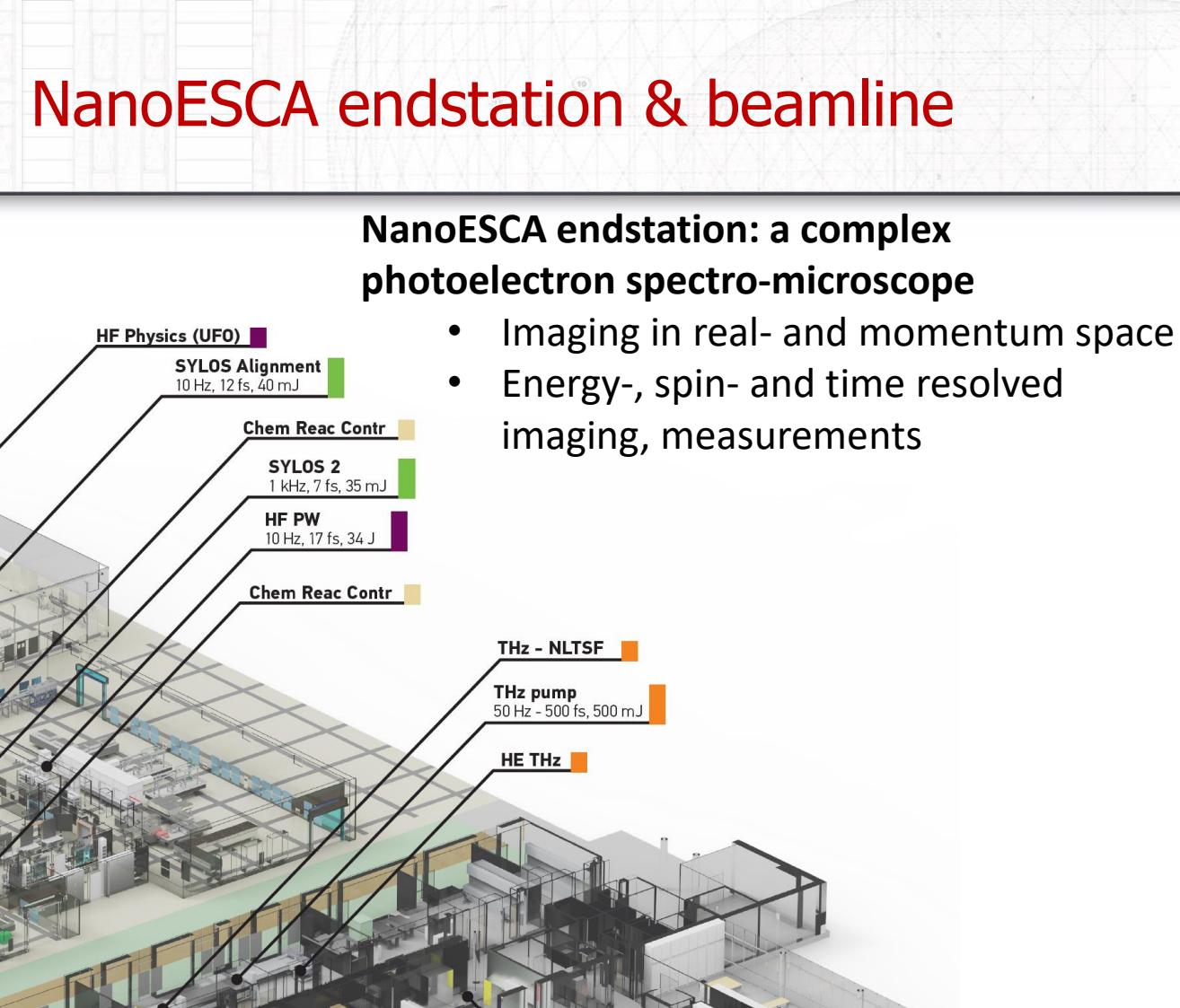
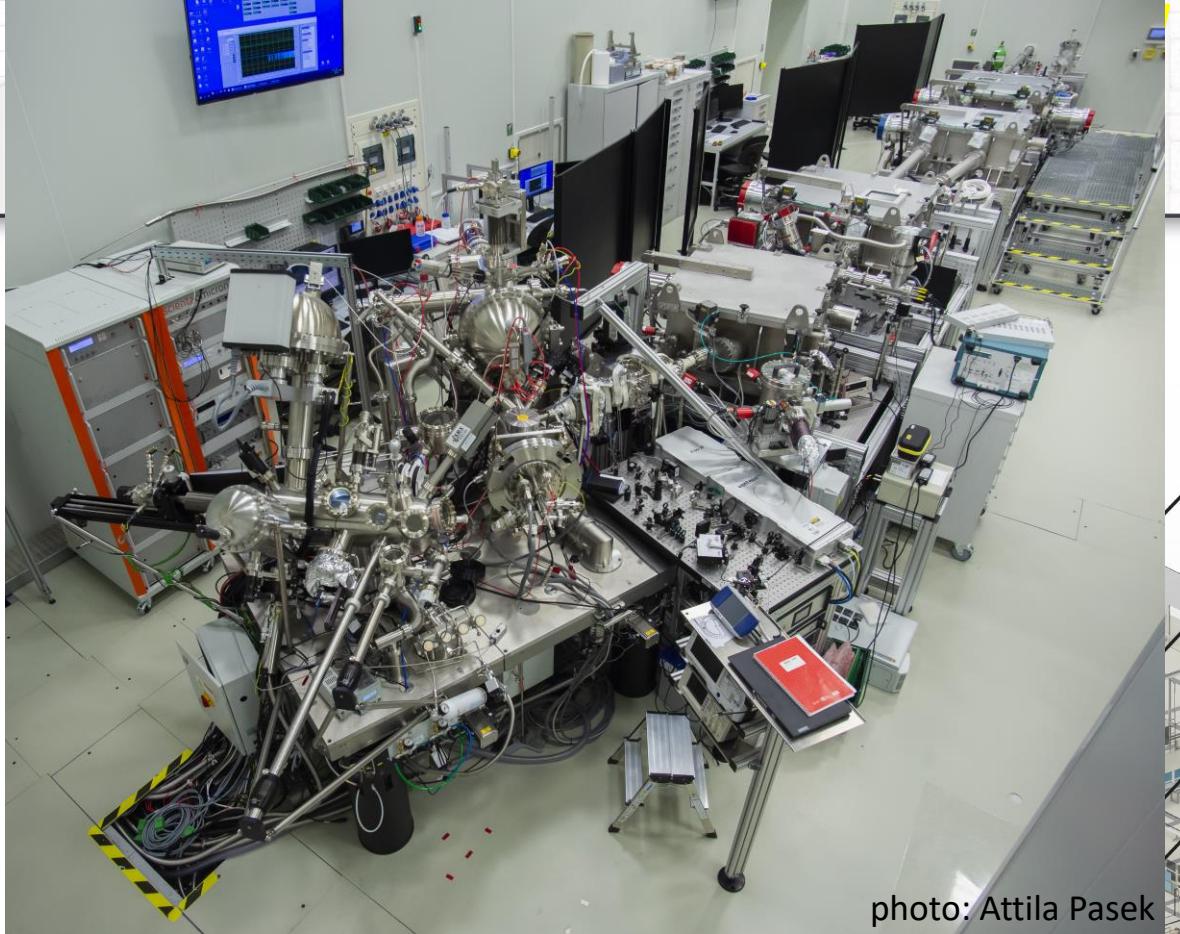
Stop Playing  
Normandie Park · 2020

Right Now  
Pick Up Game · 2019

Gimme the Look  
Gimme the Look · 2021

# Photoemission electron microscope - PEEM





IR Pump (HR1 laser)		XUV source - probe			Venteon oscillator
Wavelength	1030 nm (1.2 eV)	Spectral range of GHHG (with monochromatized option)	17-30 eV (Xe, Kr)	25-55 eV (Ar)	70-90 eV (Ne)
Repetition rate	100 kHz	Pulse energy at end station for attosecond pulse trains	15-50 pJ	5-25 pJ	3-10 pJ
Average power	100 W	Pulse energy at end station for isolated attosecond pulses	5-15 pJ	3-8 pJ	1-3 pJ
Pulse energy	>1 mJ				~2.5 nJ
Pulse duration	6.2 fs				<6 fs (CEP stabilized)

# NanoESCA end-station

## Preparation chamber sample cleaning, preparation, and characterization

### Cleaning:

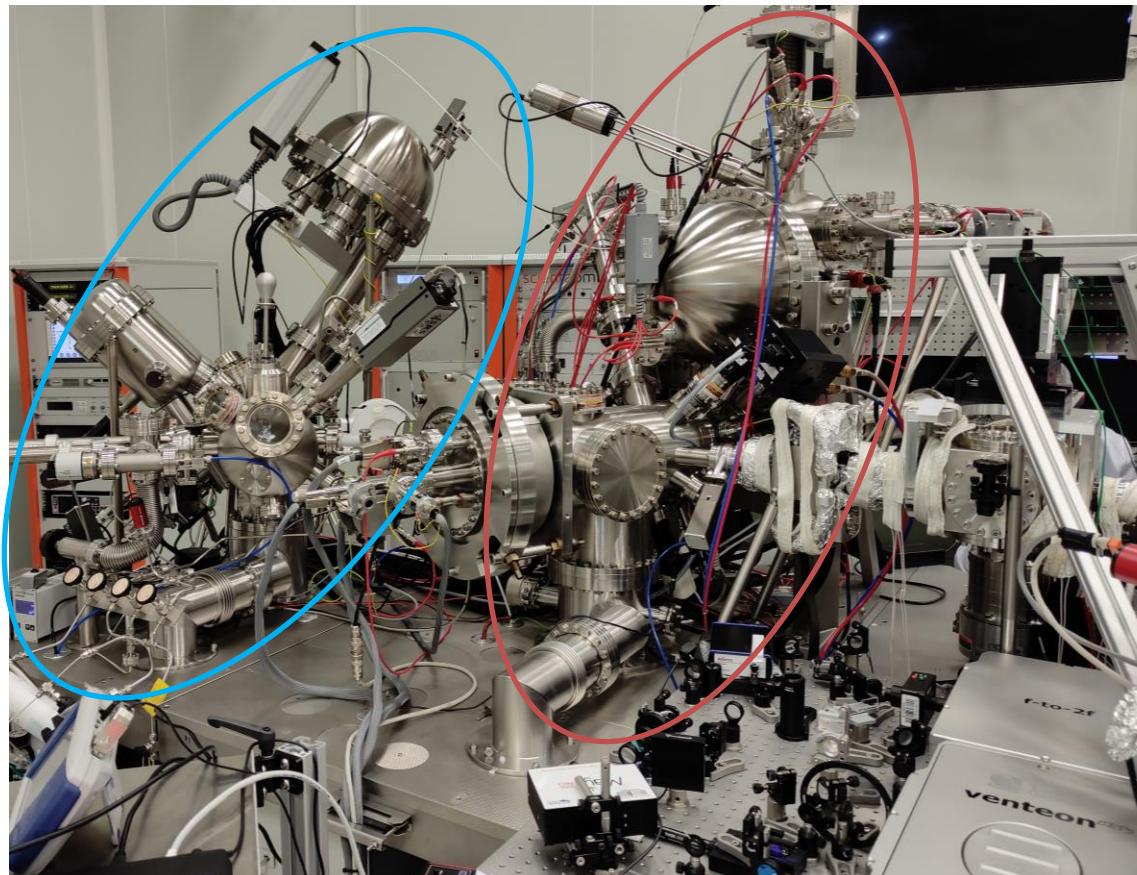
- Ar<sup>+</sup> ion sputtering
- Annealing (heat- and coolable manipulator)

### Preparation:

- **e-beam evaporator** for metal deposition
- **gas dozer** based on a capillary array
- **magnetizer**
  - Helmholtz coil
  - B field: up to 43 mT

### Characterization (laterally averaged):

- **LEED** (Low Energy Electron Diffraction): determination of surface structure
- **AES** (Auger Electron Spectroscopy): determination of surface composition
- **XPS** (X-ray photoelectron spectroscopy):
  - **quantitative chemical analysis of the surface** (top few nm)
  - monochromatic Al K<sub>α</sub> X-ray source
  - 128 detection channels
- **RGA** (Residual Gas Analyzer) by quadrupole mass spectrometer



