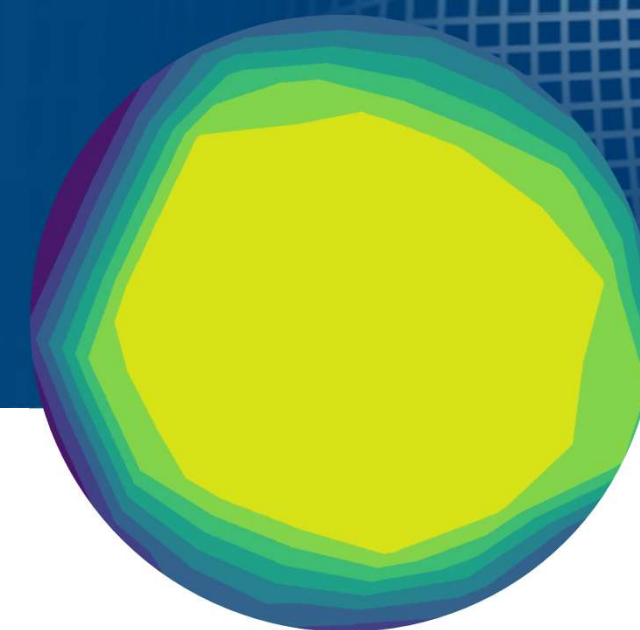


SOFT- AND HARD XPS AND XAS MEASUREMENTS ON A NA-K-SB PHOTOCATHODE

PROF. ALICE GALDI

UNIVERSITÀ DEGLI STUDI DI SALERNO, ITALY



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UNIVERSITÀ DEGLI STUDI
DI SALERNO

HZDR

Dr. Rong Xiang



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December 2025 beamtime photo

HZB - EMIL

Dr. Regan Wilks



Dr. Mihaela Gorgoi



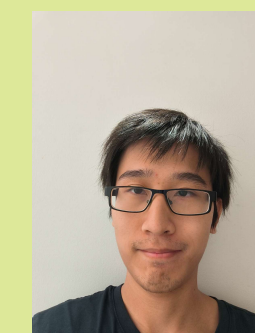
Dr. Anna Efimenko



Department of Interface Materials

Friedrich Schiller Universität, Germany

Chung Xu



Richard Schier



Prof.. Dr. Caterina Cocchi



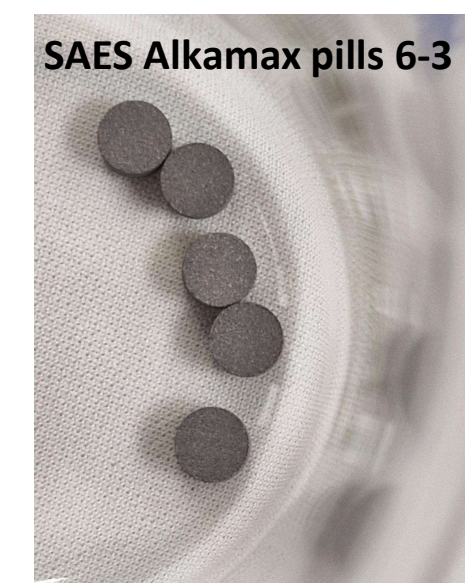
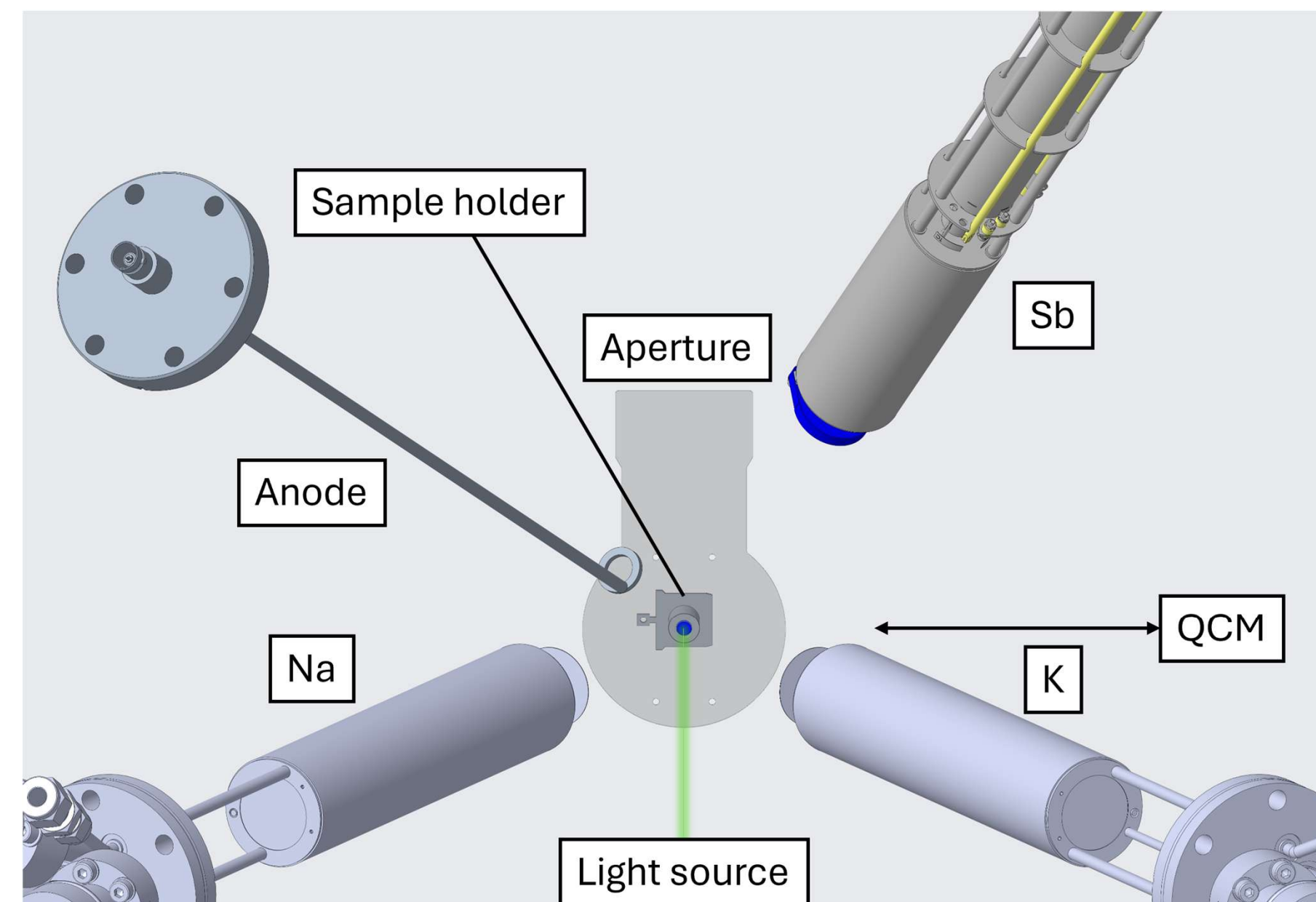
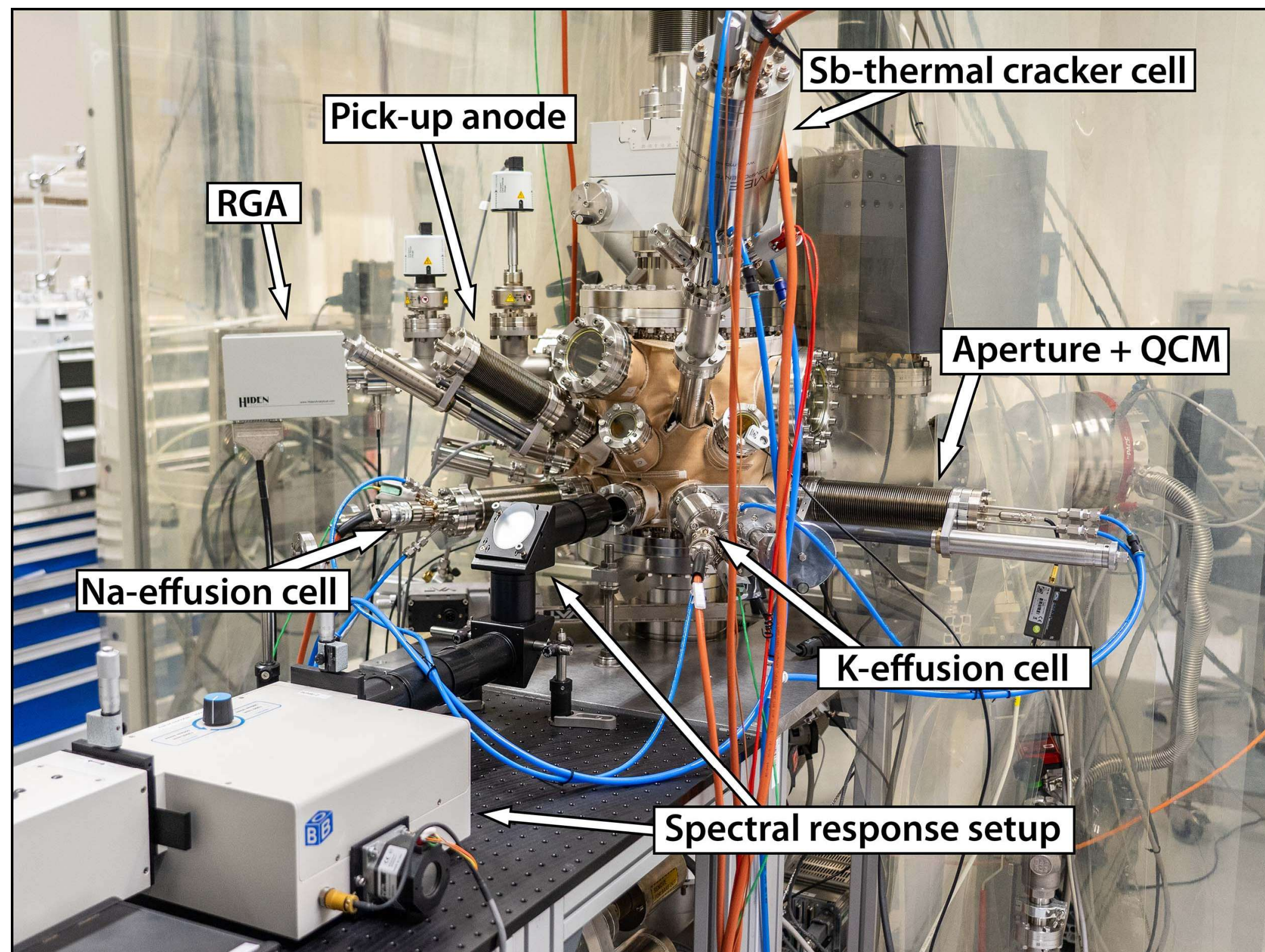
Jena Electronic Theory and Spectroscopy

<https://www.physik.uni-jena.de/en/25597/cocchi-group>

Outline

- Motivation
- Objectives
- Methods
 - **The BESSY-II synchrotron facility and EMIL laboratory**
 - **Preparation and transport of samples**
- Results
 - **X-ray photoelectron spectroscopy with soft and hard x-rays**
 - **Near edge X-ray absorption spectroscopy fine structure (XAS-NEXAFS)**
- Conclusions

- Na-K-Sb photocathodes are the choice for several linear accelerator and test facilities
 - **CBETA@Cornell University (USA) – DC photoinjector**
 - G. H. Hoffstaetter et al., 10.18429/JACoW-IPAC2018-TUYGBE2
 - **MEDUSA@Cornell University (USA) – DC gun**
 - W.H. Li, C.J. Duncan et al. Struct. Dyn. 9, 024302 (2022);
 - **SEALab@HZB (DE) – SRF photoinjector**
 - Seen in Jonas Dube's talk on Monday, J. Dube et al. Phys. Rev. Materials, 10 (7),074601(2026)
 - **Pegasus@UCLA (USA)– S-band RF photoinjector (high-gradient testing)**
- Facilities that foresee the use of Na-K-Sb photocathodes
 - **DALI@HZDR (DE)**
 - [DALI – Dresden Advanced Light Infrastructure - Helmholtz-Zentrum Dresden-Rossendorf, HZDR](#)
 - **LCLS-II-HE@Stanford University (USA)**
 - J. H. Lewellen et al., 10.18429/JACoW-NAPAC2022-TUYD3