## Analysis chamber NanoESCA – nano- Electron Spectroscopy for Chemical Analysis

### Modes (outputs):

**PEEM:** Photoemission electron microscope

**ToF-PEEM:** Time of flight + DLD analyzer (delay line detector)

**Spectroscopy for selected area:** Channeltron detector after first hemisphere

**IDEA:** Imaging with dispersive energy analyzer

**Imaging spin filter:** IDEA + spin selective mirror: gold coated Ir(100) crystal

### Light sources:

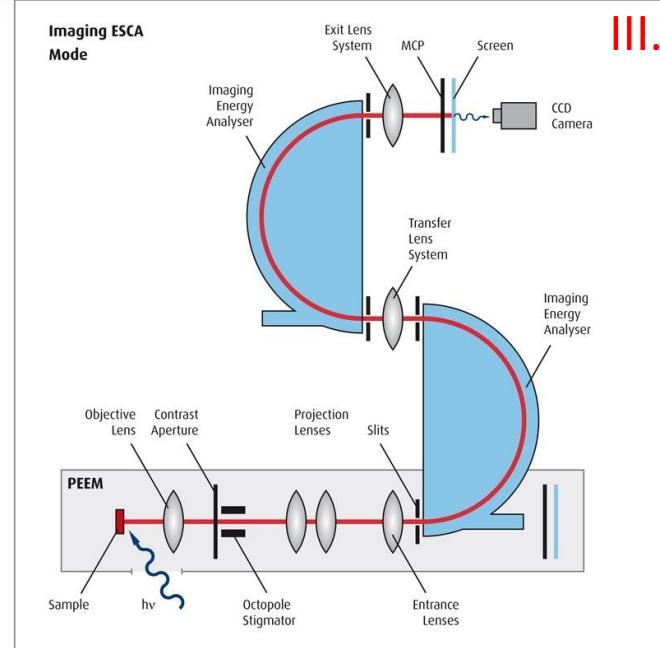
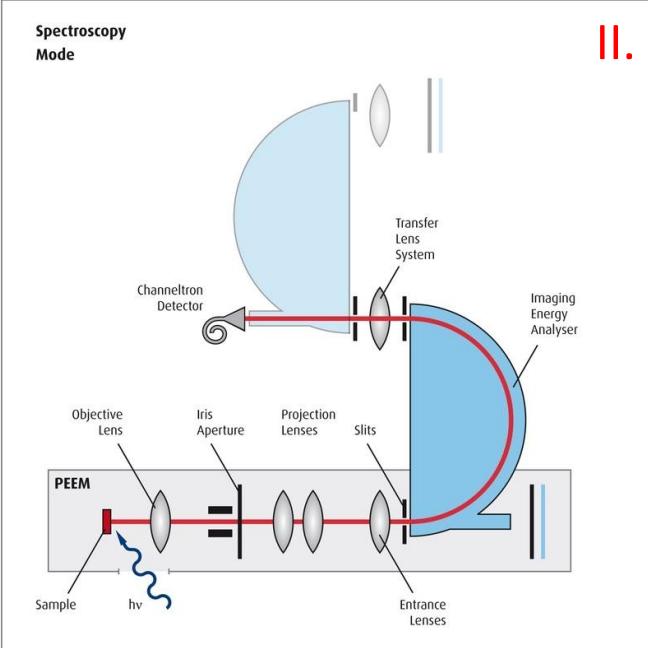
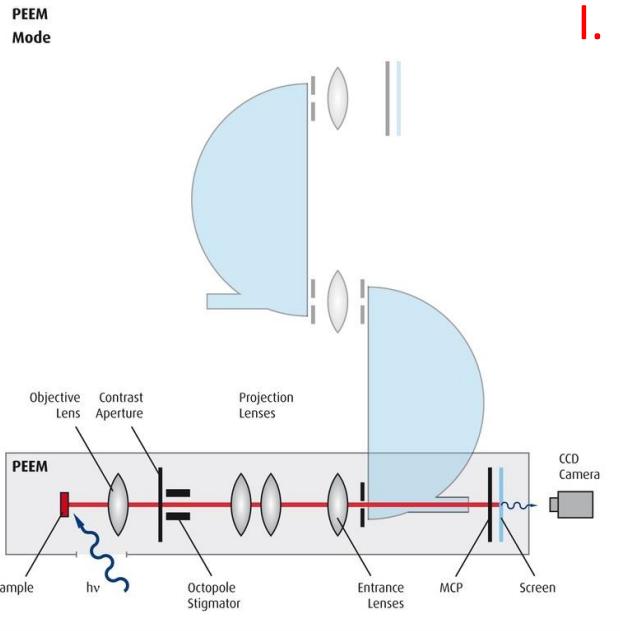
#### **Internal (CW) sources:**

- Hg arc lamp (5.2 eV – 238 nm)
- He discharge lamp
  - HeI: 21.22 eV – 58 nm
  - HeII: 40.81 eV – 30 nm

#### **Short pulsed** sources:

- pump: HR laser fundamental (1.2 eV – 1030 nm)
- probe: GHH generated XUV (20-90 eV – 62-13.8 nm) (BeamLine condensed)
- Venteon CEP5 oscillator (1.5 eV – 830 nm)

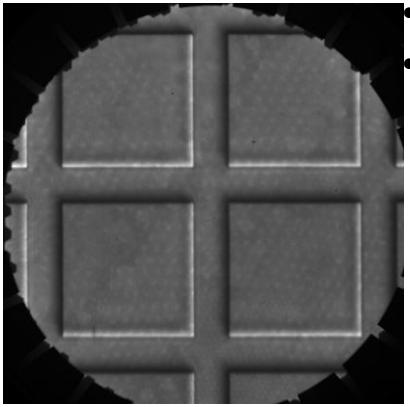
# Operating modes I-III. & provided data of NanoESCA



**I. PEEM (Photoemission electron microscope) - imaging WITHOUT energy filtering:**

Outputs:

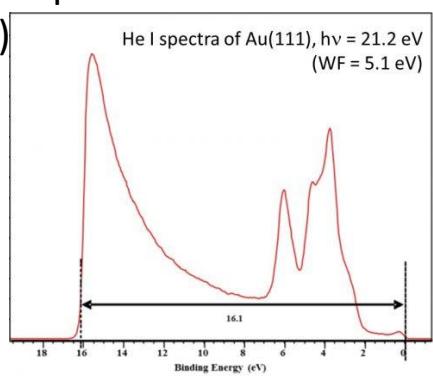
- single images (1MP, 16 bit)
- metadata (ASCII)



**II. Spectroscopy mode**

Outputs:

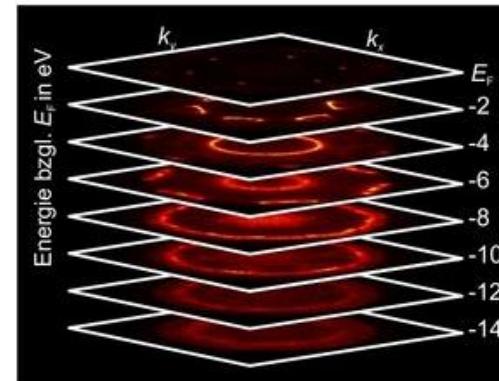
- laterally averaged spectra
- metadata (ASCII)



**III. Imaging with dispersive energy filtering mode (IDEA)**

Outputs:

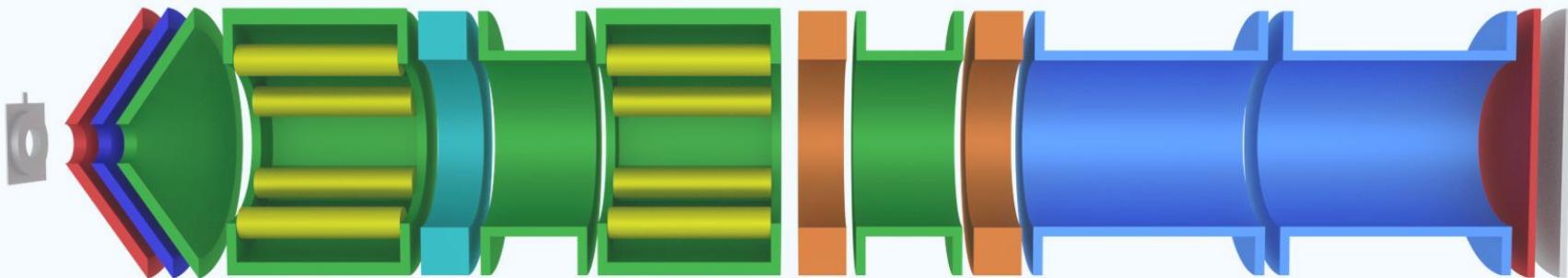
- images stacks (~900)
- metadata (ASCII)



# ToF-PEEM & spin-filter

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IV.

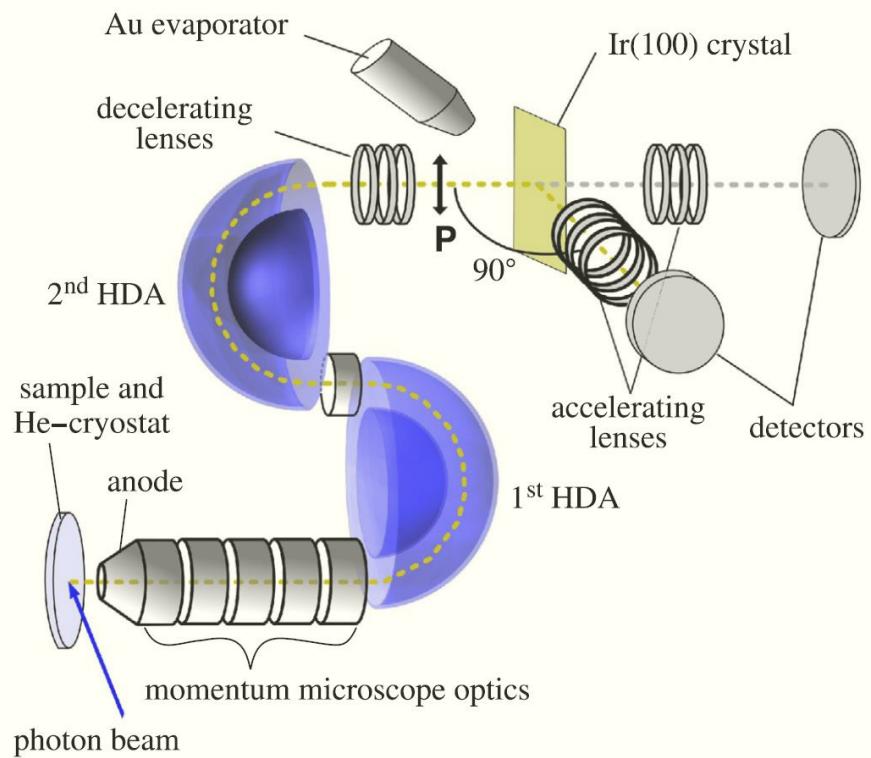


**IV. ToF - PEEM (Time of flight analyzer with imaging (delay line detector - DLD))**

Outputs:

- image stacks (~900 images)
- metadata (ASCII)

V.