- Na, K
- 10 per effusion cell
- stable in air
- QCM calibration

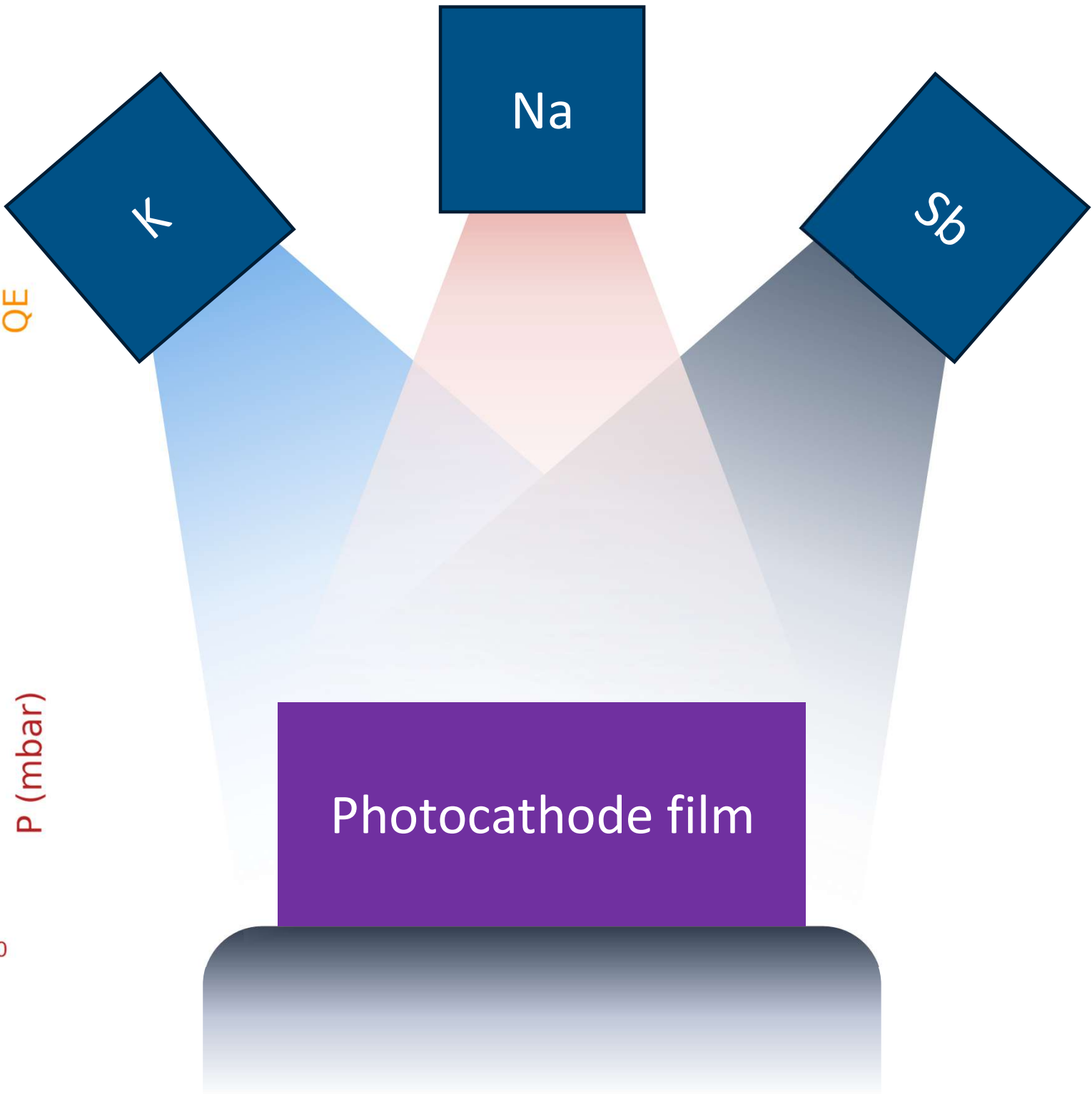
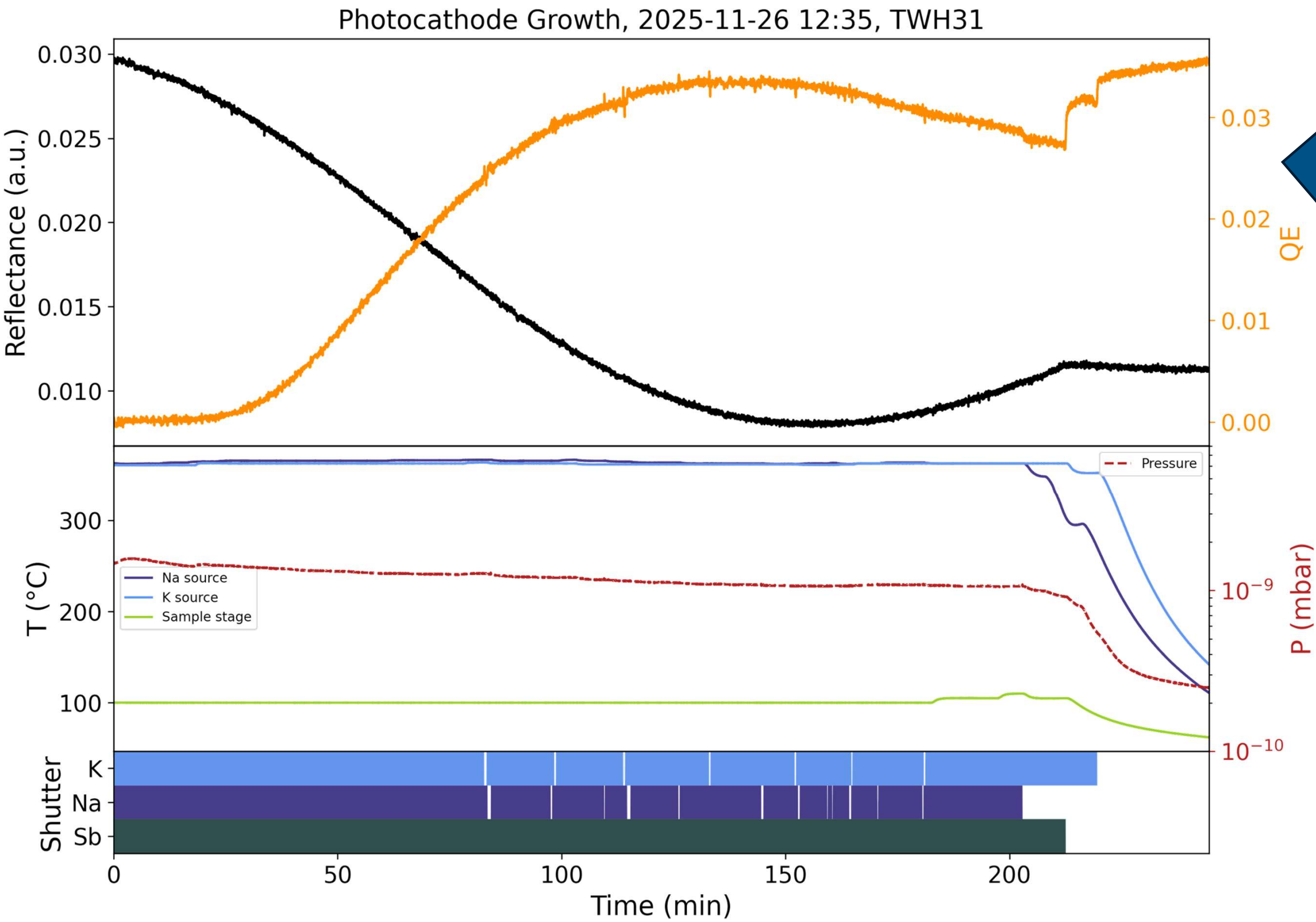
Dube et al., J. Appl. Phys. 138 (2025) 045704.

Wang, C. et al., J. of Phys. D: Applied Physics 59.7 (2026) 075102.

Triple-evaporation growth at HZB

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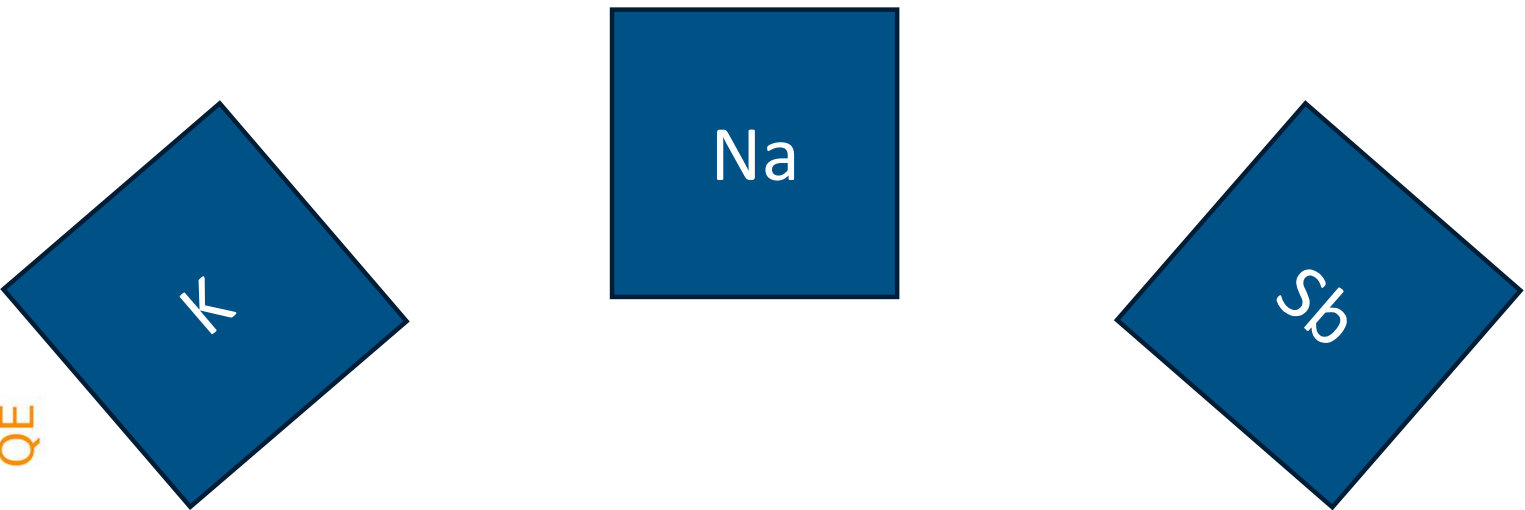
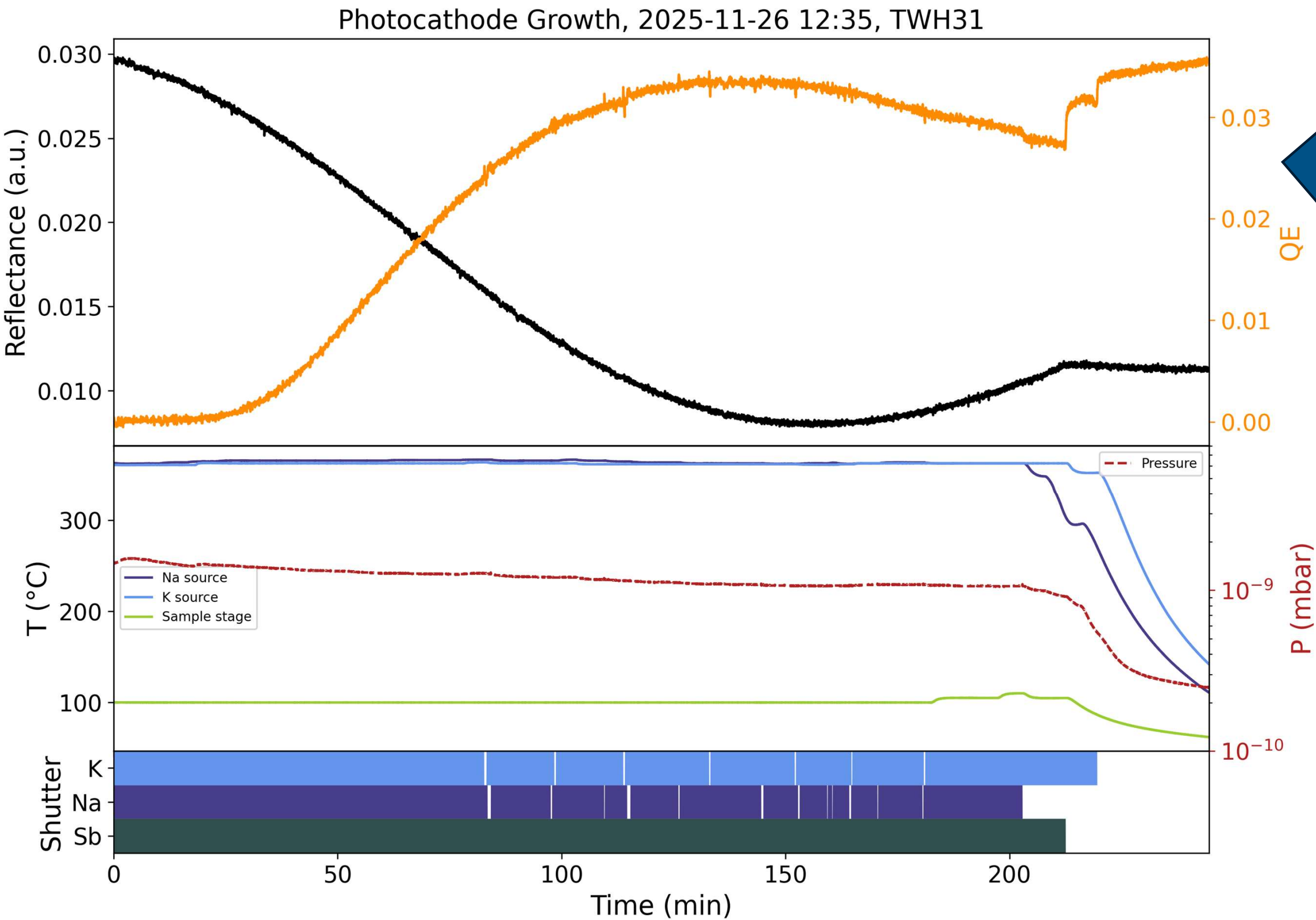