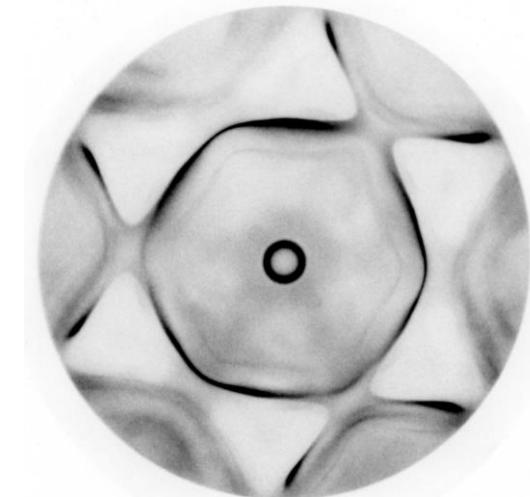
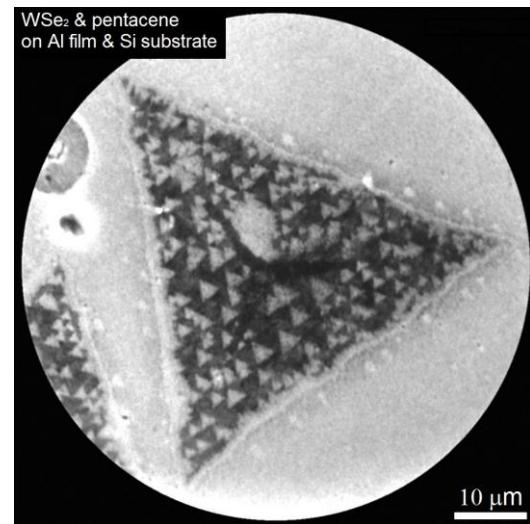
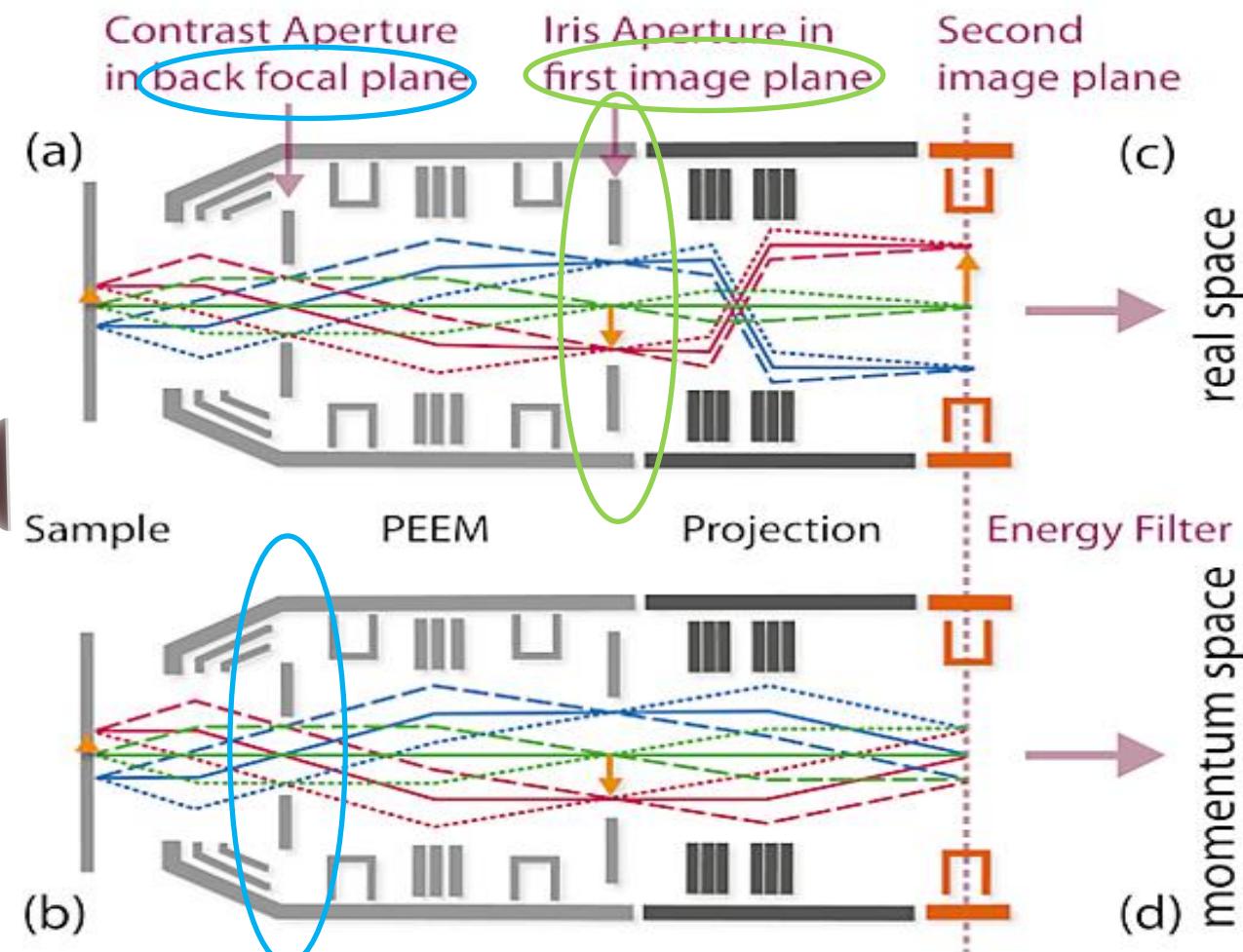
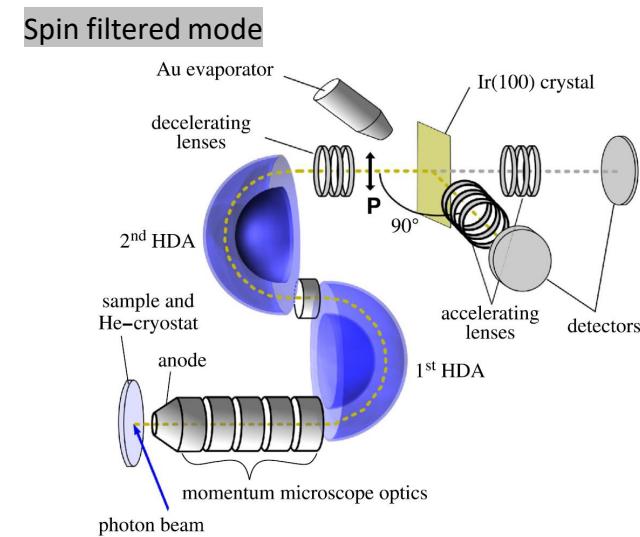
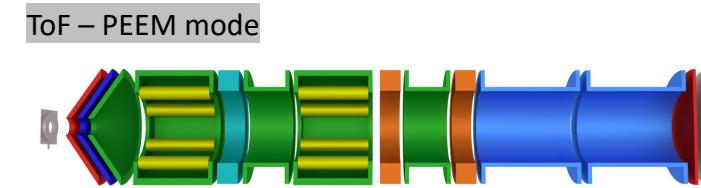
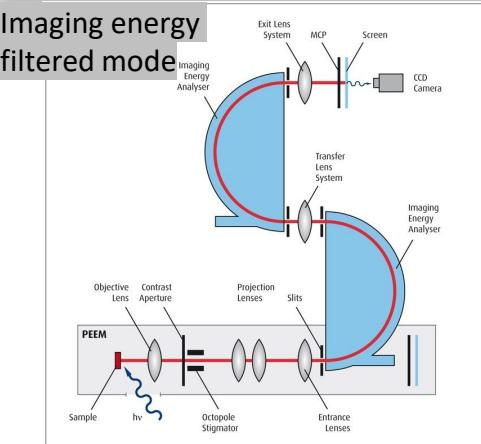
## V. Spin filtered mode

Outputs:

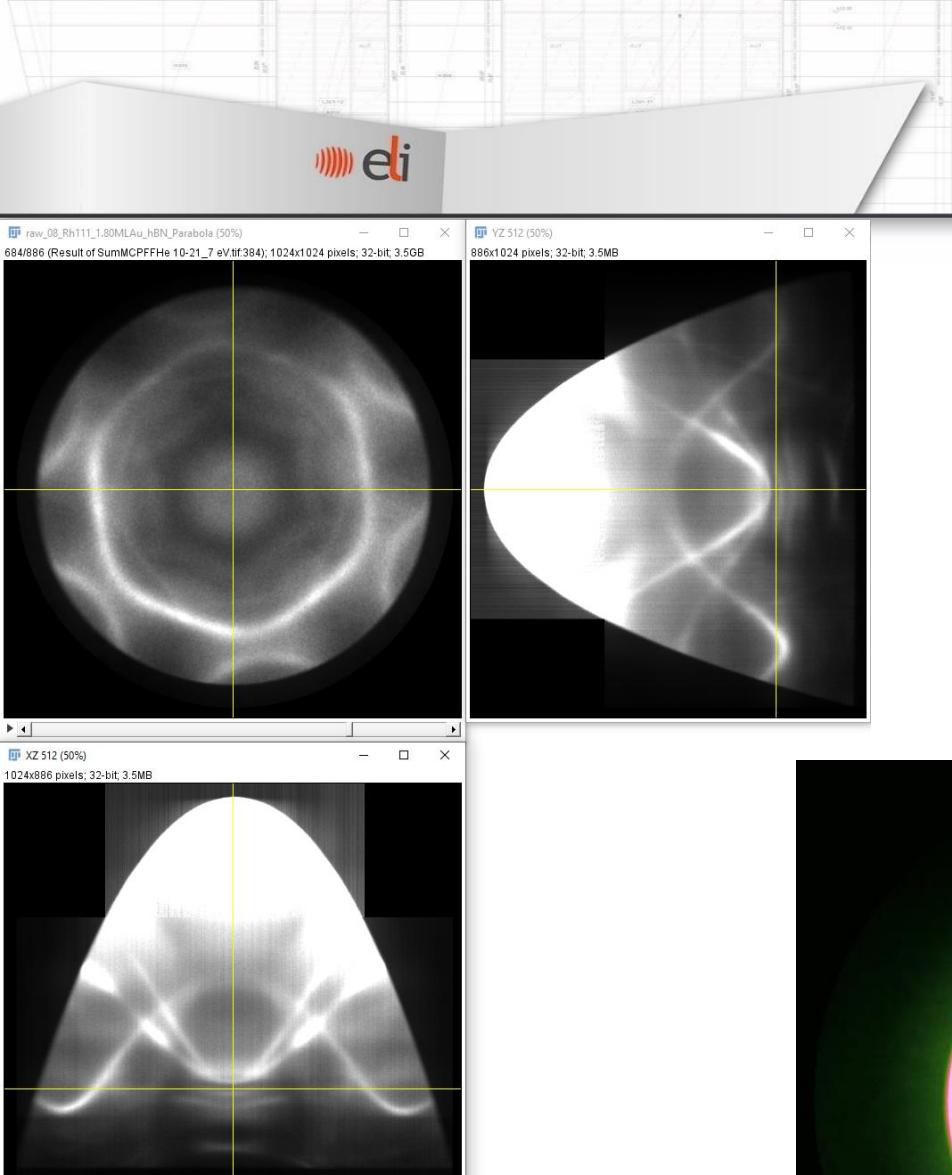
- images stacks (2 spin orientations)
- metadata (ASCII)

# Real space vs. momentum space

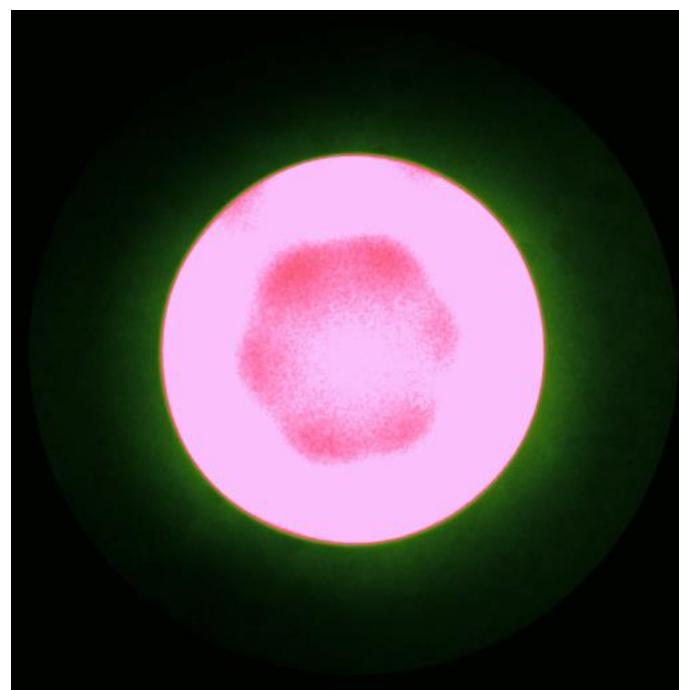
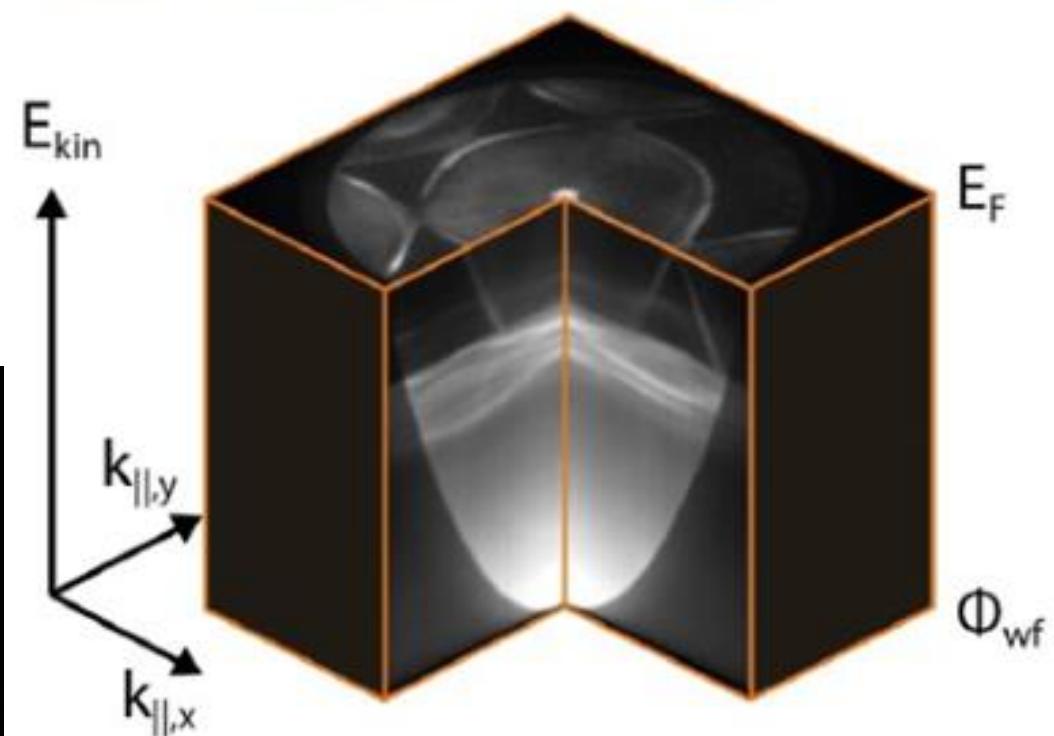
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# Band structure



## Band structure mapping



# Metadata connected to a NanoESCA in different phase of the project

## Initiation and project preparation phase:

- Experimental plan – planned parameter scans, conditions, etc.
- Sample preparation recipes & sample handling @previous studies & users' knowhow
- Results of preliminary simulations – if relevant

## Sample preparation phase:

- Sample preparation metadata & laterally averaged measurement data @LEED PC & XPS PC & handwritten notes – e-LogBook

## Experimental phase:

- Automatically stored NanoESCA metadata in an ASCII files @NanoESCA PC
- Automatically stored environmental parameters @Archiving service of ELI-ALPS
- Further relevant but not automatically stored parameters (e.g. positions/status of manually adjusted components) @handwritten notes & e-LogBook
- Metadata of photon sources (internal lamps & laser & secondary sources) @handwritten notes & e-LogBook

## Postprocessing & analysis phase:

- Image corrections, calibrations
- Simulations

## Publishing phase:

- Final cross sections selection, filtering, etc.

# Metadata of initiation

Sample preparation recipes & sample handling @previous studies & users' knowhow

Example I.

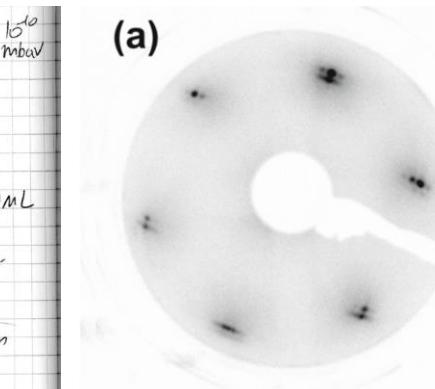
Cleaning	
Sample cleaning = sputtering 15 min	1.0kV $1.8 \times 10^{-6}$ mbar Ar, 17 mA
$P_{\text{PC}}$	$2.9 \times 10^{-10}$ mbar
$P_{\text{MC}}$	$8.4 \times 10^{-11}$ mbar
Oxidation of sample ✓	@ $5.0 \times 10^{-7}$ mbar or 20 min ~ 550°C
Sputtering ✓	
Oxidation 2th ✓	
Sputtering 2th ✓	
Annealing ✓	
Notes	
Sample annealing 1.7A / 400V / 7.1mA for 20min	
sample sputtering 1.0kV / 25mA / 17mA for 20 min	
annealing 1.7A / 400V / 4.1mA for 20 min	

Preparation

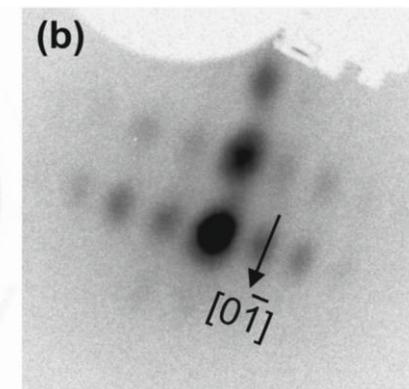
Ce degass = 1.2A / 1kV / 400mA flux 1MA,  $P_{\text{PC}} = 9.7 \times 10^{-10}$  mbav  
4 digit for microbalance:  
3'39" 3'55" 3'45" 3'46" 3'35" 3'46"  
Cedeportation @ 200°C,  $1.0 \times 10^{-6}$  mbar O<sub>2</sub>  
Deposition time = 8'38" ~ 9.2 digit ~ 0.2 mL  
position  $X=7$   $Y=8.75$   $Z=14.25$   $\theta=80^\circ$ ,  
Sample heating 1.65A for 5 min  $\rightarrow$  1.25A  
After deposition, keep for 2min, cooling down  
in O<sub>2</sub> atmosphere for 10 min.

Reference (LEED)

(a)



(b)



Example II.

- Rh(111) cleaning with Ar<sup>+</sup> sputtering & annealing cycles
- Au deposition @500K & annealing @1000K, afterwards
- Borazine exposure @1000-1050 K
- decomposition of borazine (B<sub>3</sub>N<sub>3</sub>H<sub>6</sub>) at ~1050 K

R. Gubó, G. Vári, J. Kiss, A. P. Farkas, K. Palotás, L. Óvári, A. Berkó, Z. Kónya, *Phys.Chem.Chem.Phys.* 2018, **20**, 15473.

The preparation chambers and its subsystems differs in all institute (temperature calibration is the most critical), so the recipes has to be fine tuned to our system to reproduce the sample, which could be time consuming.

# Metadata of sample preparation & laterally averaged sample analysis

## Au788 cleaning:

- sputtering 1kV 5mA 1.2E-5mbar 3.8uA 20min [0; 1.5; 24; 270]
- annealing 4.10A 6.3V 10min
- sputtering 0.8kV 5mA 1.3E-5mbar 3.6uA 20min [0; 1.5; 24; 270]
- annealing 4.10A 6.2V 10min

## XPS cleaned Au788:

- 14kV 14mA leak=545uA
- [-0.4; 4.42; 516; 0] sample plate orientation: ear outside
- file: Au788\_cleaned
- Au live intensity: 313 kcps (87eV CAE100 0.5s)
- spectra (1503s):
  - 1x survey 1100-20:0.5eV CAE50eV 0.1s
  - 3x Ce3d 925-875:0.05eV CAE50eV 0.3s
  - 1x O1s 0.05eV CAE50eV 0.3s
  - 2x C1s 0.05eV CAE50eV 0.3s
  - 2x Au4f 94-78:0.05eV CAE50eV 0.3s
  - 2x UPS 12-1:0.05eV CAE50eV 0.3s

CeO<sub>2</sub> deposition: ML

- Magnetoplasma parameters
    - I<sub>flux</sub>; I<sub>fil</sub>
    - U, I<sub>em</sub>
    - T<sub>sample</sub>
  - p<sub>base</sub>
  - p<sub>O<sub>2</sub></sub> level
  - Evaporation t
  - Hold
  - Cooling down
- [0; 1; 23; 235]  
1.0 uA , 1.37 A  
775 V/ 39.5 mA (38.9)  
2.45A 2.85V 158oC (max.: 165 oC)  
1.3x10<sup>-9</sup> mbar  
5x10<sup>-7</sup> mbar (IGP off)  
42:27 (mm:ss)

XPS Au788 + 8 ML CeO<sub>2</sub> -> calculated coverage 8 ML (calc.based on Au int.decay)

- 14kV 14mA leak= 545uA
- [-0.4; 4.35; 516; 0] sample plate orientation: ear outside
- file: Au788\_8MLCeO2
- Au live intensity: 129 kcps (87eV CAE100 0.5s)
- spectra:
  - 1x survey 1100-20:0.5eV CAE50eV 0.1s
  - 3x Ce3d 925-875:0.05eV CAE50eV 0.3s
  - 0x Ce4d 135-104:0.05eV CAE50eV 0.3s
  - 4x O1s 542-522:0.05eV CAE50eV 0.3s
  - 4x C1s 298-278:0.05eV CAE50eV 0.3s
  - 2x Au4f 9135-1044-78:0.05eV CAE50eV 0.3s
  - 3x UPS 12-1:0.05eV CAE50eV 0.3s

LEED Au788 + 2MLCeO<sub>2</sub>

- [2.5, 0.25, 257.25; 97]
- 40-200:1 eV
- I<sub>fil</sub>=1.45 Usr=4.5kV

Ethanol adsorption I. on 8ML CeO<sub>2</sub> on Au788

- positions:[-6, 2.5, 256.5, 312, dozer: 30]
- t=15 min
- P<sub>ethanol</sub>=6E<sup>-8</sup> mbar
- p<sub>base</sub> 1.3x10<sup>-9</sup> mbar
- T<sub>sample</sub>: 35°C
- IGP OFF

XPS I. Au788 + 8 ML CeO<sub>2</sub> -> calculated coverage 8 ML (calc.based on Au int.decay)

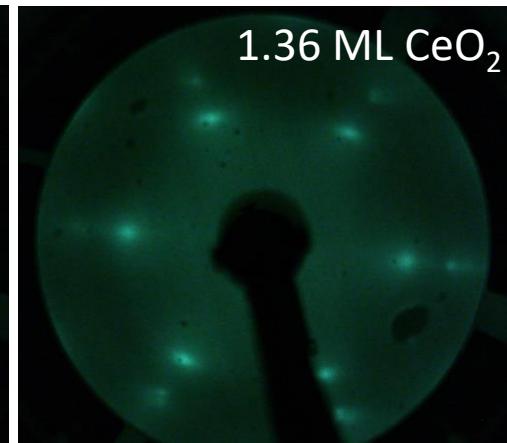
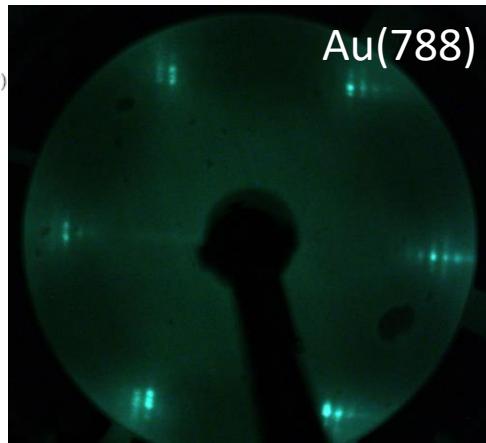
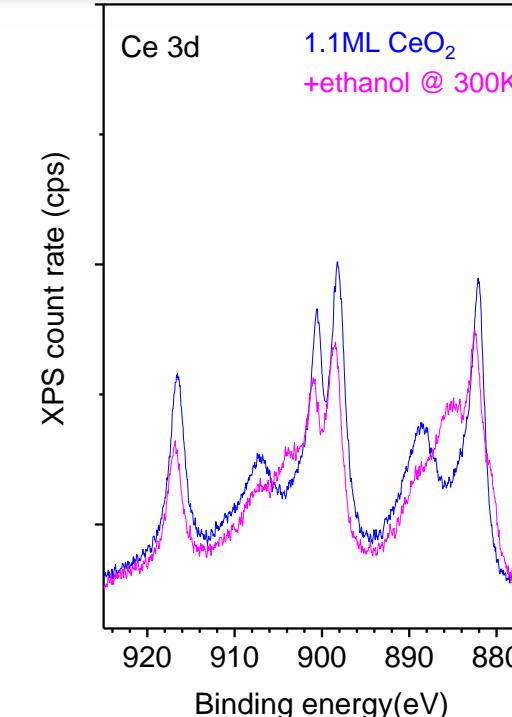
- 14kV 14mA, leak= 538uA , I<sub>fil</sub>: 4.1A
- [-0.4; 4.35; 516; 0] sample plate orientation: ear outside
- file: Au788\_8MLCeO2+ethanol 15min
- p<sub>base</sub>: 2.64x10<sup>-9</sup> mbar
- Au live intensity: cps (87eV CAE100 0.5s)
- spectra:
  - 1x survey 1100-20:0.5eV CAE50eV 0.1s
  - 3x Ce3d 925-875:0.05eV CAE50eV 0.3s
  - 0x Ce4d 135-104:0.05eV CAE50eV 0.3s
  - 2x O1s 542-522:0.05eV CAE50eV 0.3s
  - 10x C1s 301-278:0.05eV CAE50eV 0.3s
  - 2x Au4f 9135-1044-78:0.05eV CAE50eV 0.3s
  - 3x UPS 12-1:0.05eV CAE50eV 0.3s