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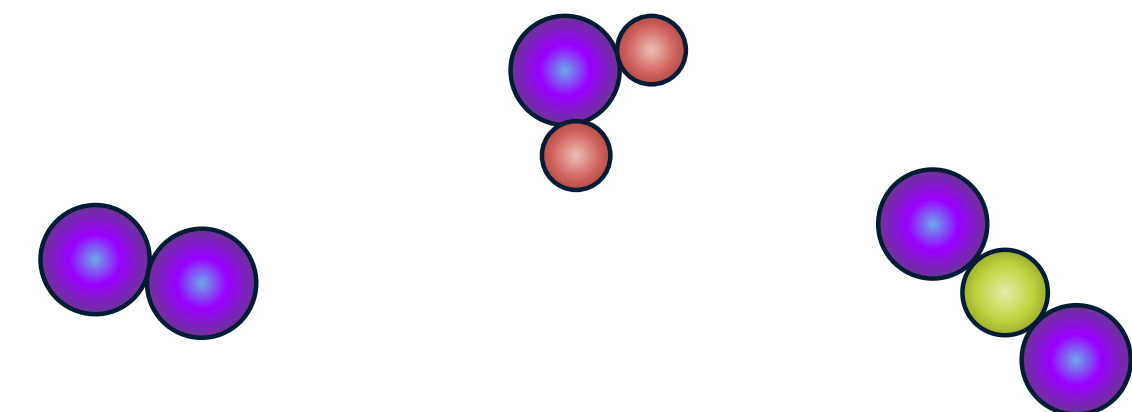
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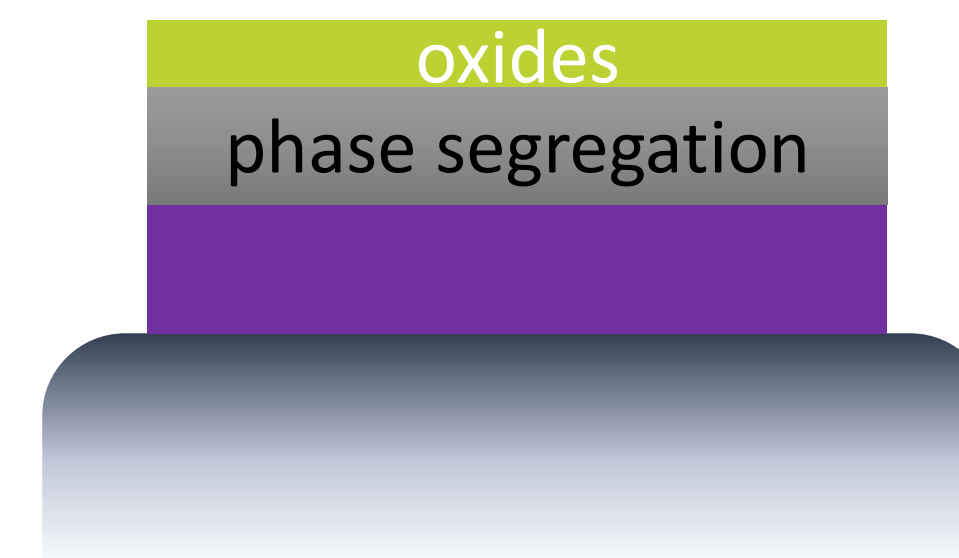
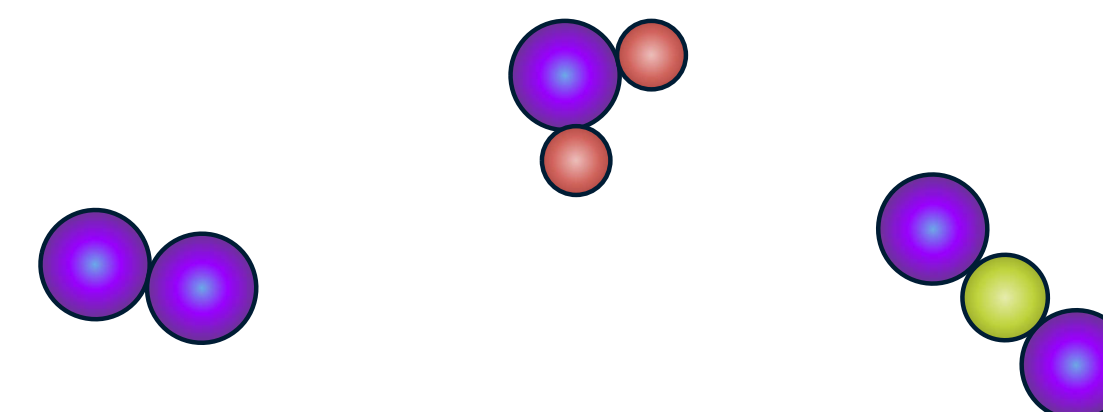
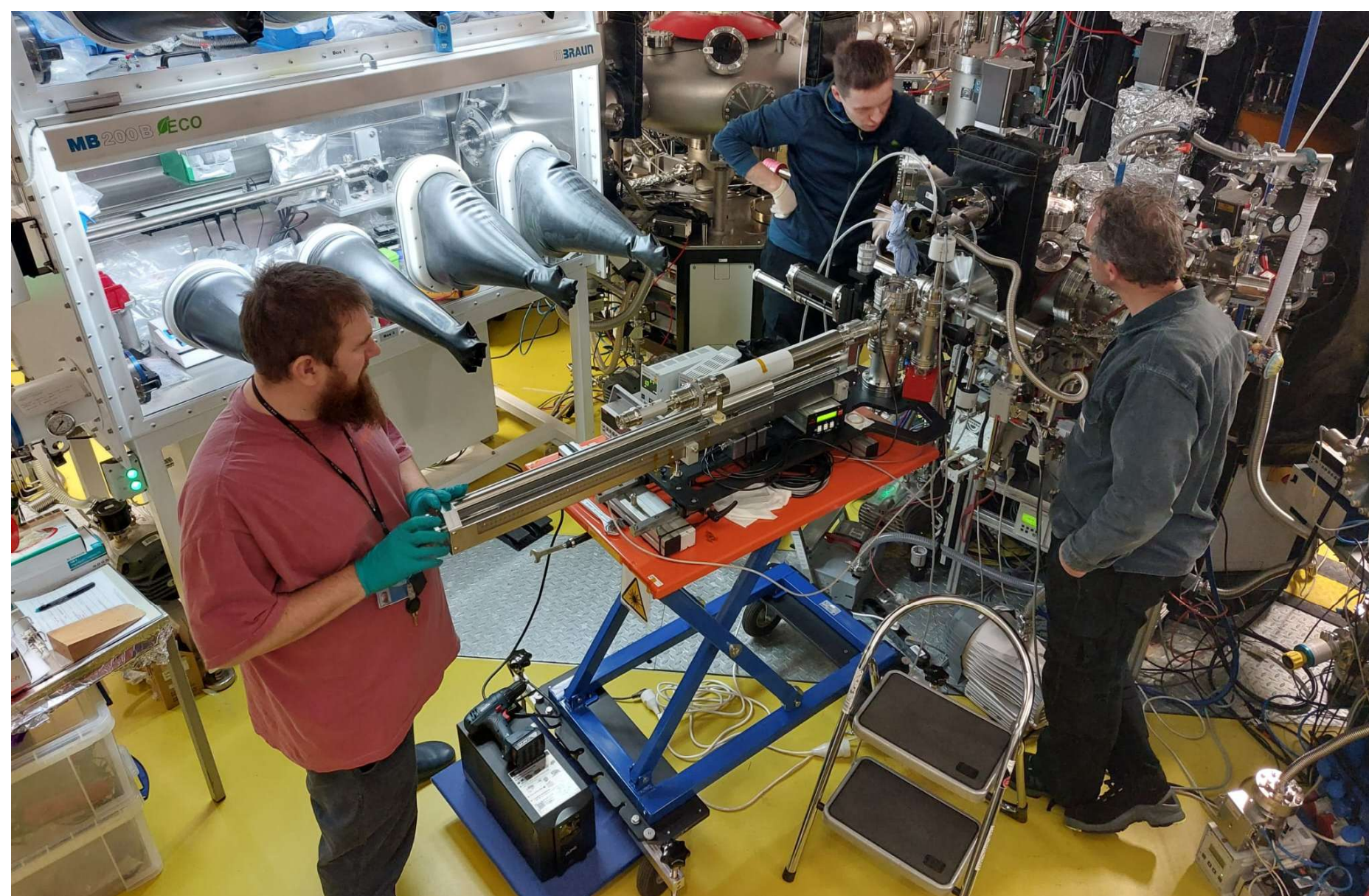
Final stoichiometry?
Uniformity?
Composition profile?



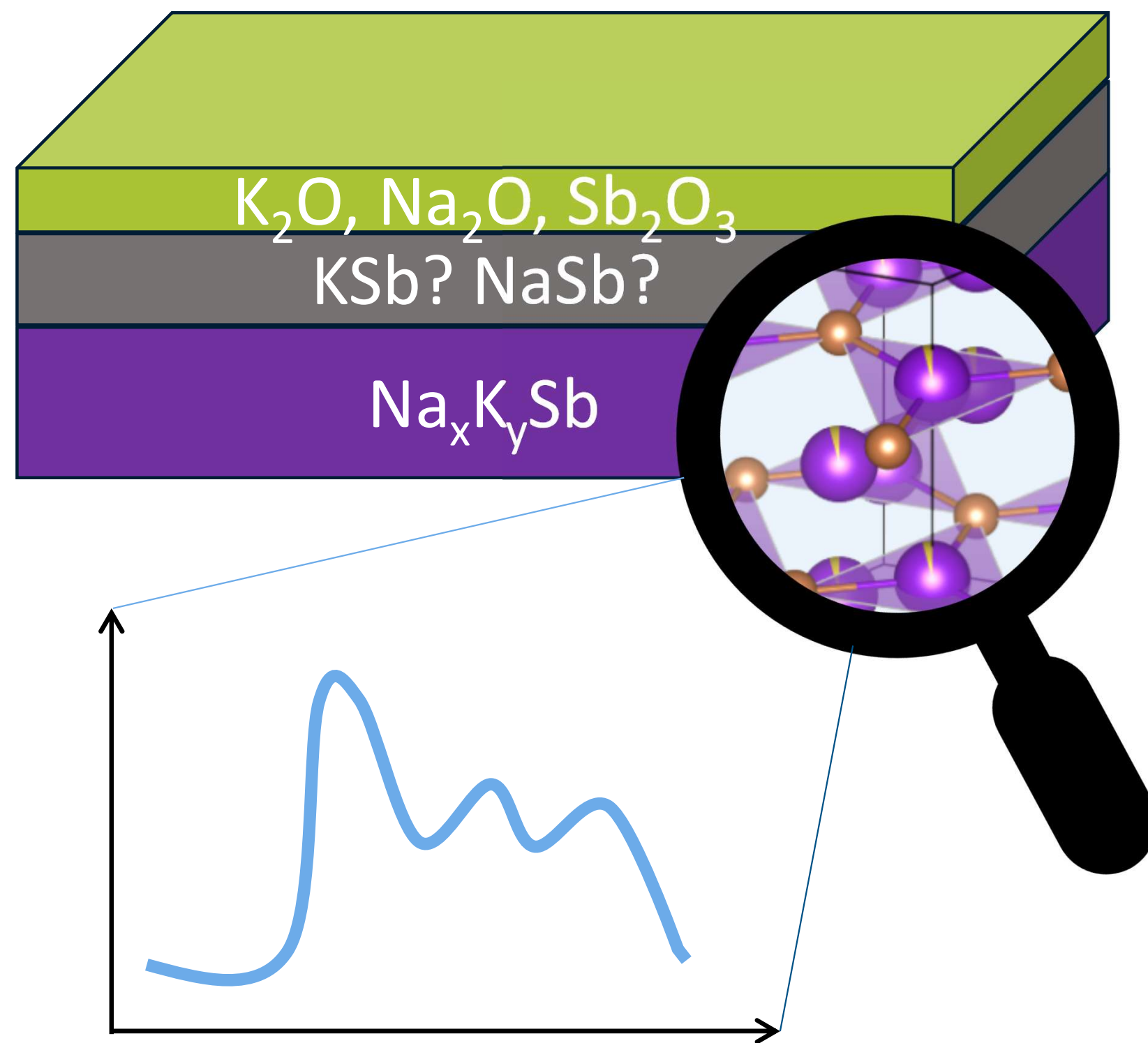
Photocathode transfer and ageing



Photocathode transfer and ageing



Objectives



- Model the composition profile of Na-K-Sb photocathodes
 - **Origin: growth procedure, surface oxidation, ageing**
 - **Connect to: QE, lifetime, MTE**
- Experimental verification of structural and electronic properties
 - **Valence states**
 - **Crystal symmetry**
 - **Band structure**