Ethanol adsorption II. on 8ML CeO<sub>2</sub> on Au788

- positions:[-6, 2.5, 256.5, 312, dozer: 30]
- t=15 min
- P<sub>ethanol</sub>=6E<sup>-8</sup> mbar
- p<sub>base</sub> 1.7x10<sup>-9</sup> mbar
- T<sub>sample</sub>: 27.6°C
- IGP OFF

XPS II. Au788 + 8 ML CeO<sub>2</sub> -> calculated coverage 8 ML (calc.based on Au int.decay)

- 14kV 14mA, leak= 538uA , I<sub>fil</sub>: 4.1A
- [-0.4; 4.35; 516; 0] sample plate orientation: ear outside
- file: Au788\_8MLCeO2+ethanol 15 +15 min
- p<sub>base</sub>:
- Au live intensity: 118 kcps (87eV CAE100 0.5s)
- spectra:
  - 1x survey 1100-20:0.5eV CAE50eV 0.1s
  - 3x Ce3d 925-875:0.05eV CAE50eV 0.3s
  - 0x Ce4d 135-104:0.05eV CAE50eV 0.3s
  - 2x O1s 542-522:0.05eV CAE50eV 0.3s
  - 10x C1s 301-280:0.05eV CAE50eV 0.3s
  - 2x Au4f 9135-1044-78:0.05eV CAE50eV 0.3s
  - 2x UPS 12-1:0.05eV CAE50eV 0.3s



# Metadata of NanoESCA measurements

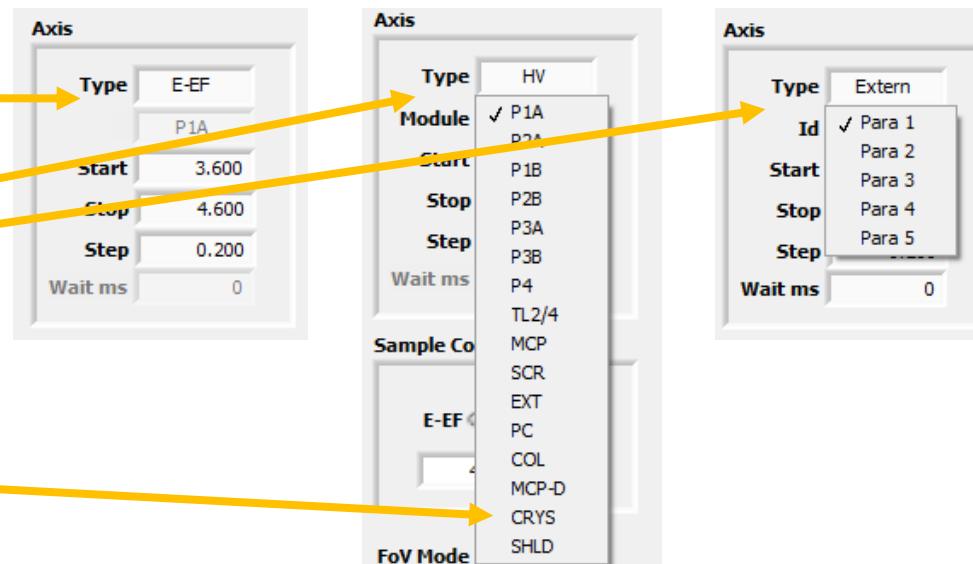
Automatically stored NanoESCA metadata in an ASCII file and display in the history window

e.g.:

- Electron-optical parameters (voltage of the lenses & components)
- Exposure-time
- Number of averaged images
- ...
- Parameter-scan range (single loop: start – end, step size; nesting loops: under development)

History window:

Axis	Name	E-EF	Operator	VCs	Instrument Mode	Energy Filtered Mode
	Start	21.100	Sample	Au(111)	N Scan	100
	Stop	21.100	Detector Mode	Camera	Dwell Time	10000 ms
	Step	0.000	Slit EA1	0.5 mm	Photon Energy	21.218750 eV
			Slit EA2	3.0 mm	Iris Diameter	20.0 μm
	E-EF :	-> Axis	TRANS :	-> Track	Epass :	50.000eV
	EXT :	20000.0V	P1A :	476.0V	FL1 :	-> Track
	FOC :	-> Track	P1B :	1600.0V	FL2 :	-> Track
	COL :	2000.0V	P2A :	12.0V	TL2/4 :	210.0V
	COL2 :	---	P2B :	1100.0V	TL3 :	-> Track
	COL-T :	-> Track	RP :	-> Track	RP2 :	-> Track
	R1 :	544.0V	R3 :	280.0V	Shld :	50.0V
	R2 :	280.0V	R4 :	544.0V	Crys :	0.0V
	Stig1 Vx :	-2.590	Stig2 Vx :	0.090	Def Ax :	-0.060
	Stig1 Vy :	-4.170	Stig2 Vy :	-1.280	Def Ay :	-0.110
	Stig1 Sx :	-0.120	Stig2 Sx :	0.000	Def Bx :	-0.240
	Stig1 Sy :	0.010	Stig2 Sy :	0.150	Def By :	-0.220
	Apert. X :	-58.3μm	Apert. Y :	2395.4μm	Sample X :	6.1μm
	Extern 1 :	Off	Extern 2 :	Off	Extern 3 :	Off
					Sample Y :	9.4μm
					Extern 4 :	Off
					Extern 5 :	Off



ASCII:

```

MOD01_NAME = "COL-T"
MOD01_ADDR = "050"
MOD01_PARA1_NAME = "UNOM"
MOD01_PARA1_VALUE = 1000.000000
MOD02_NAME = "P1a"
MOD02_ADDR = "051"
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MOD02_PARA1_VALUE = 471.500000
MOD03_NAME = "P2a"
MOD03_ADDR = "053"
MOD03_PARA1_NAME = "UNOM"
MOD03_PARA1_VALUE = 8.000000
MOD04_NAME = "P1b"
MOD04_ADDR = "052"
MOD04_PARA1_NAME = "UNOM"
MOD04_PARA1_VALUE = 1500.000000

```

# Data structure of raw measured data (images) & its metadata

**Experiment List**

Name	Instr. Mode	Event C.	Axis	Start	Stop	Step	FoV	Dwell [ms]	N Scan	Time	...
15-0_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-1_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-2_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-3_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-4_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-5_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-6_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-7_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-8_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-9_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
16-0_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
14-0ref_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6--4-6eV_ul	Energy Filtered Mode	Off	E-EF	3.600000	4.600000	0.200000	k-Space	10000	8	00:08:00	
15-0ref_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6-0eV_ulp-CEP	Energy Filtered Mode	Off	E-EF	3.000000	6.000000	0.100000	k-Space	10000	8	00:41:20	
21_R5-F1_IDEA_RS_PE100_S1_20kV_FoV83_Hg01_4-85eV_MCP1800_FOC3020	Energy Filtered Mode	Off	E-EF	4.850000	4.850000	0.000000	Realspace	500	1200	00:10:00	
17_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-2--5-4eV_FSw15	Energy Filtered Mode	Off	E-EF	3.200000	5.400000	0.100000	k-Space	10000	2	00:07:40	
05_R5-F1_IDEA_KS_PE100_S1_20kV_FoV2-1_V_4-0eV_FSw0--24	Energy Filtered Mode	Off	Extern	0.000000	24000000.000	2000000.000	k-Space	10000	1	00:02:10	

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- [2022-08-23\_nRhombs\_R5\_V\_RS-KS\_3rd]
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  - [02\_R5-F1\_IDEA\_RS\_PE100\_S1\_20kV\_FoV83\_V\_4-3eV\_IMG\_220823\_161308]
  - [03\_R5-F1\_IDEA\_RS\_PE100\_S1\_20kV\_FoV83\_V\_4-3eV\_IS40um\_220823\_161518]
  - [04\_R5-F1\_IDEA\_KS\_PE100\_S1\_20kV\_FoV2-1\_V\_4-0eV\_cent\_220823\_161930]
  - [05\_EXP\_4-0eV\_FSw0-24\_220823\_162645]
  - [06\_EXP\_3-6eV\_FSw15\_20deg\_220823\_165922]
  - [07\_EXP\_3-6eV\_FSw15\_30deg\_220823\_171744]
  - [08\_EXP\_3-6eV\_FSw15\_40deg\_220823\_172405]
  - [09\_EXP\_3-6eV\_FSw15\_50deg\_220823\_173127]
  - [10\_EXP\_3-6eV\_FSw15\_60deg\_220823\_174310]
  - [11\_EXP\_3-6eV\_FSw15\_70deg\_220823\_175448]
  - [12\_R5-F1\_IDEA\_KS\_PE100\_S1\_20kV\_FoV2-1\_V\_4-0eV\_img\_220823\_181853]
  - [13\_EXP\_3-6eV\_FSw15\_20deg\_220823\_184603]
  - [14\_EXP\_3-2-5-4eV\_FSw15\_20deg\_220823\_185323]
  - [15\_EXP\_3-2-5-4eV\_FSw15\_40deg\_220823\_185845]
  - [16\_EXP\_3-2-5-4eV\_FSw15\_50deg\_220823\_190352]
  - [17\_EXP\_3-2-5-4eV\_FSw15\_60deg\_220823\_190859]
  - [18\_R5-F2\_IDEA\_RS\_PE100\_S1\_20kV\_FoV83\_V\_4-3eV\_IS40um\_220823\_192319]
  - [19\_EXP\_R5-F2\_3-6eV\_FSw14-16\_220823\_194259]
    - [14-0\_R5-F2\_IDEA\_KS\_PE100\_S1\_20kV\_FoV2-1\_V\_3-6-0eV\_220823\_194259]
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  - [14-1\_R5-F2\_IDEA\_KS\_PE100\_S1\_20kV\_FoV2-1\_V\_3-6-0eV\_220823\_202529]

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14-0_R5-F2_IDEA_KS_PE100_S1_20kV_FoV2-1_V_3-6-0eV_AV_018	TIF	2,097,403	2022-08-23 20:25	-a--
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# Metadata of NanoESCA measurements



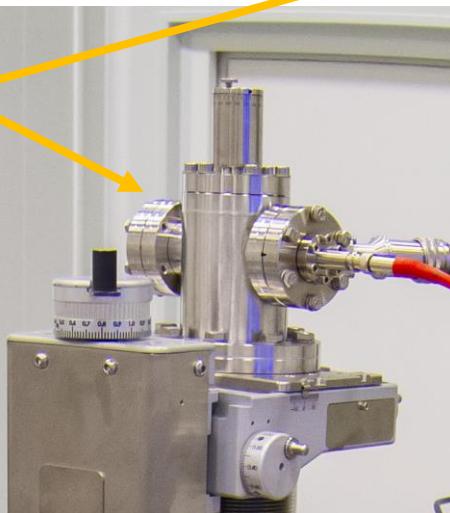
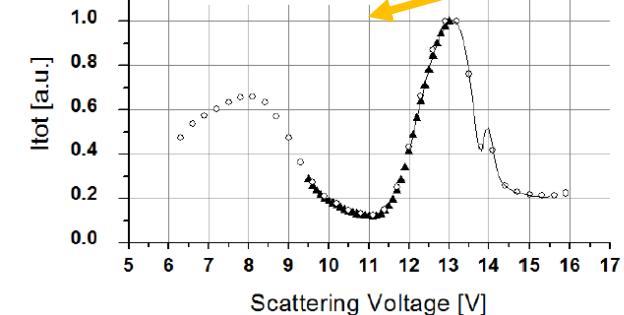
Automatically stored 'environmental' parameters:

- Chamber pressures (Grafana)
- Sample temperatures (Preparation chamber: Grafana, analysis chamber: local log file, notes)
- Vacuumpump (current & speed) and cooling parameters (pressure, temperature, flow rate)
- Status of the pneumatic gate valves
- Laboratory temperature, air pressure, humidity

Further relevant but not automatically stored parameters

- Sample position
- Spin-filter position
- Spin filter preparation (cleaning, evaporation, annealing) & IV curve

Enable	Axis	Position	Unit	Step Size	Job Velocity
<input checked="" type="checkbox"/>	X	3.437671	mm	0.03	0.1
<input checked="" type="checkbox"/>	Y	0.285620	mm	0.01	0.1
<input checked="" type="checkbox"/>	Z	2.195930	mm	0.1	0.1
<input checked="" type="checkbox"/>	Polar	-0.000234	°	0.5	1



# Metadata of NanoESCA photon sources I.

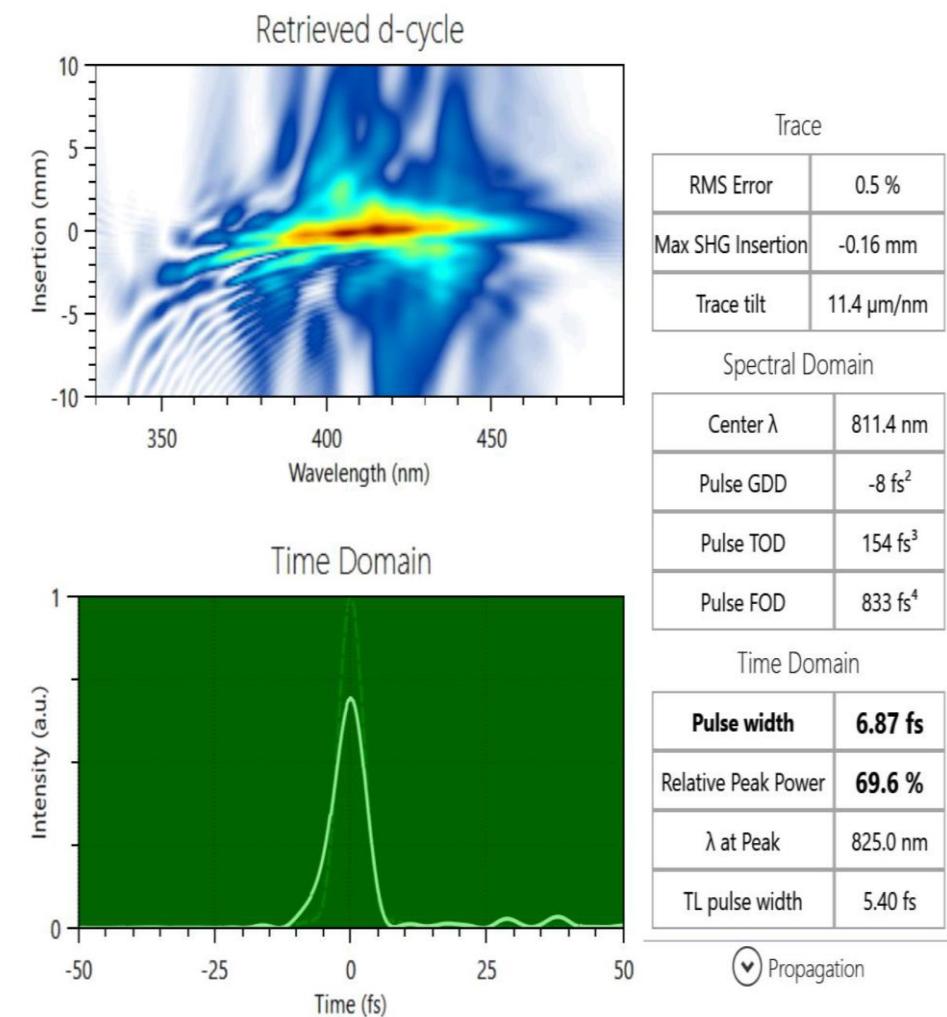
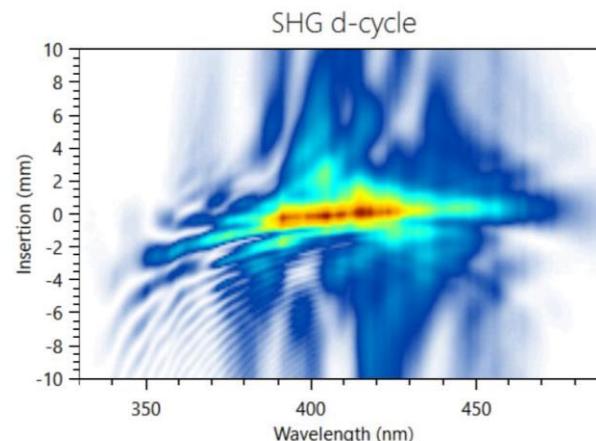
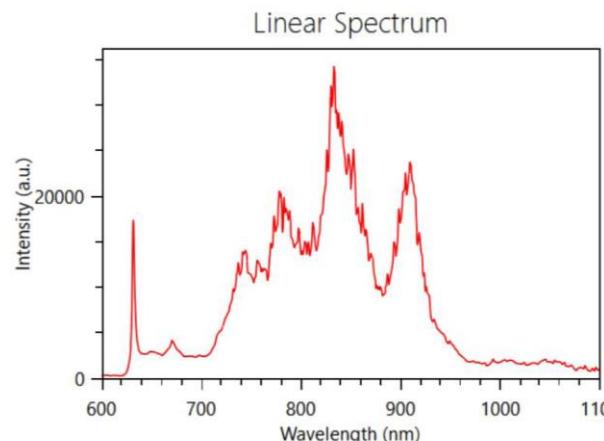
## CW & laser sources (e-LogBook & handwritten notes)

Continuous wave sources for static measurements:

- Hg arc lamp: ON/OFF; intensity determined by the filter (100%, 10%, 1%) – manually stored
- He discharge lamp: current & voltage & pressures - manually stored

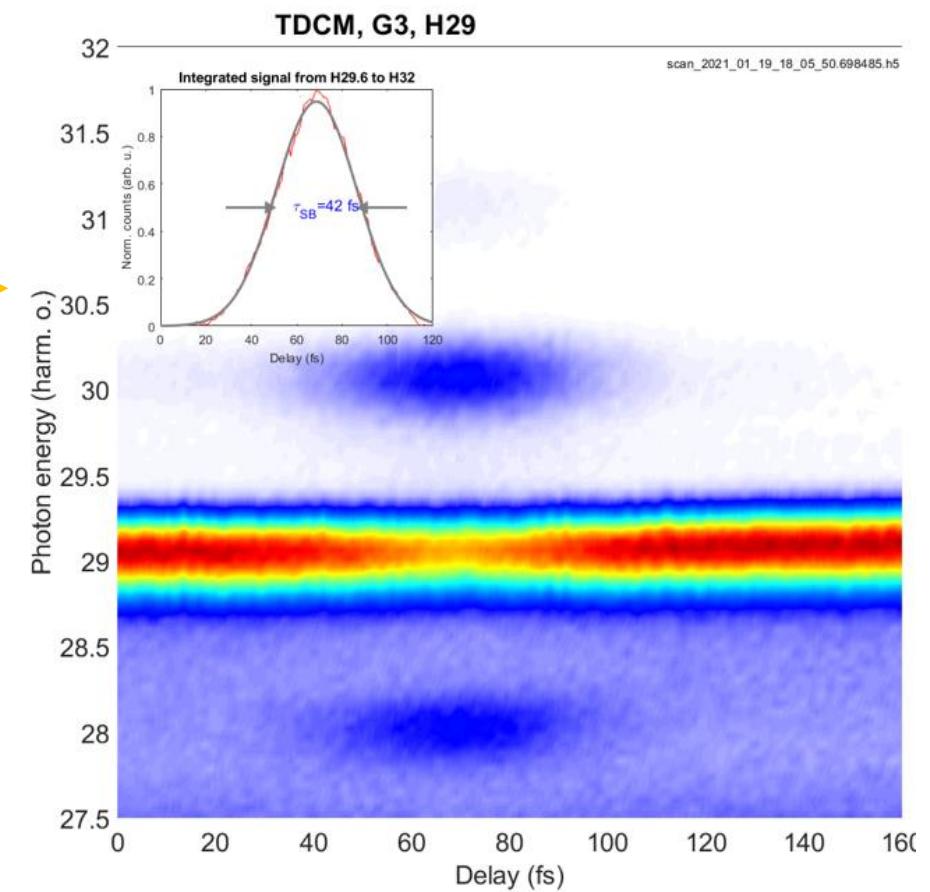
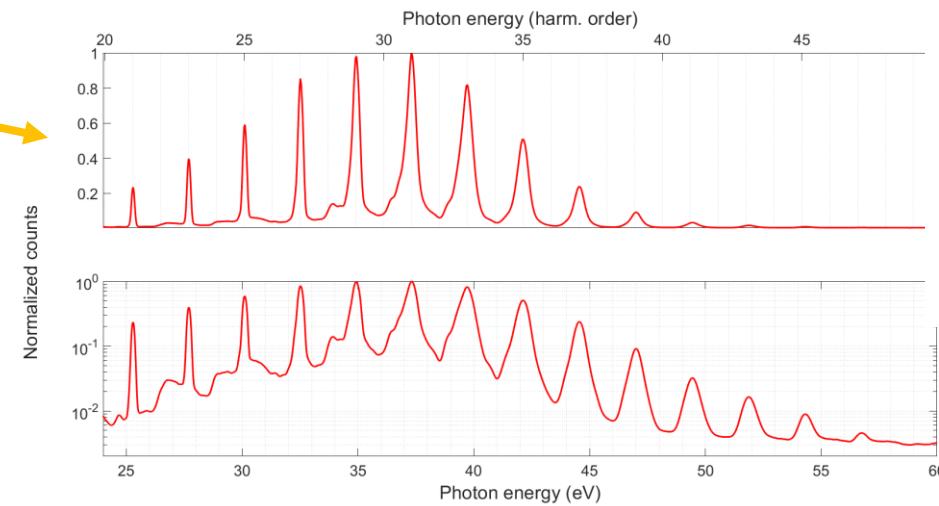
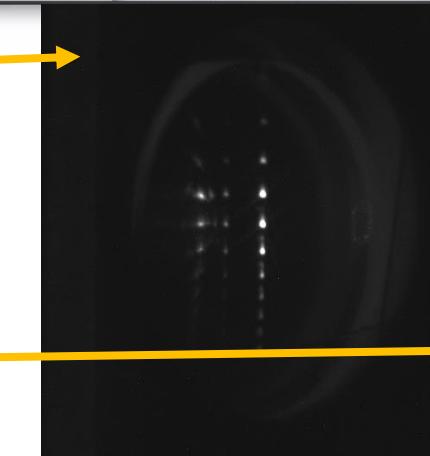
Parameters of laser sources (pump pulse):

- spectrum
- pulse length
- beam profile
- other (mirrors & wedge positions; pressures in the multi-pass cells)



# Metadata of NanoESCA photon sources II. Characterization of XUV source (e-LogBook)

- Beam profile (gas: Xe):  
fluorescence of diffracted  
harmonics on Ce:YAG crystal
- Pulse length: IR-XUV cross-  
correlation spectrogram
- Spectrum
- Operation mode & position  
of the optical components
- Applied gas
- Position of gas cell
- Intensity of IR & XUV
- Pressure in the target  
chamber
- Applied filters

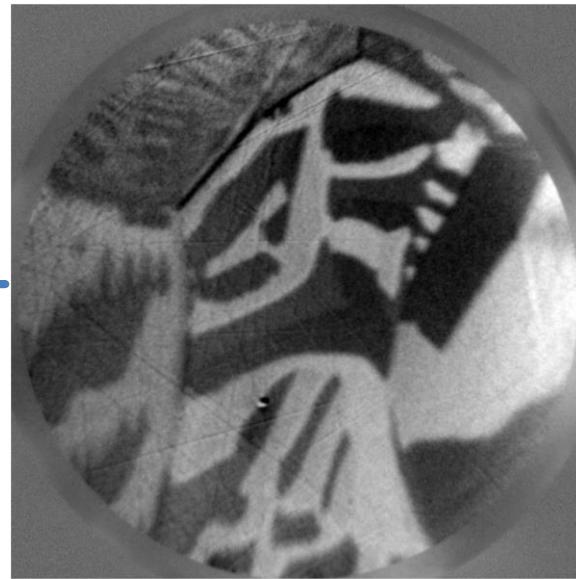


# Post processing

- Flatfield correction
- Calibration of energy scale and the lateral scales
- Correction of sample tilting & rotation
- Correction of distortions (elliptical distortion of electron optics)
- Calculation of Fermi-edge & work function
- Preparation of spin-contrast images



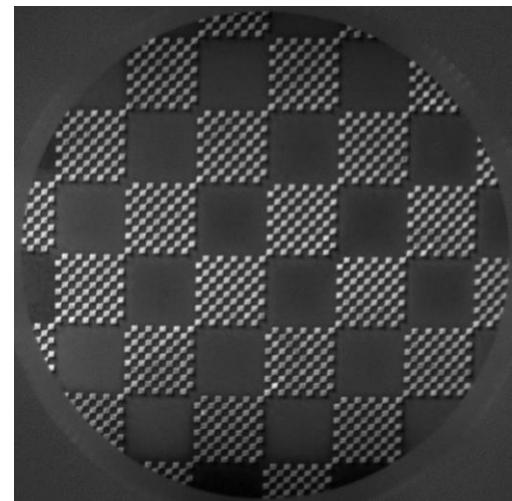
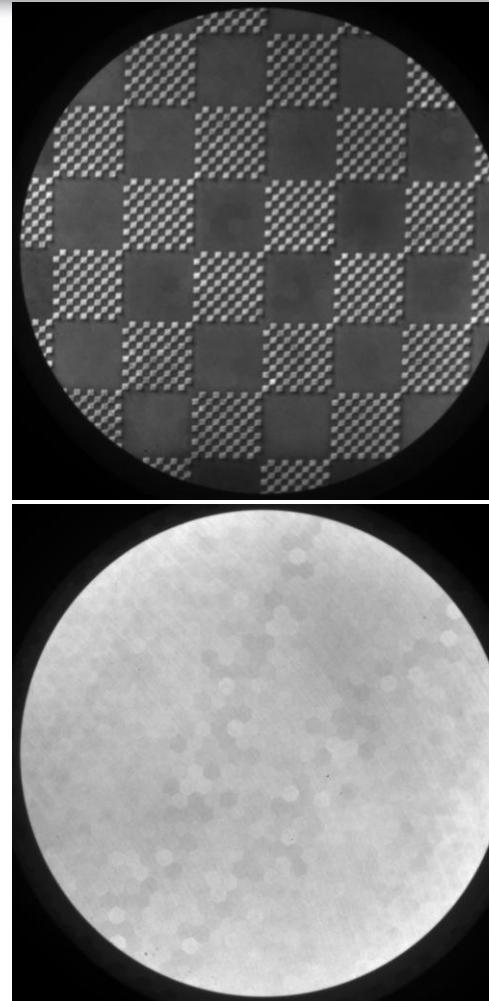
Working point I ( $S > 0$ )



Spin polarization map

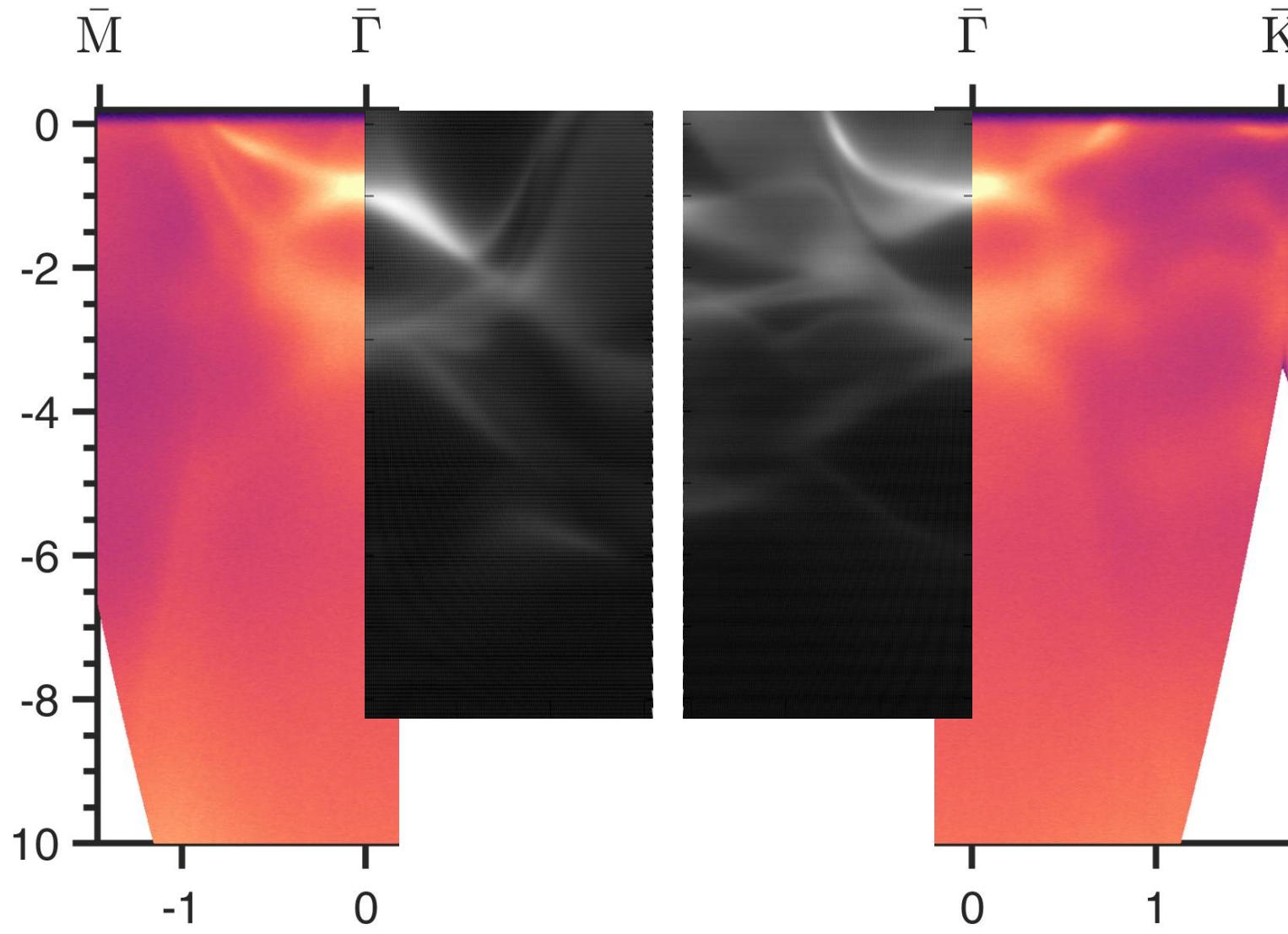


Working point II ( $S < 0$ )