HZB: Wilhelm-Conrad-Röntgen-Campus Berlin-Adlershof

EMIL

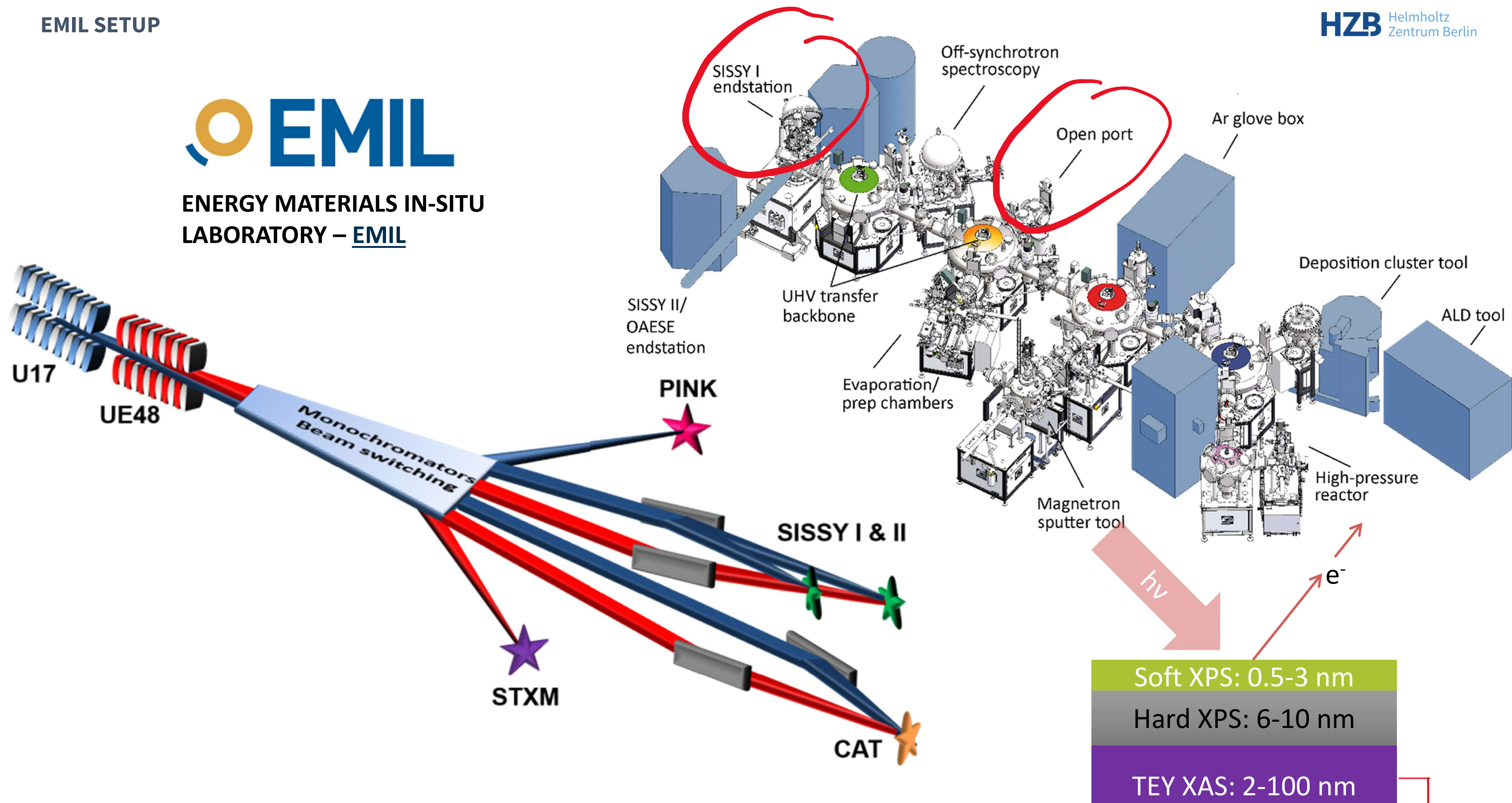
BESSY II

PHOTOCATHODE LAB
MTE LAB

SEALAB

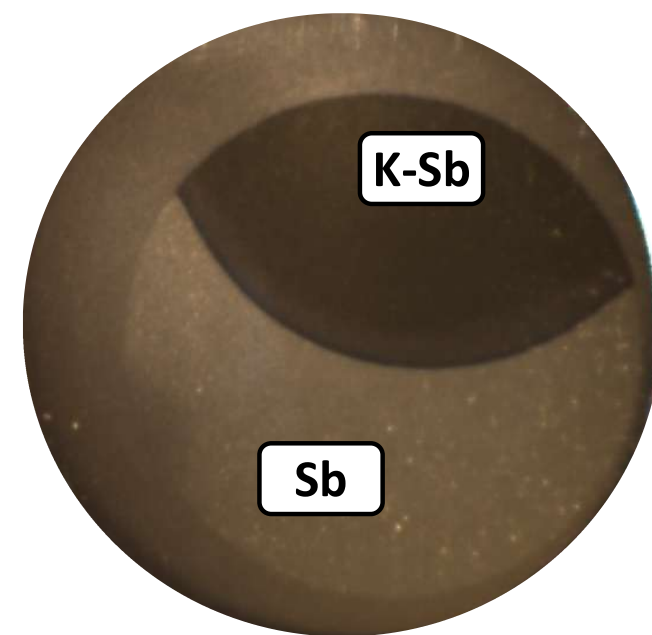


ENERGY MATERIALS IN-SITU
LABORATORY – EMIL



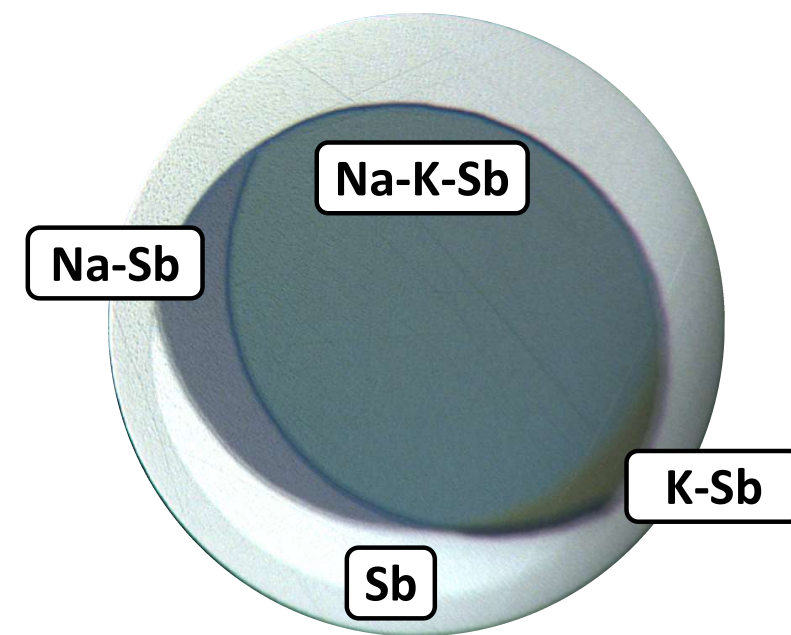
Soft XPS: 0.5-3 nm
Hard XPS: 6-10 nm
TEY XAS: 2-100 nm

TWH28



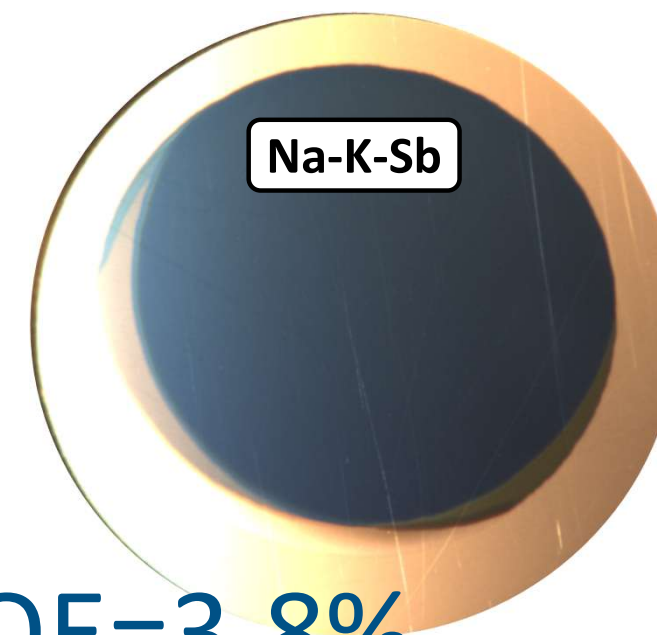
pure Sb
with „K₃Sb“

TWH29



“library approach”
with “NaK₂Sb”

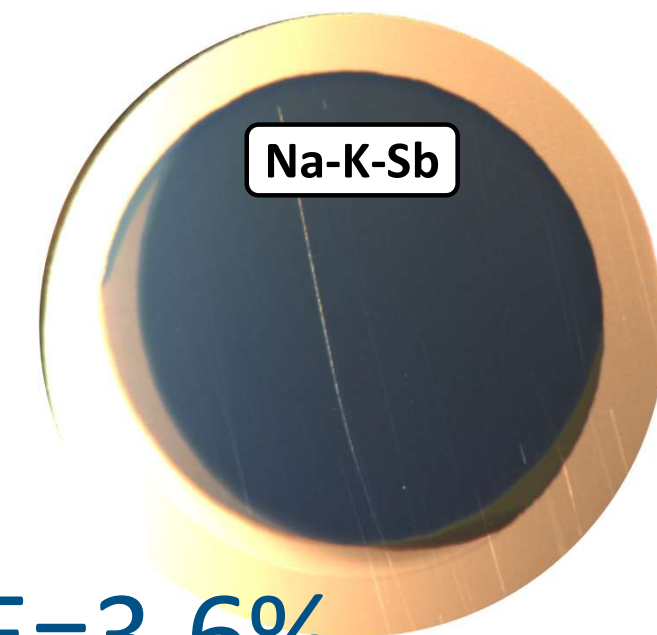
TWH30



QE=3.8%

“Na₂KSb”

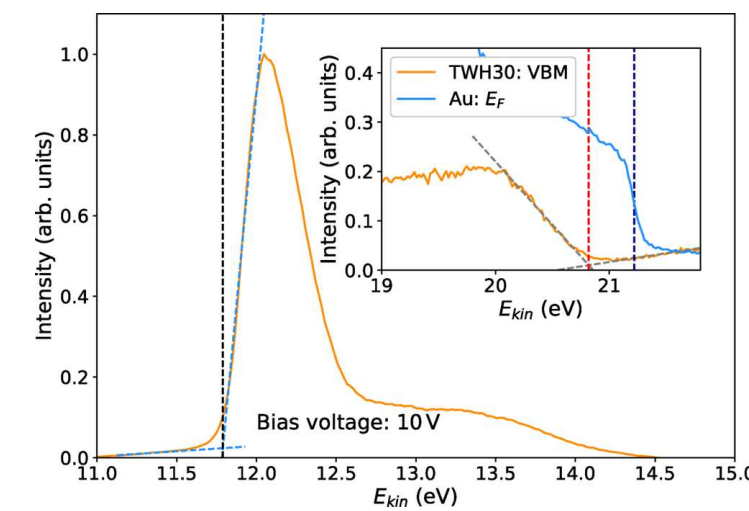
TWH31



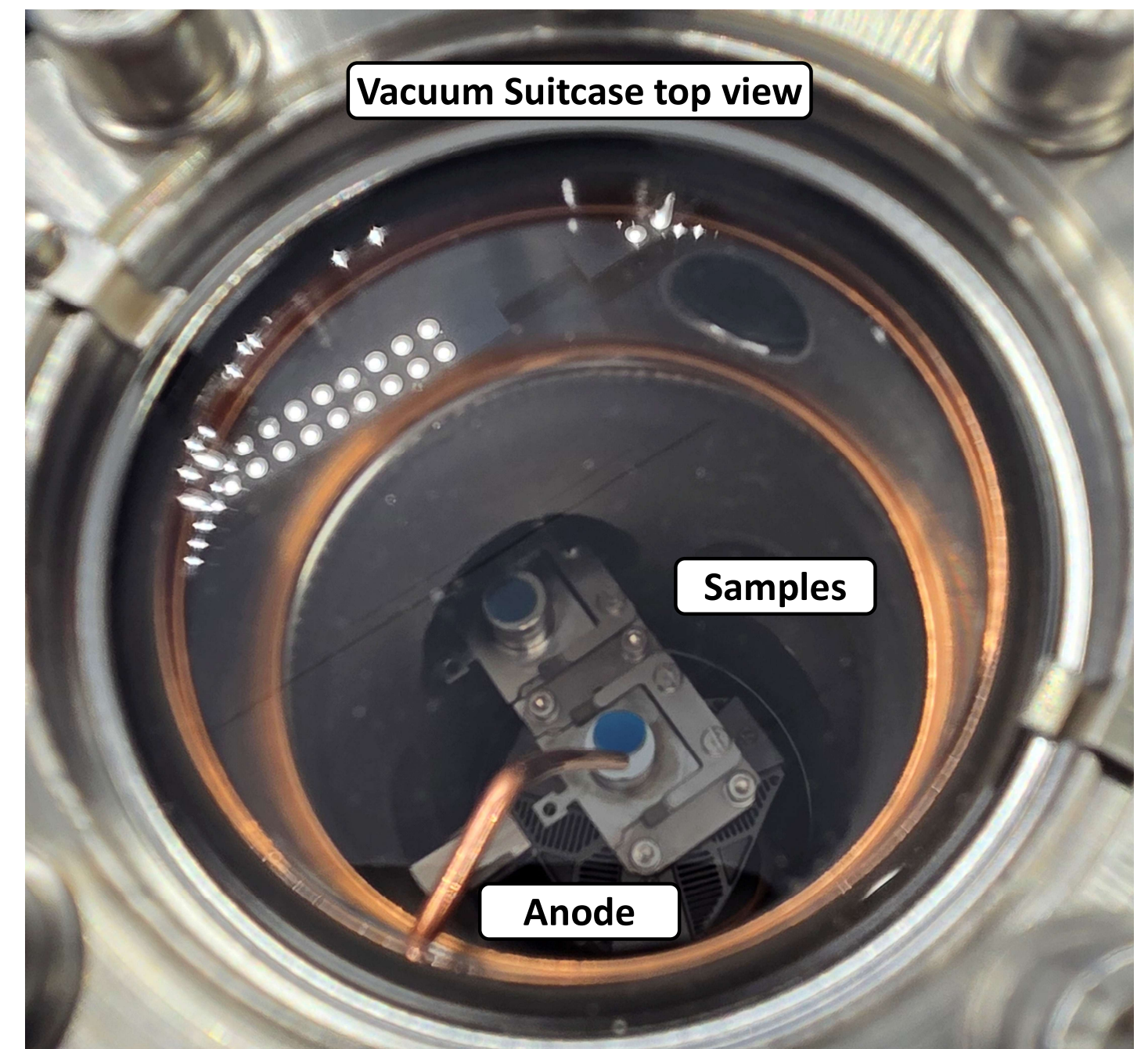
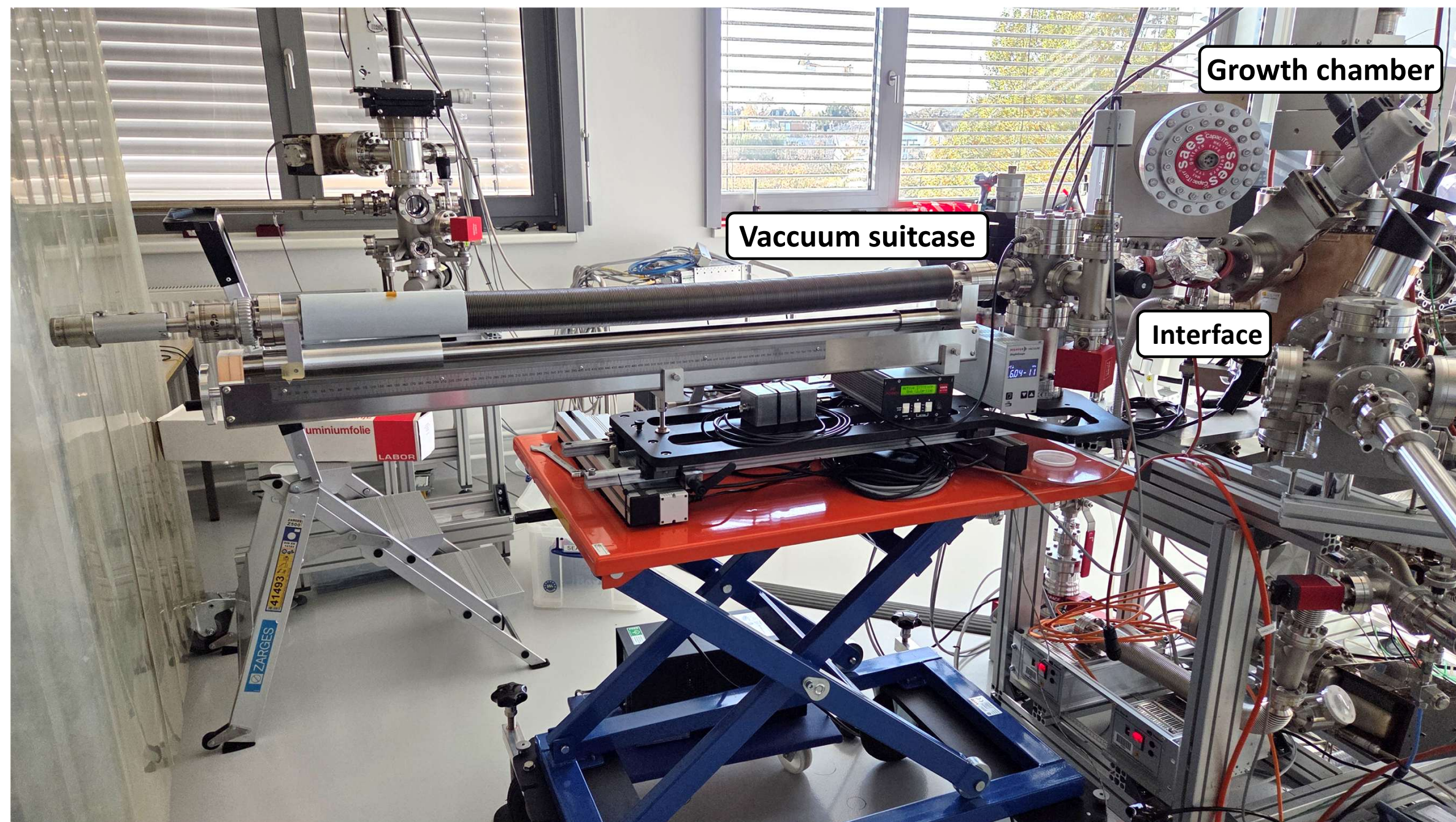
QE=3.6%

“Na₂KSb”

UPS@EMIL



Dube, et al., *Phys. Rev. Materials* 10.7 (2026) 074601.