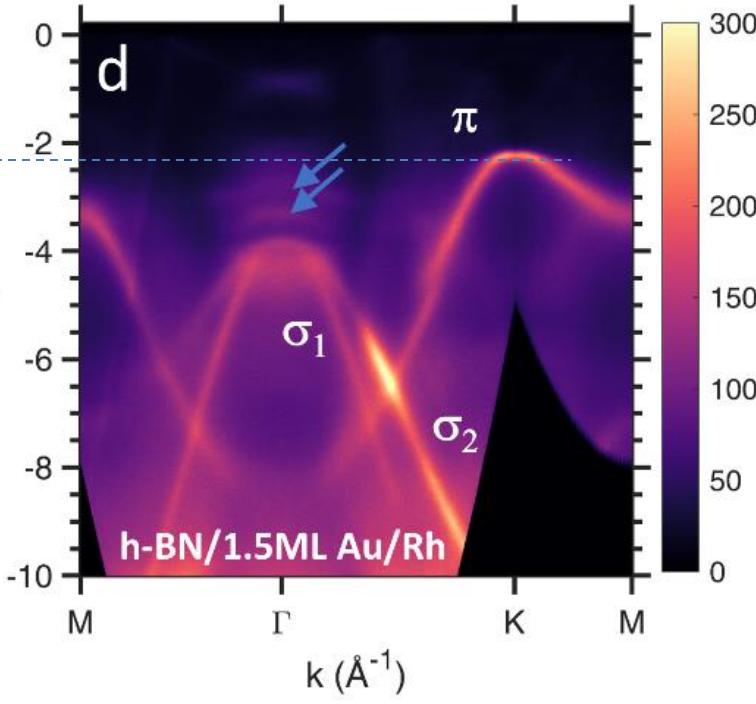
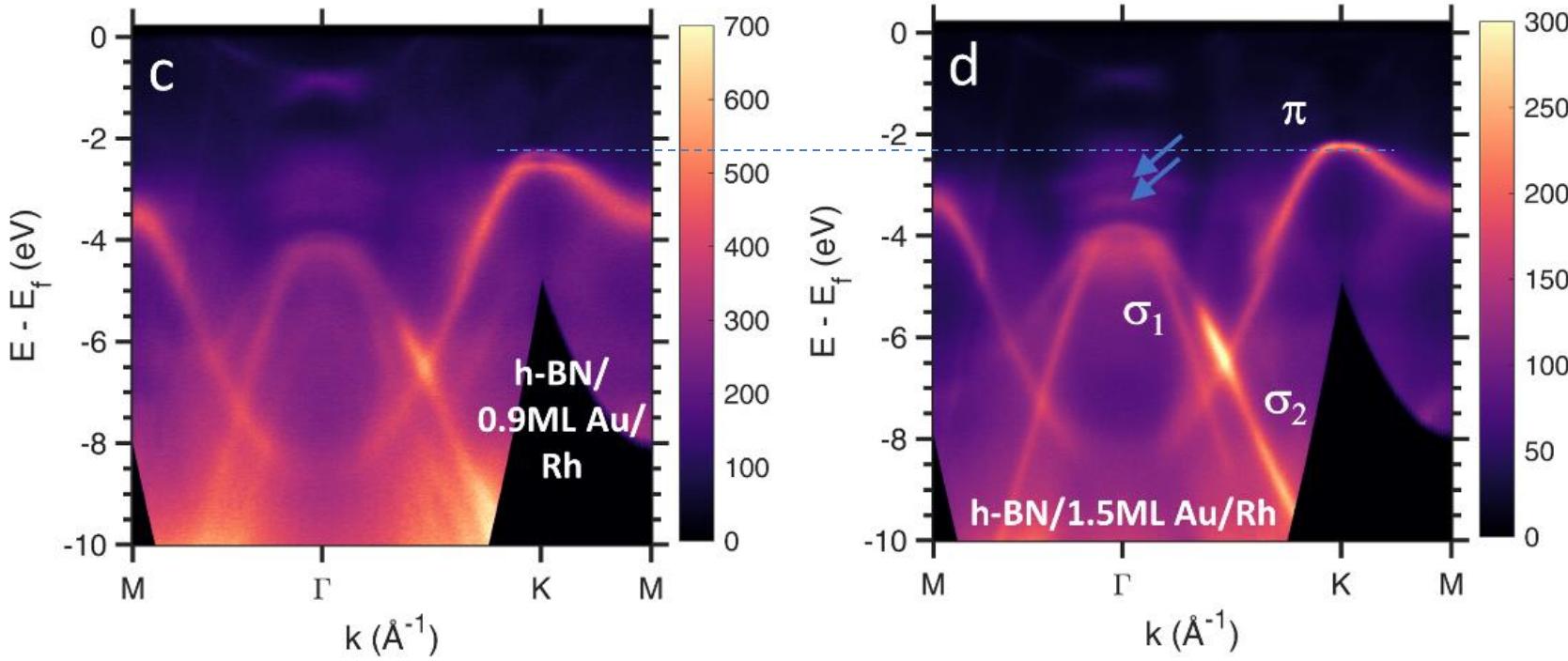
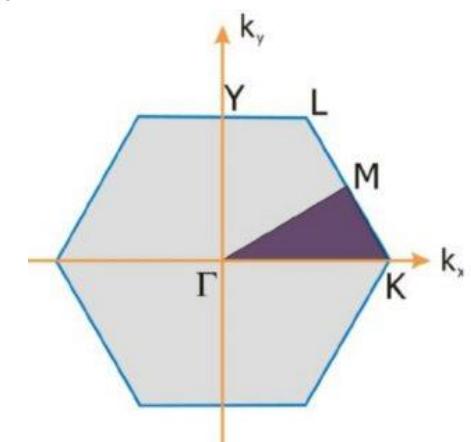
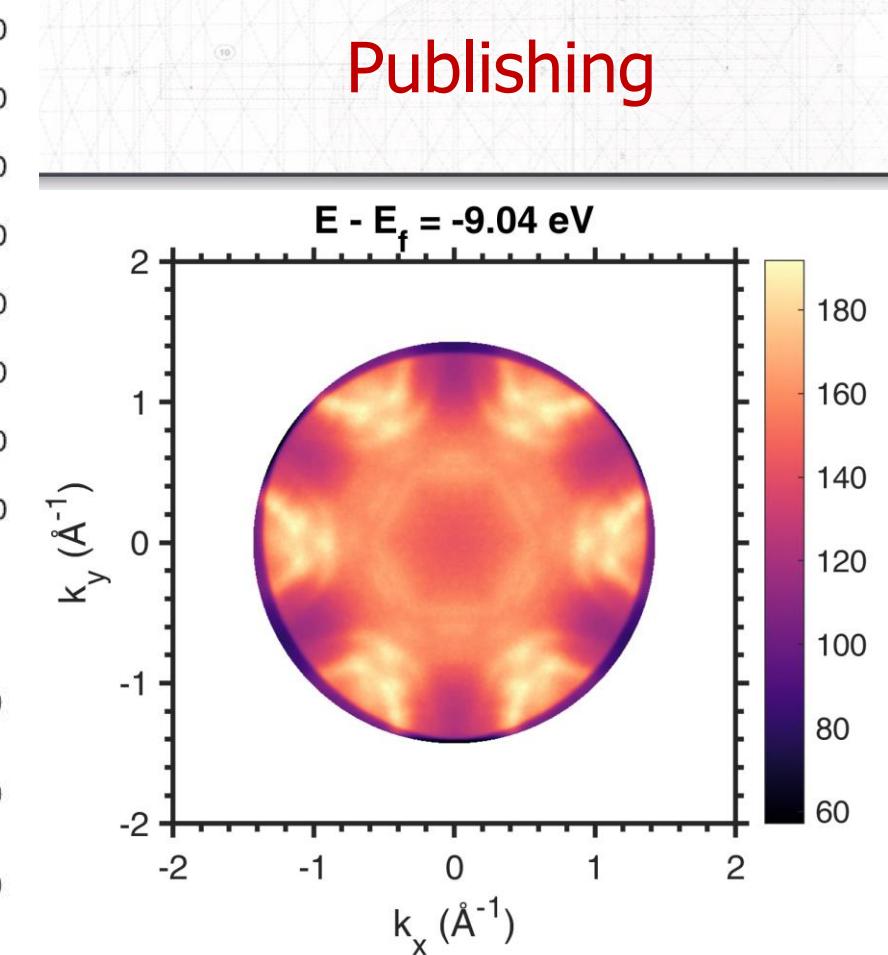
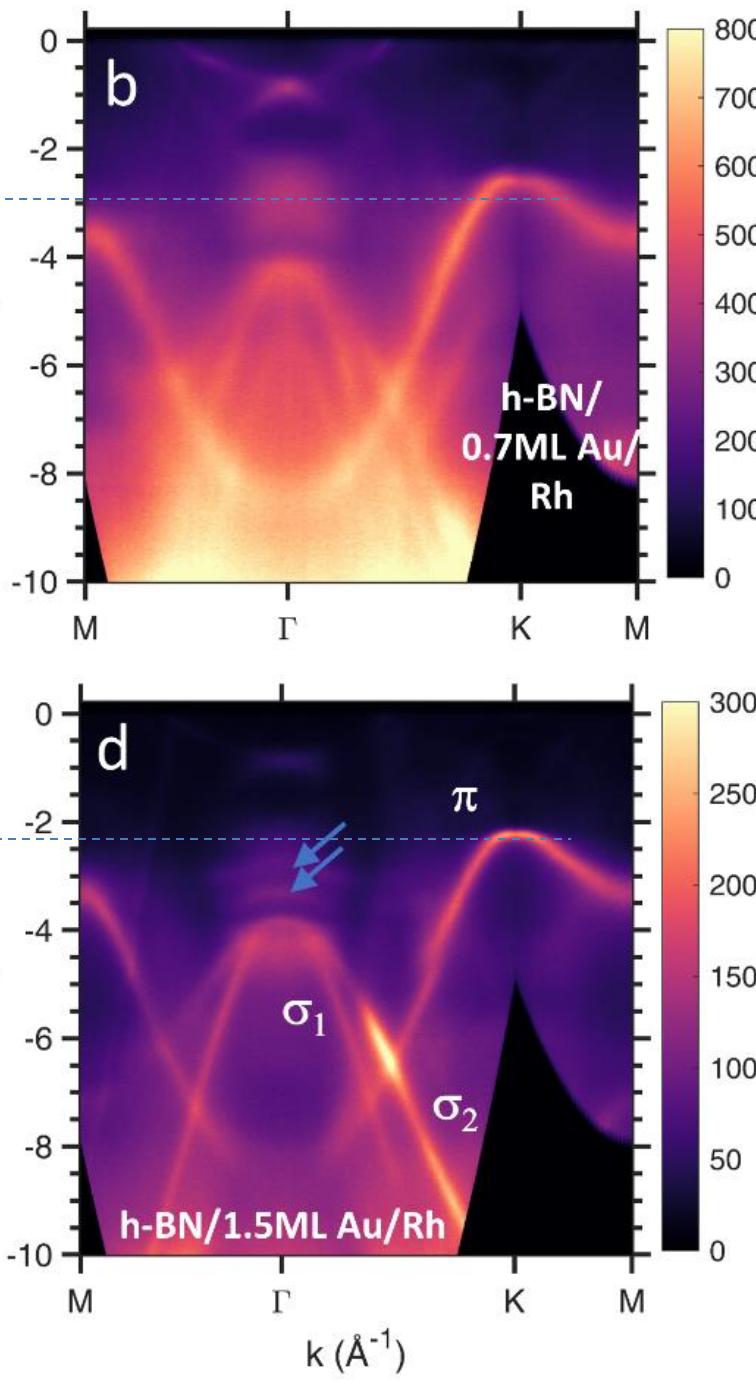
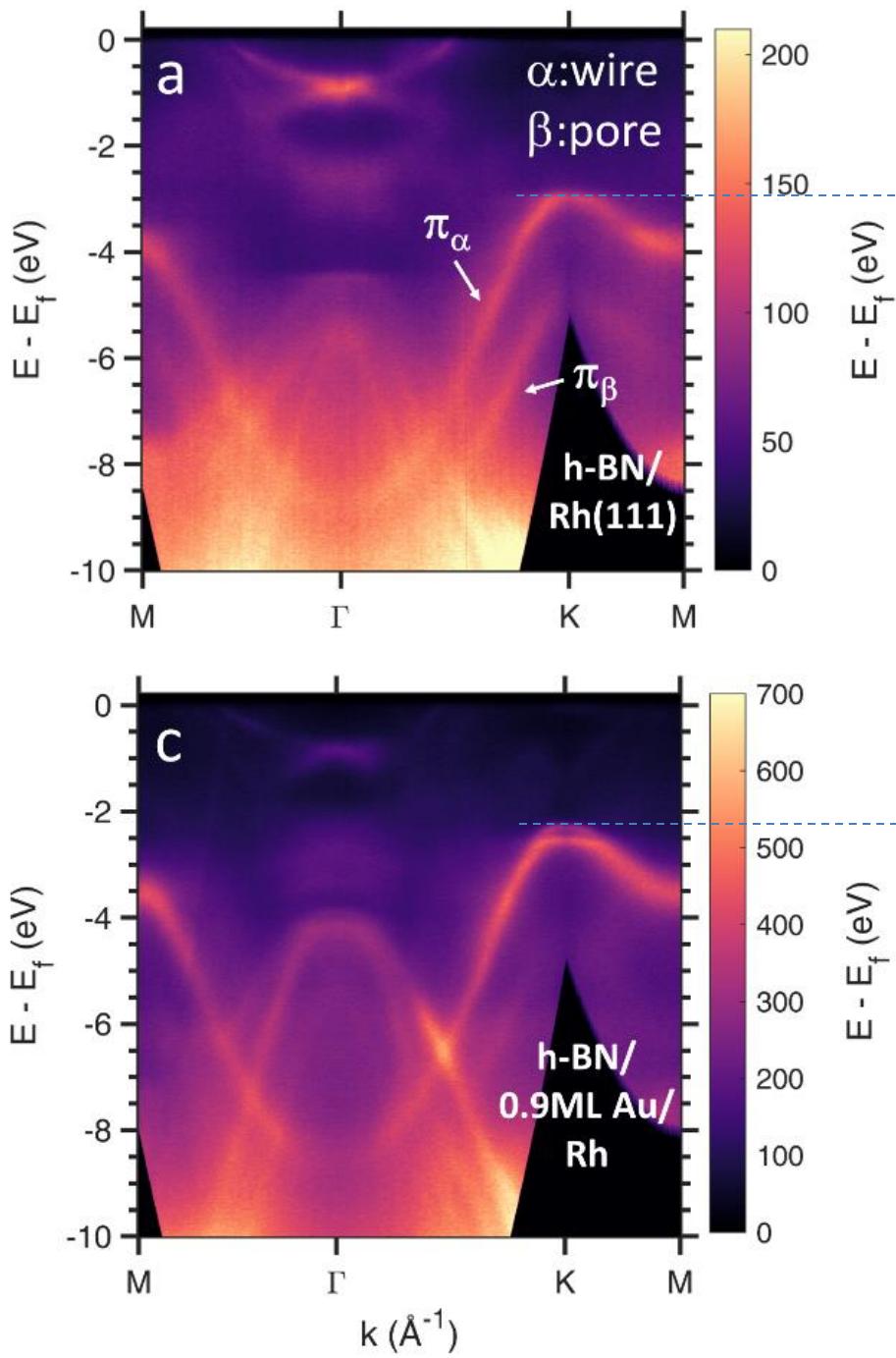


# Simulations – cooperation with our simulation group

Example: measured (colored) and simulated (grayscale) band structure of Rh(111)



Publishing



# Public access to the data

**Requirements with the shared NanoESCA data (& metadata):**

- Searchable
- Universal/known data structure (ontology)
- Contains all relevant data (and their metadata) for further analysis
  - Sample preparation recipes & result of preliminary analysis (XPS, AES, LEED)
  - Metadata of NanoESCA measurements and photon sources
  - Steps of image correction
- The related data has to link together
- It has to be understood for a specialist in the relevant research field
- Information for the **reproducibility**
- ...

**Challenges:**

Store all the relevant data in universal structure including data from different sources:

- Main data & metadata of NanoESCA - in progress with our software engineers
- Metadata from e-LogBooks – templates with automatic importing possibilities
- Metadata from laser & secondary sources & instruments
- Handwritten notes are not acceptable – has to be eliminate

Ontology:

- New techniques in an existing structures: the structures has to modified (ARPES vs. spectro-microscope)



# Thank you for your kind attention!



HUNGARIAN  
GOVERNMENT

**European Union**  
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