- Vacuum level $< 1\text{E-}10\text{mbar}$
- height adjustable for different purposes: Growth, PhoTEX, EMIL
- Manipulator with bellow instead of transfer arm: better vacuum during transfer motion
- Pincer for omicron flag-style sample holder
- Sample garage with 4 slots
- QE measurement via anode
- UPS for gauge, IGP and QE-measurement

TWH31: QE = 3% after transfer to EMIL!

Measurements results



Preliminary XPS results

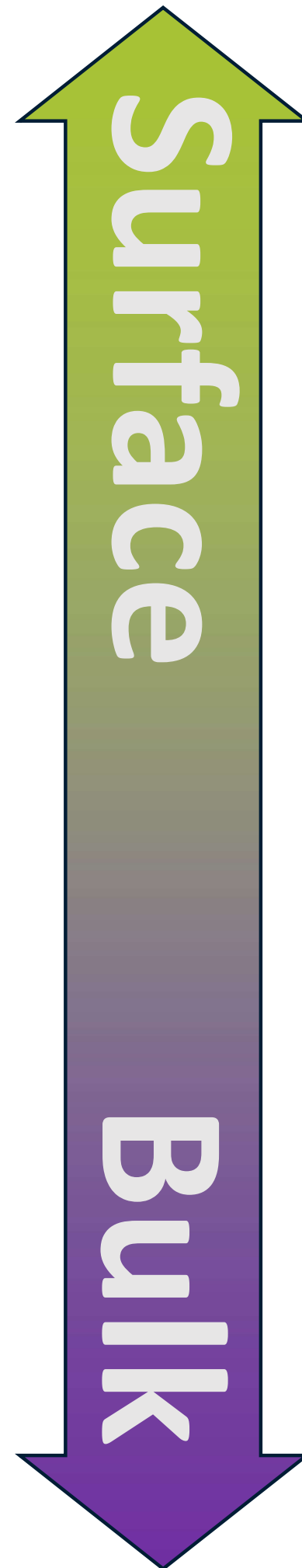
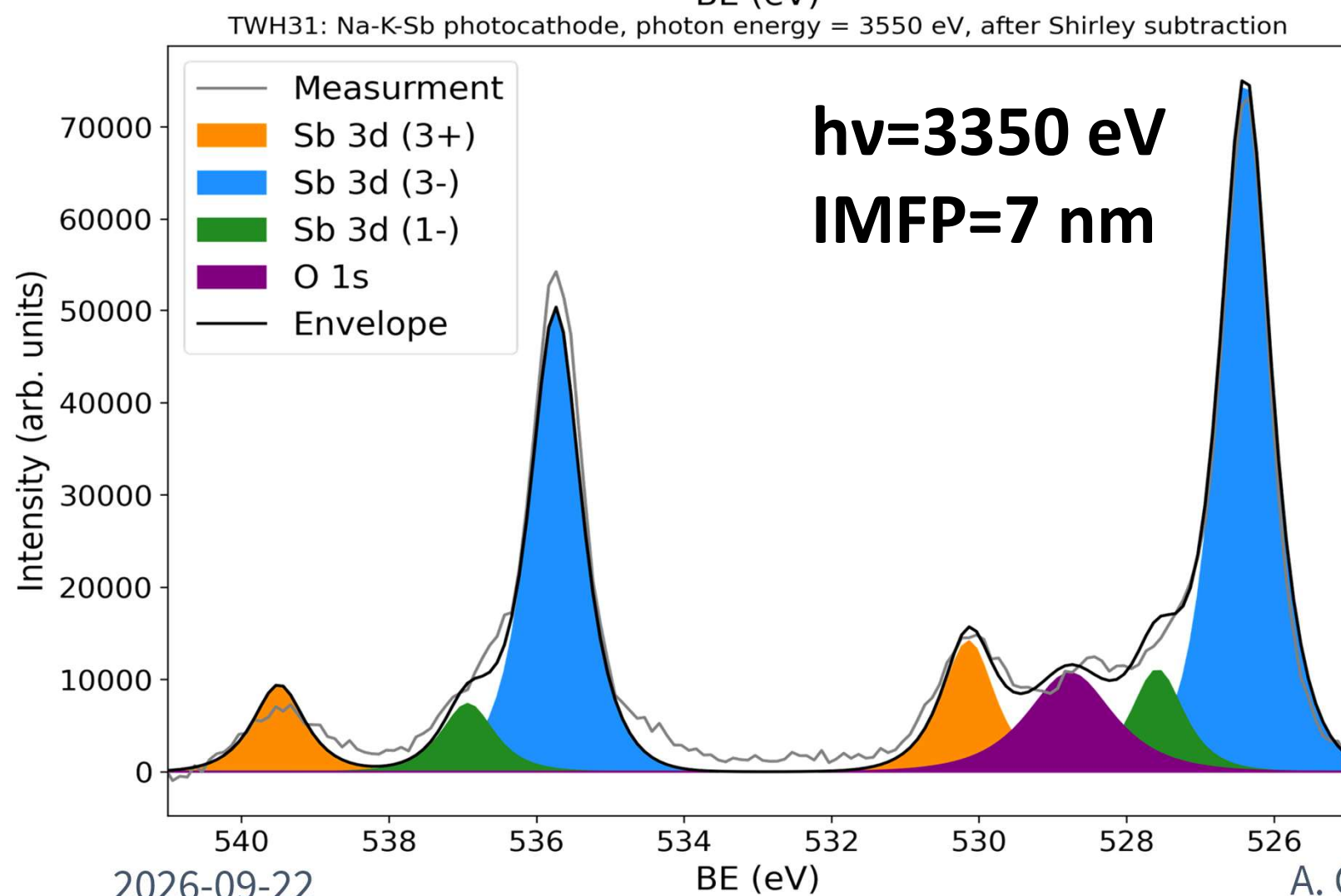
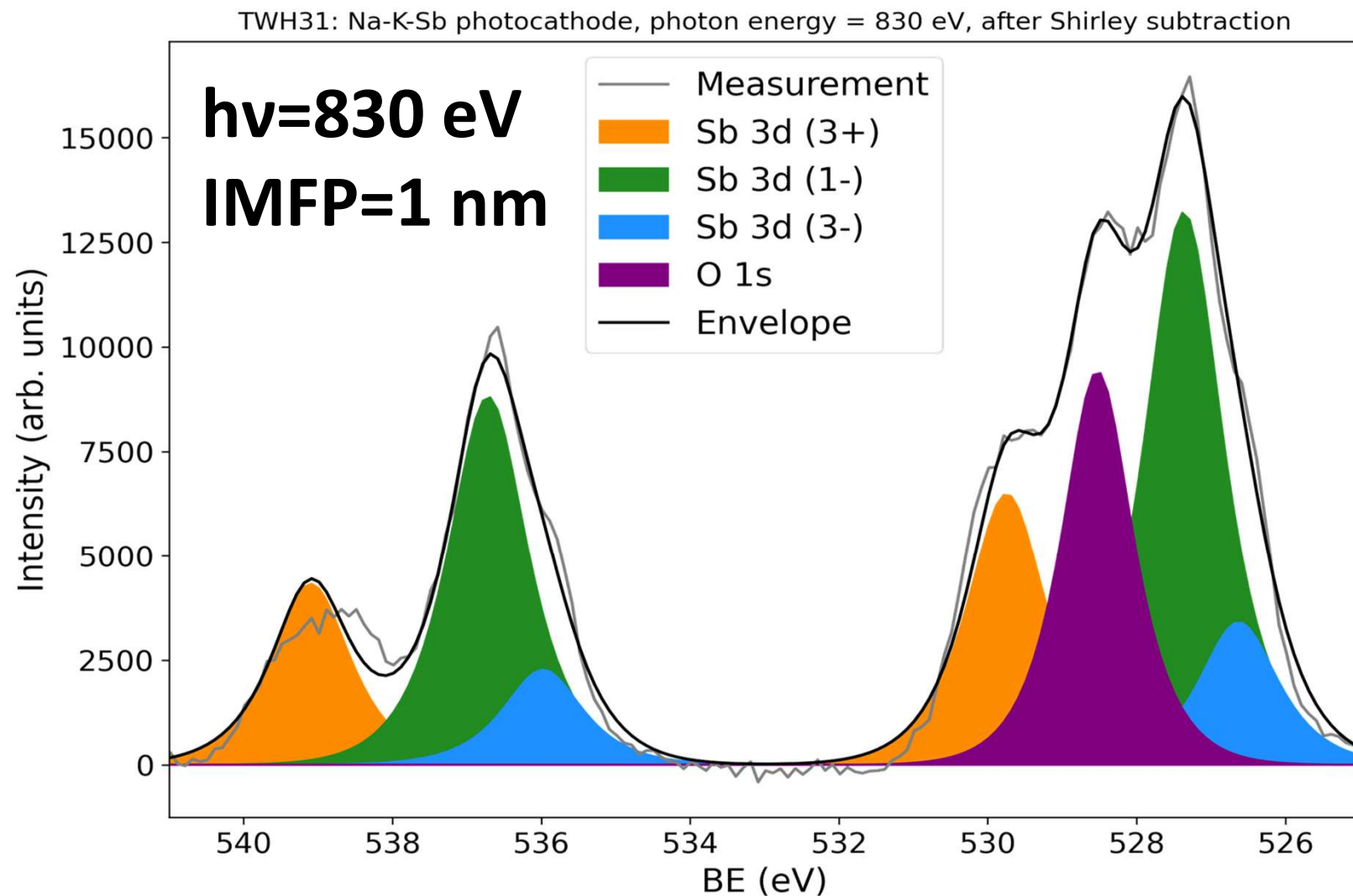


Preliminary XAS results



Comparison with theory

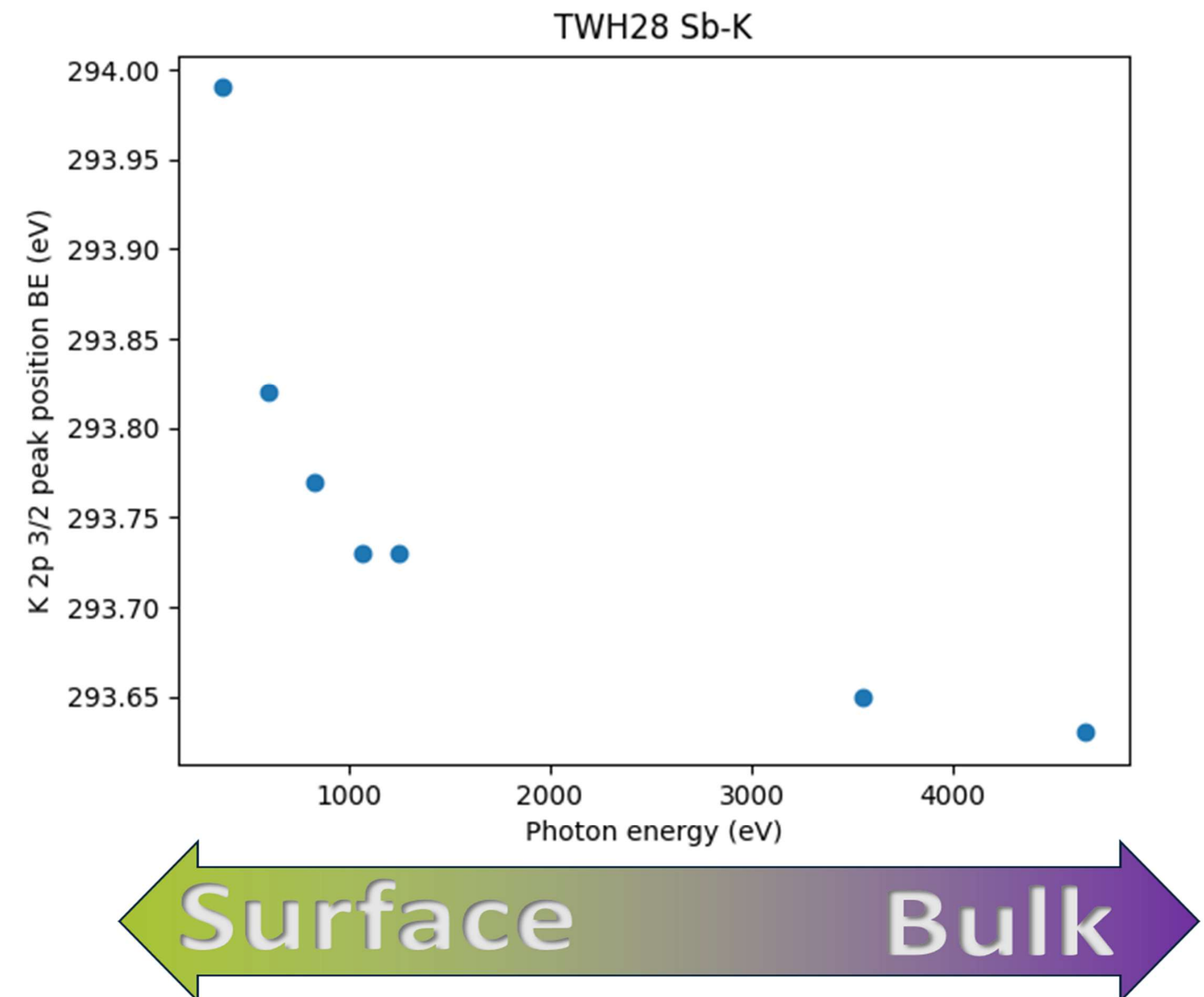
XPS RESULTS



- XPS measurements with varying photon energy: **370 eV to 4660 eV**
- IMFP from **0.5 nm to 10 nm**
- Allow to extend the probed depth beyond the limits of laboratory sources (1254 – 1487 eV)

Preliminary results on K-Sb (TWH28)

- Peak position of the K 2p_{3/2} as a function of photon energy (ref. to Au 4f)
- Lower BE for higher photon energy
- Possibly connected to the formation of potassium oxides on the surface
- Verified in controlled oxidation experiments in the photocathode lab



Preliminary results on K-Sb (TWH28)

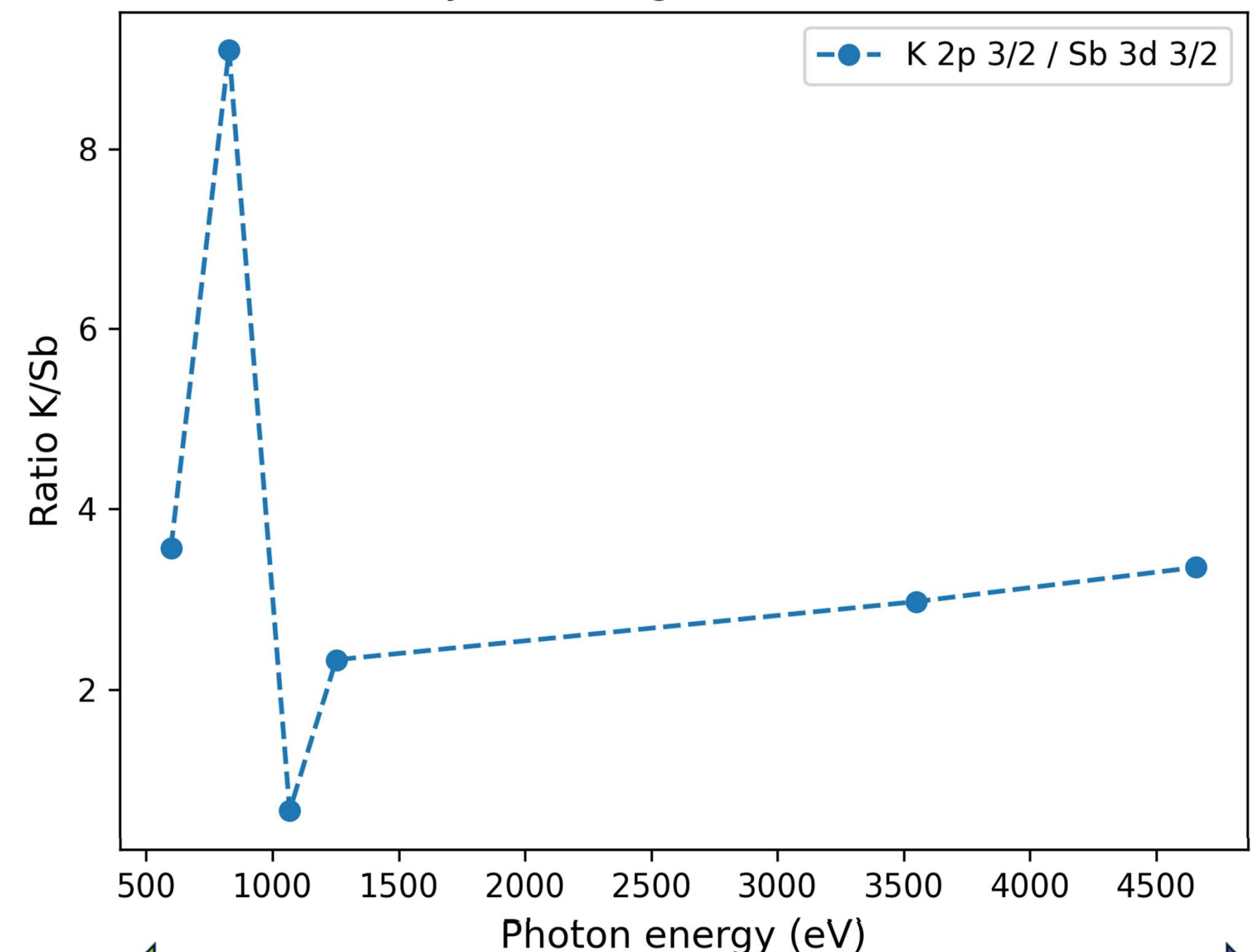
- K/Sb ratio as a function of photon energy
- Calculation of the ratios done by the following formula

$$A = \frac{Ar_A}{TF_A CS_A IMFP_A}, \quad B = \frac{Ar_B}{TF_B CS_B IMFP_B}$$

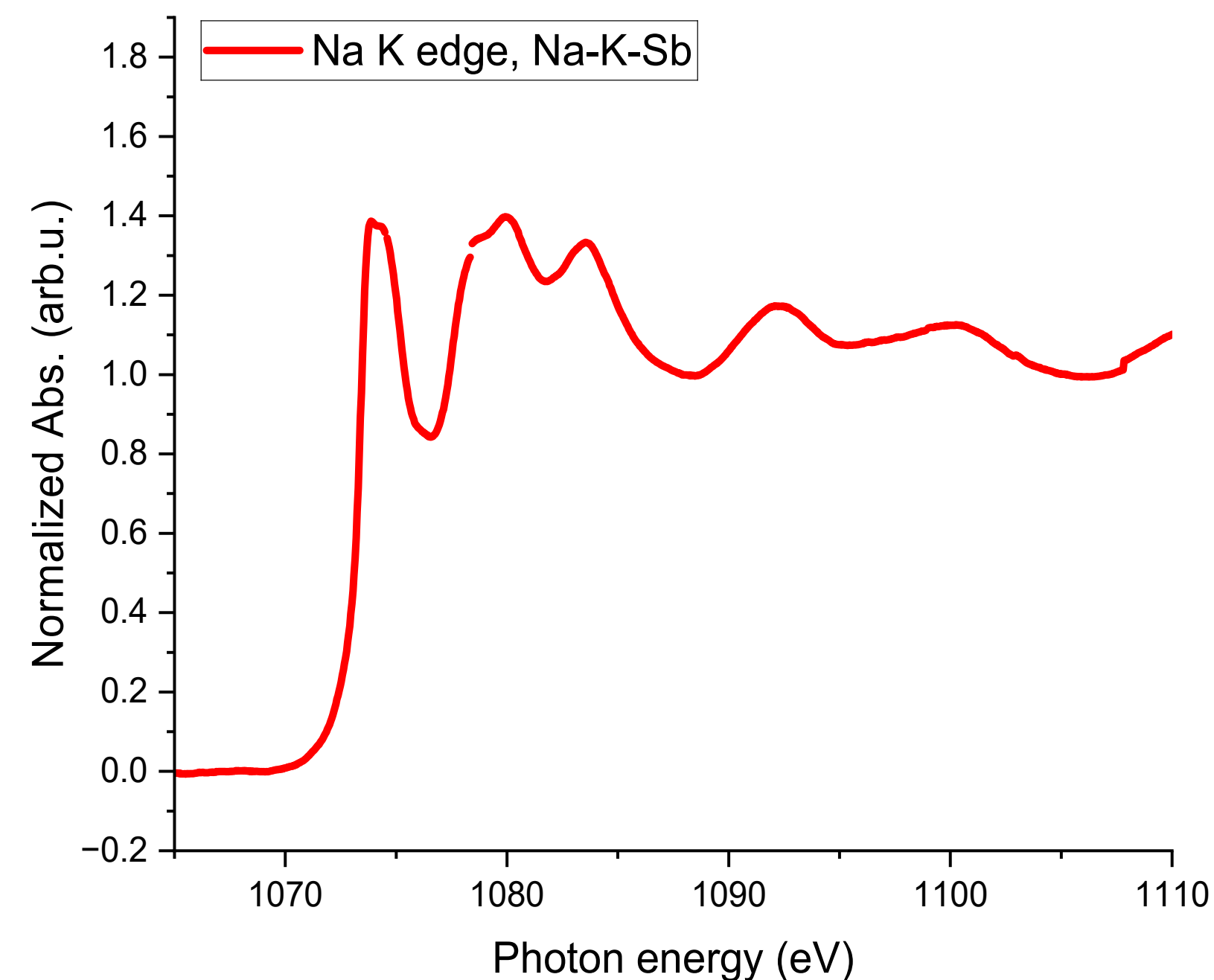
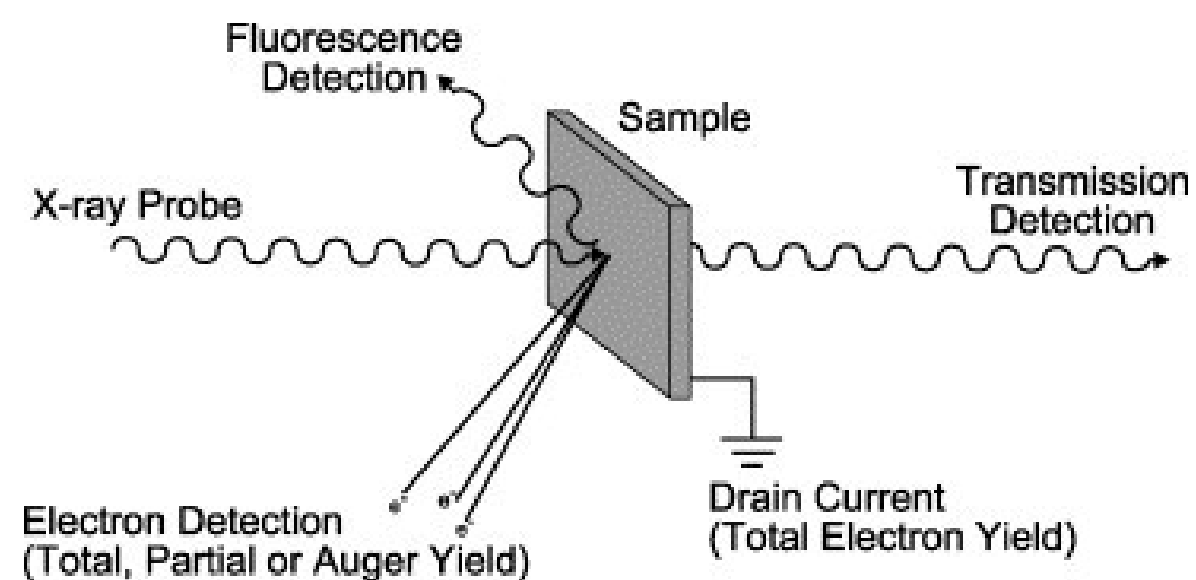
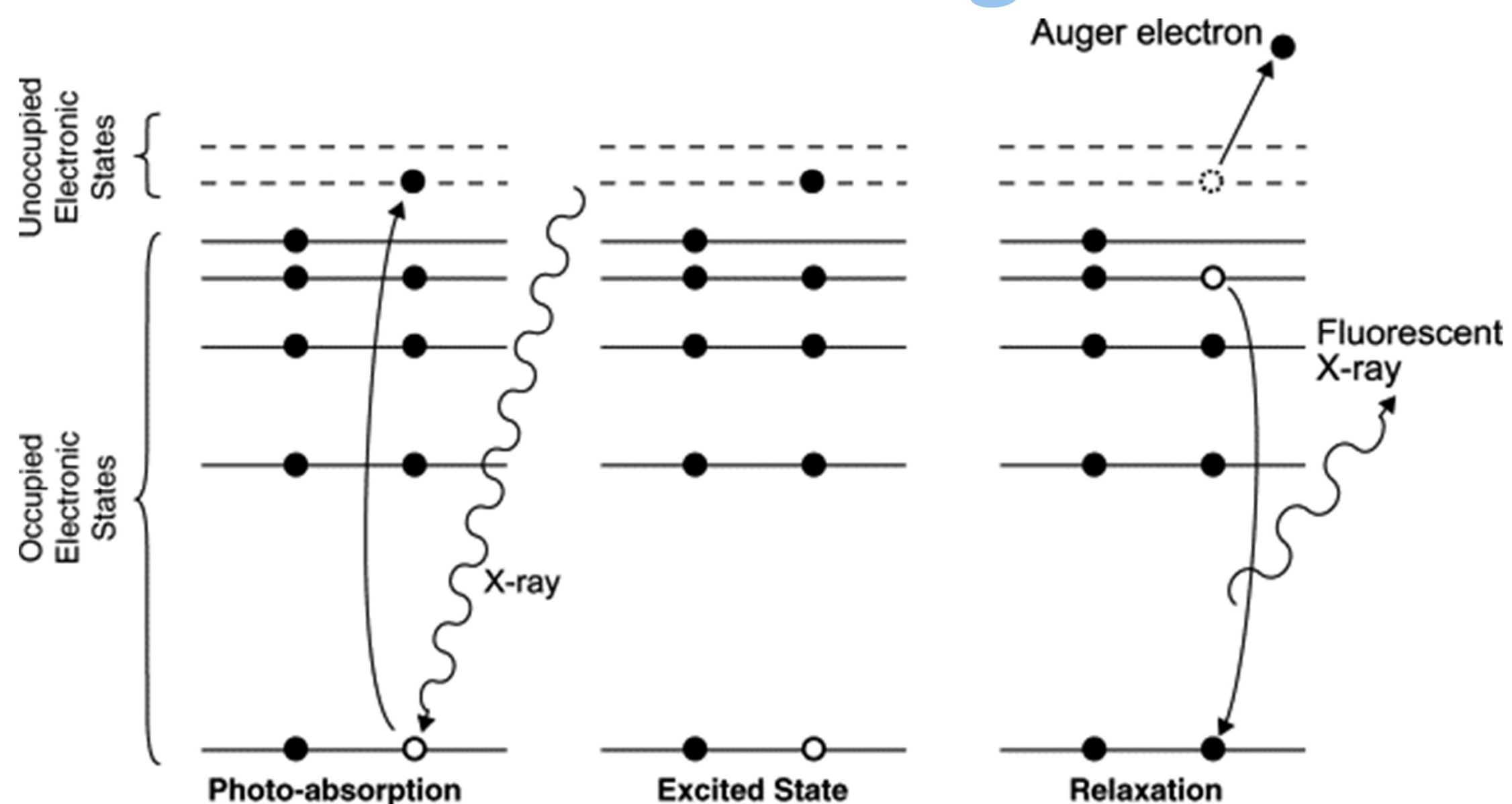
$$Ratio = \frac{A}{B}$$

- Strong variations at low photon energy
- At high photon energy K/Sb $\rightarrow$ 3

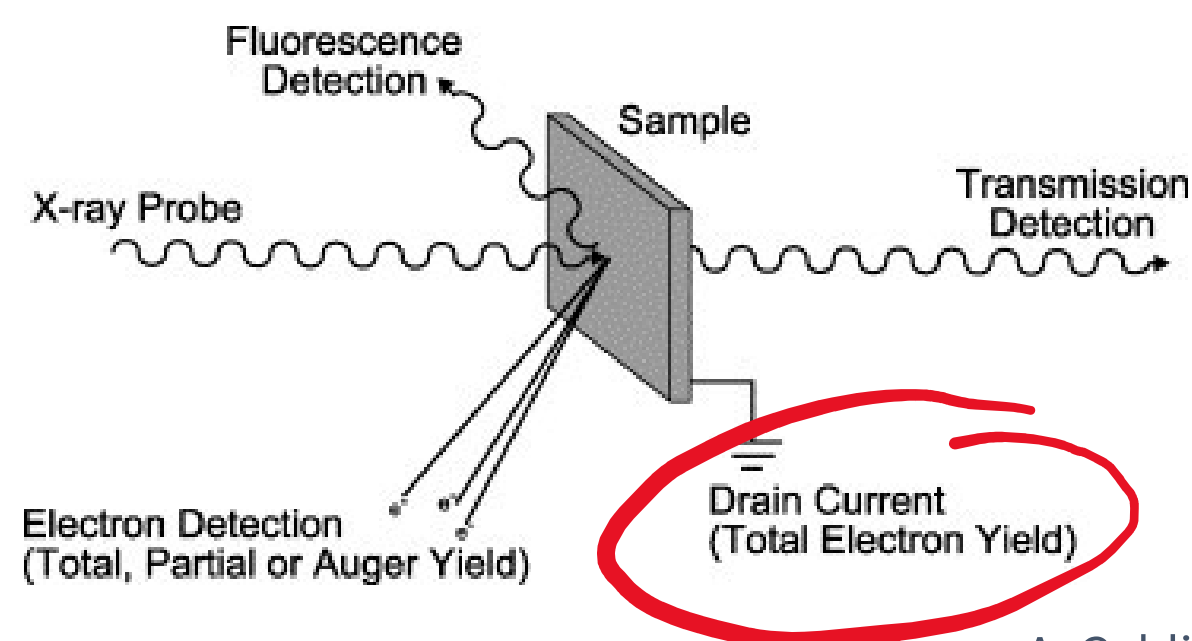
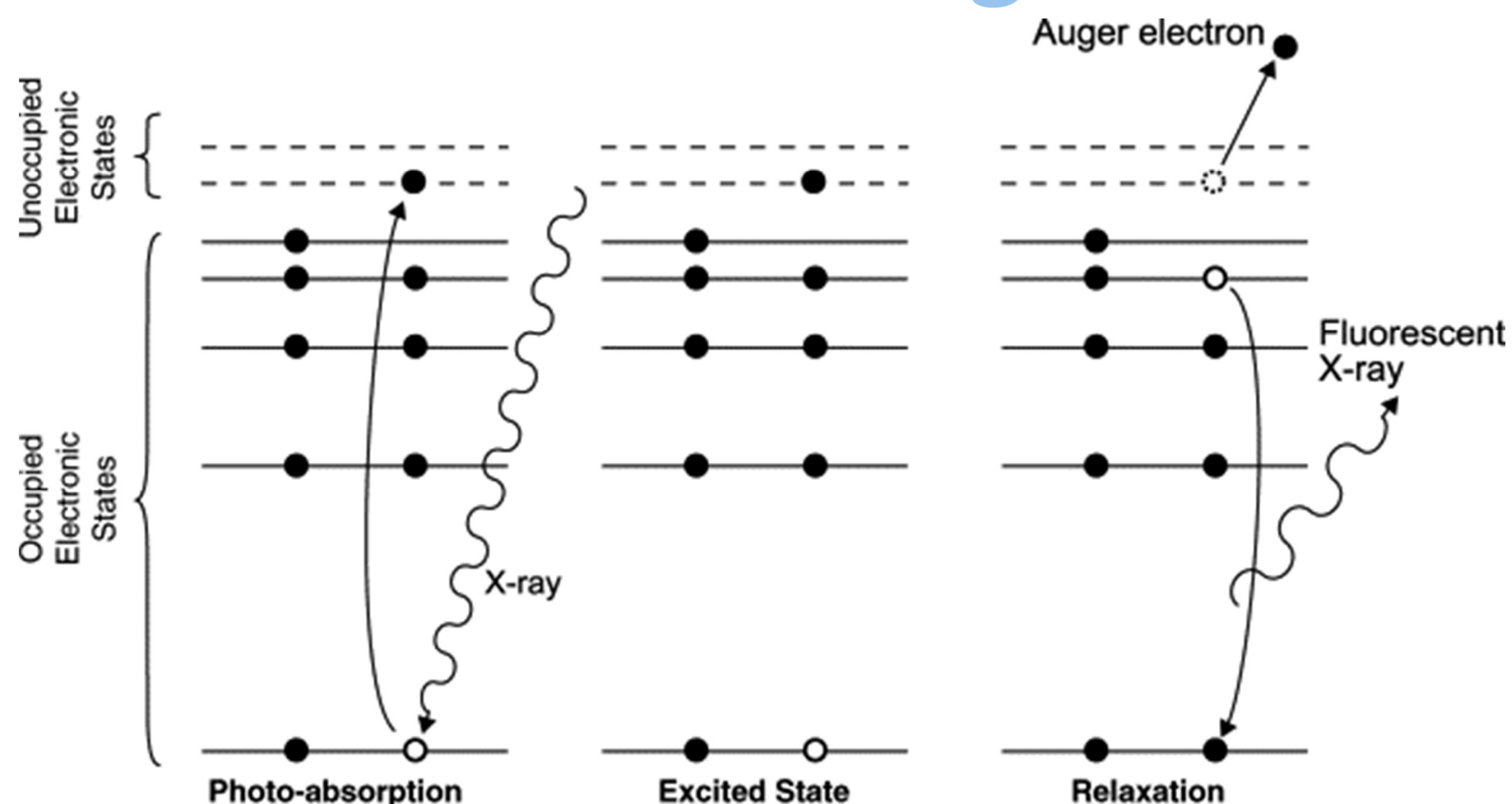
TWH28 Sb-K, corrected with TF, cross section and IMFP
K3Sb with density of 2.618 g/cm³ was used for IMFP calc



Near-edge fine structure in XAS

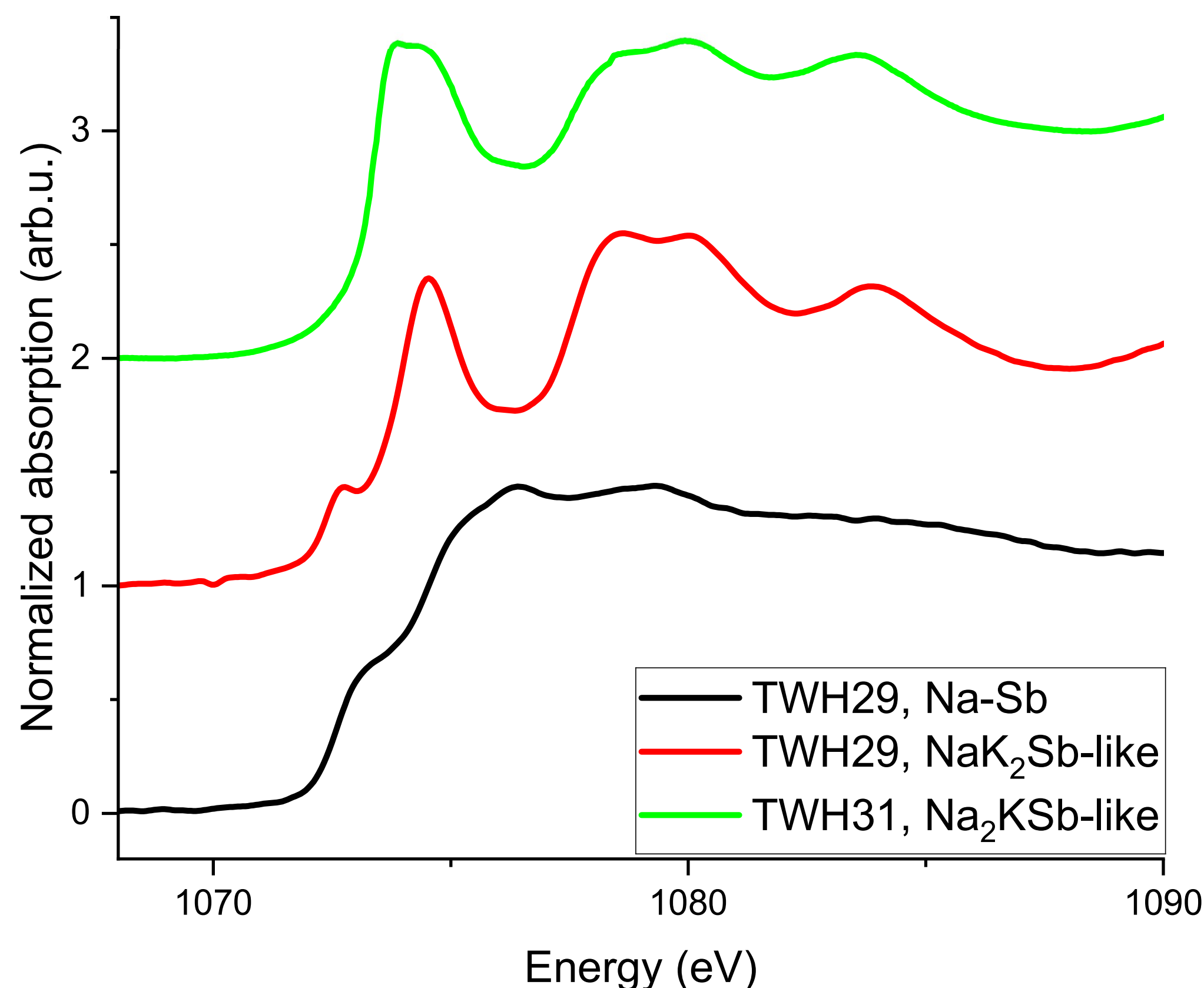


Near-edge fine structure in XAS



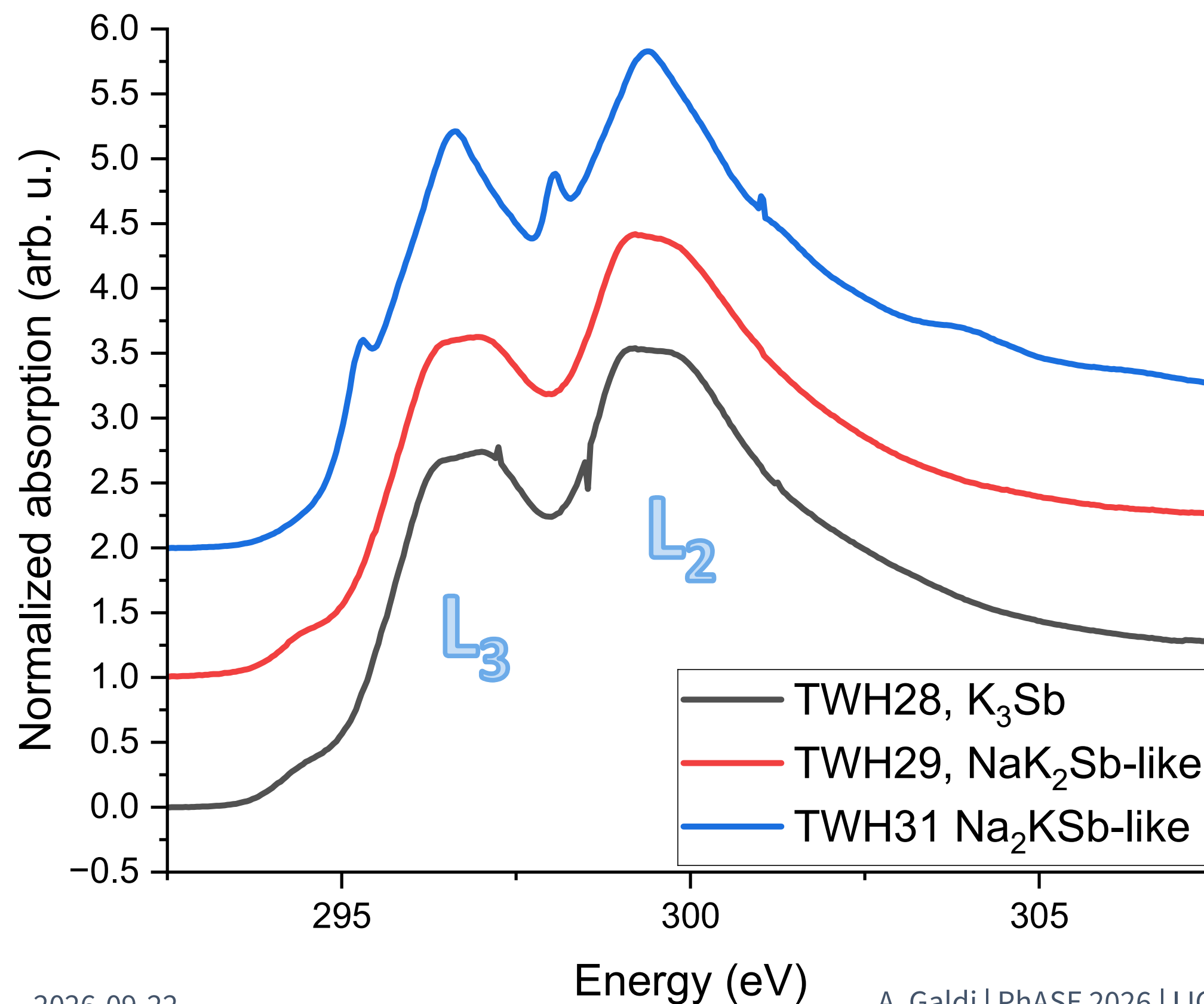
- **K-edge**
From 1s state (Na, K)
- **L_{2,3}-edge**
From 2p state (K, Sb)
- **L₁ edge**
From 2s state (Sb)
- **M_{4,5}-edge**
From 3p state (Sb)

K-edge measurements



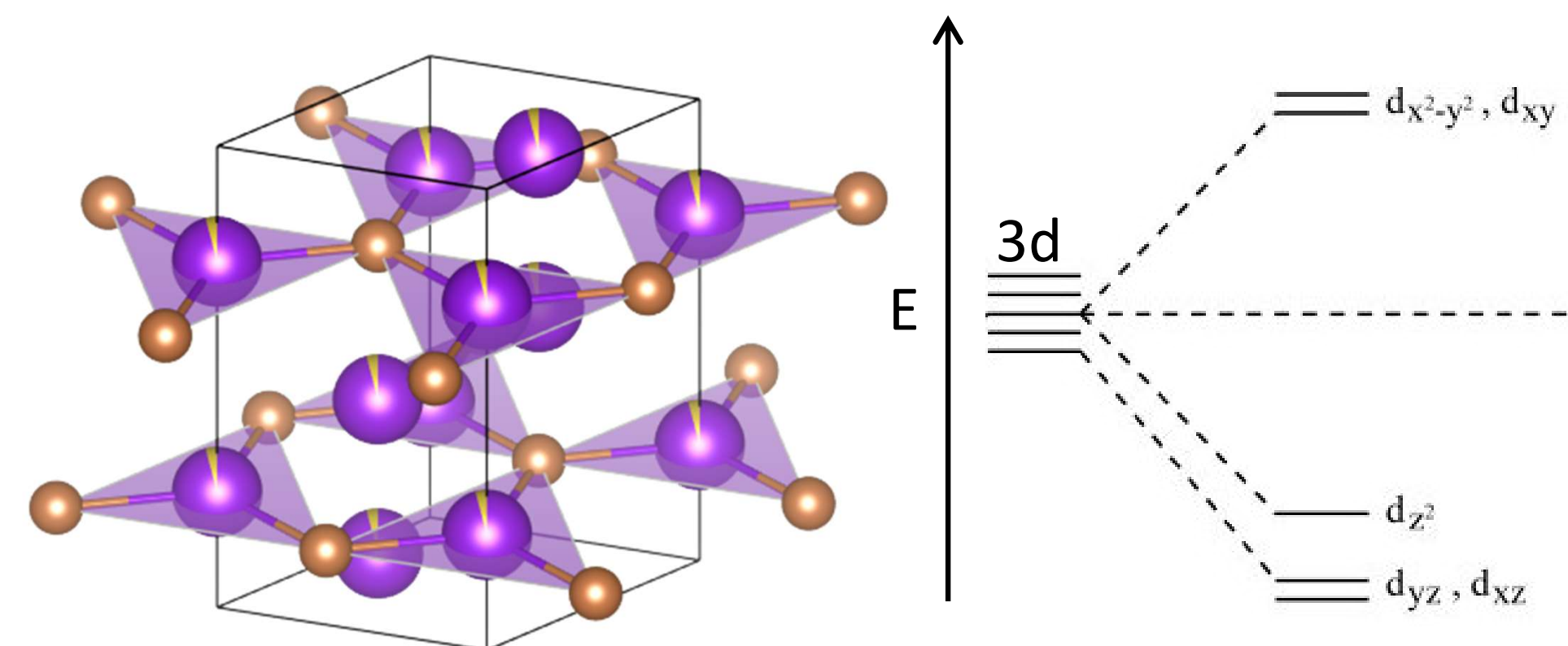
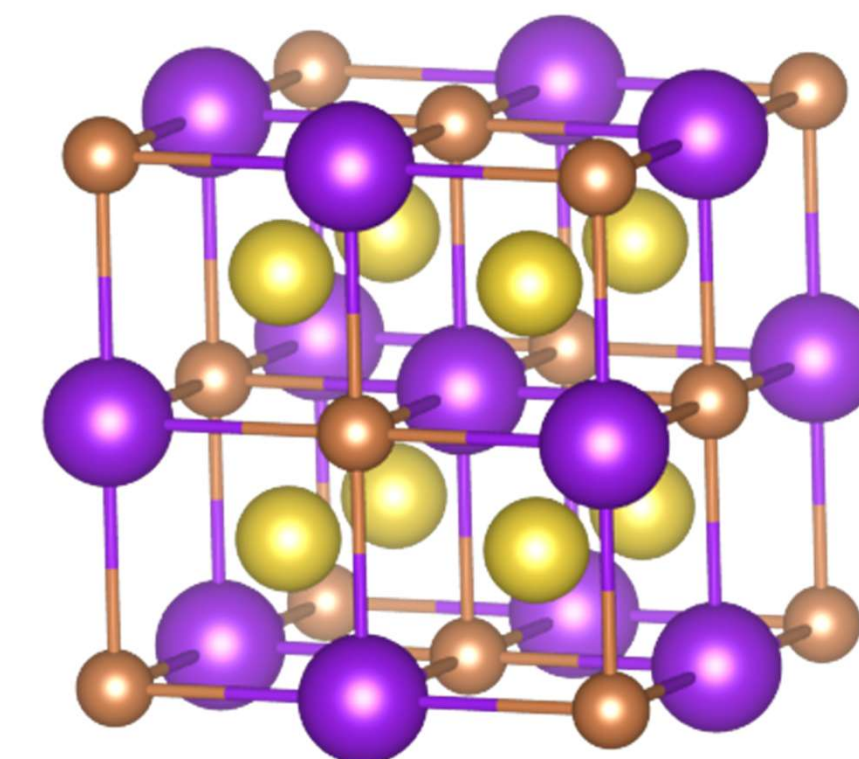
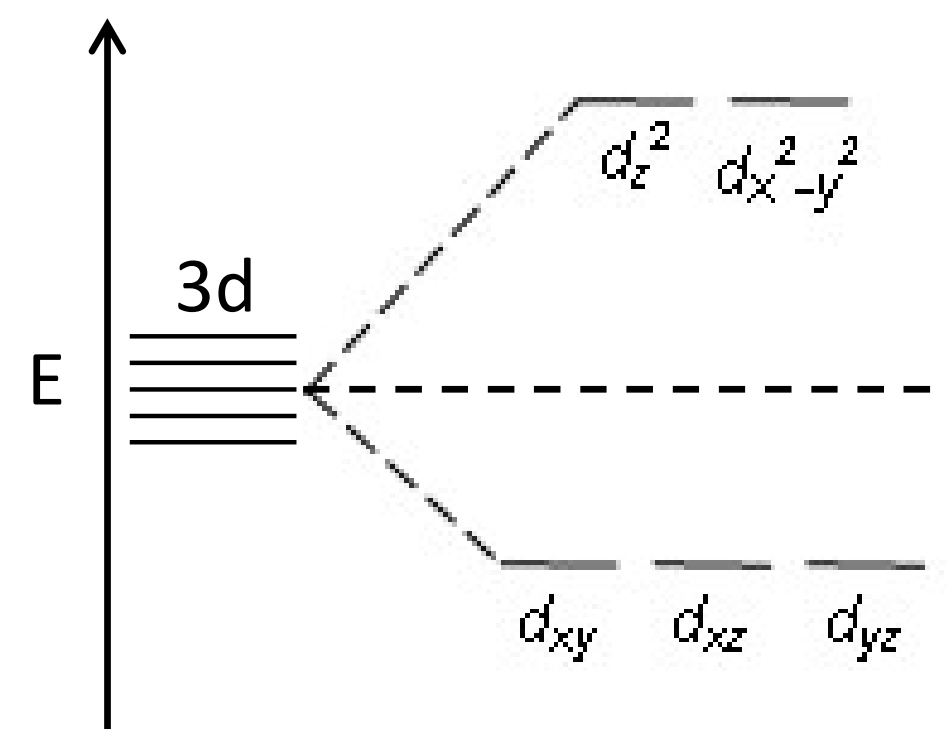
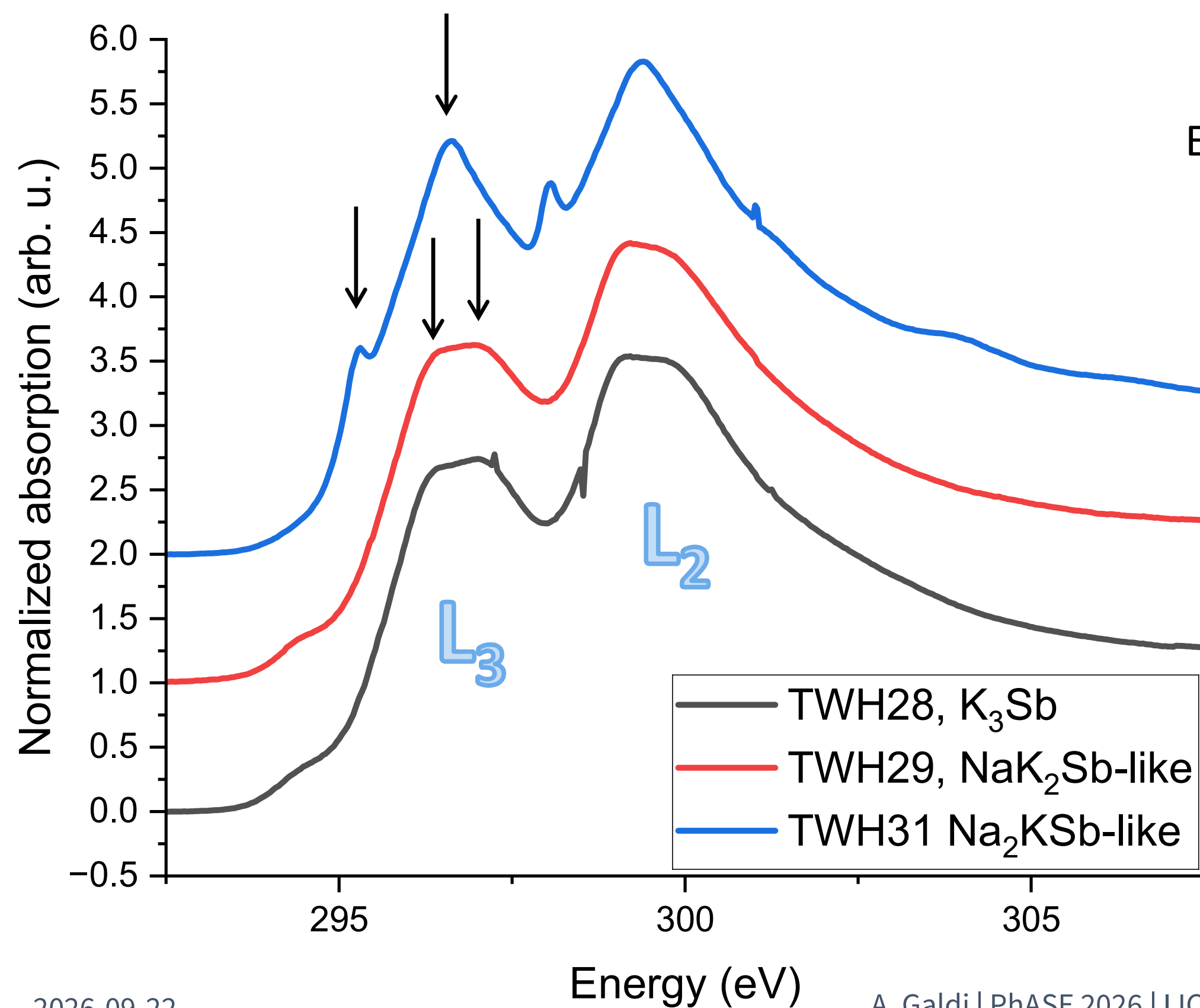
- **Na⁺ K-edge (1070 – 1100 eV)**
main transition:
 $1s^2 3p^0 \rightarrow 1s^1 3p^1$
- **MPD $\approx$ 3 nm**
- **Na-K-Sb spectra much richer than Na-Sb**
- **NaK₂Sb – Na₂KSb spectra appear markedly different**
- **K-edge reproduces the features of the DOS reflecting the hybridization of metal and ligand ions**

$L_{2,3}$ -edge measurements

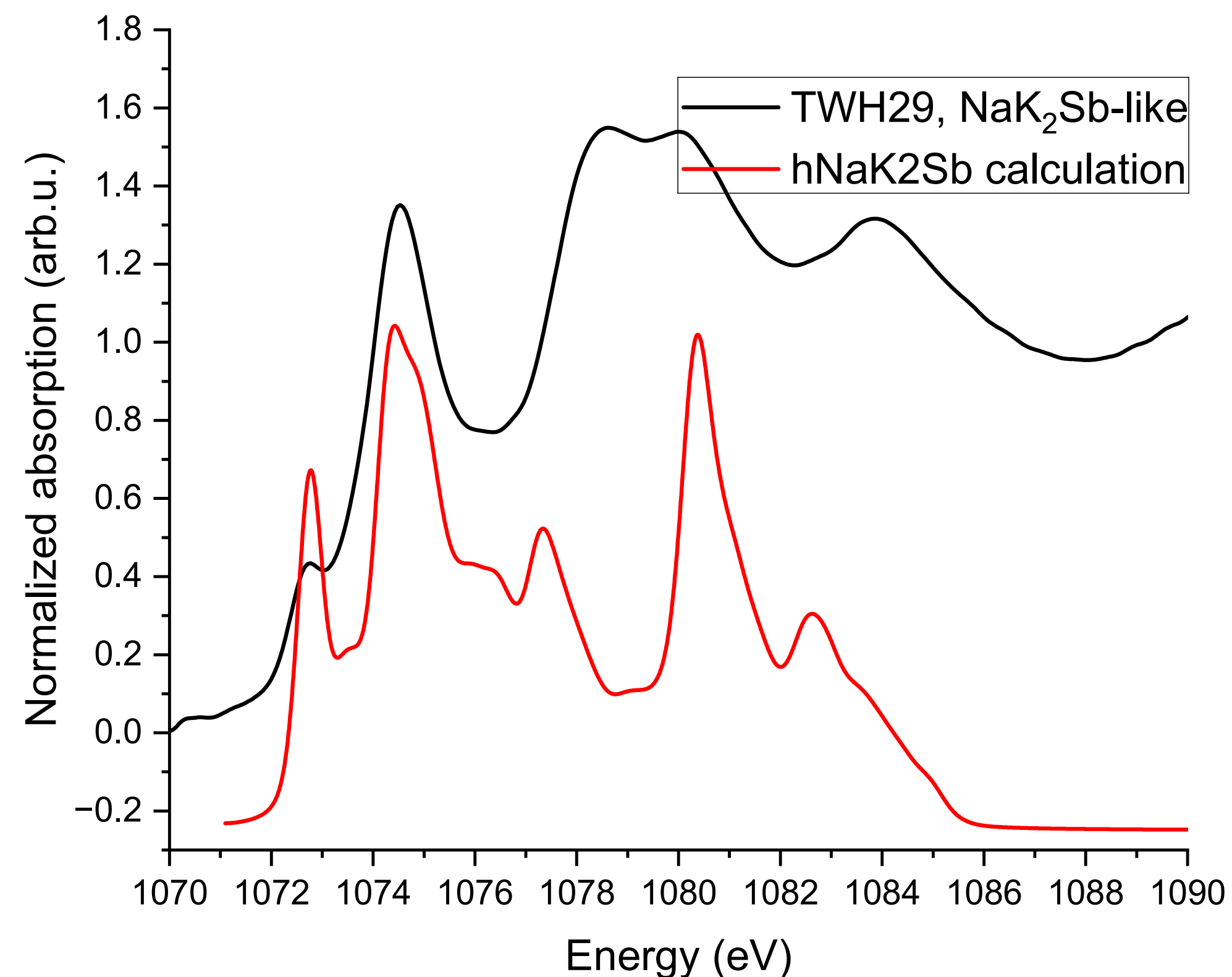
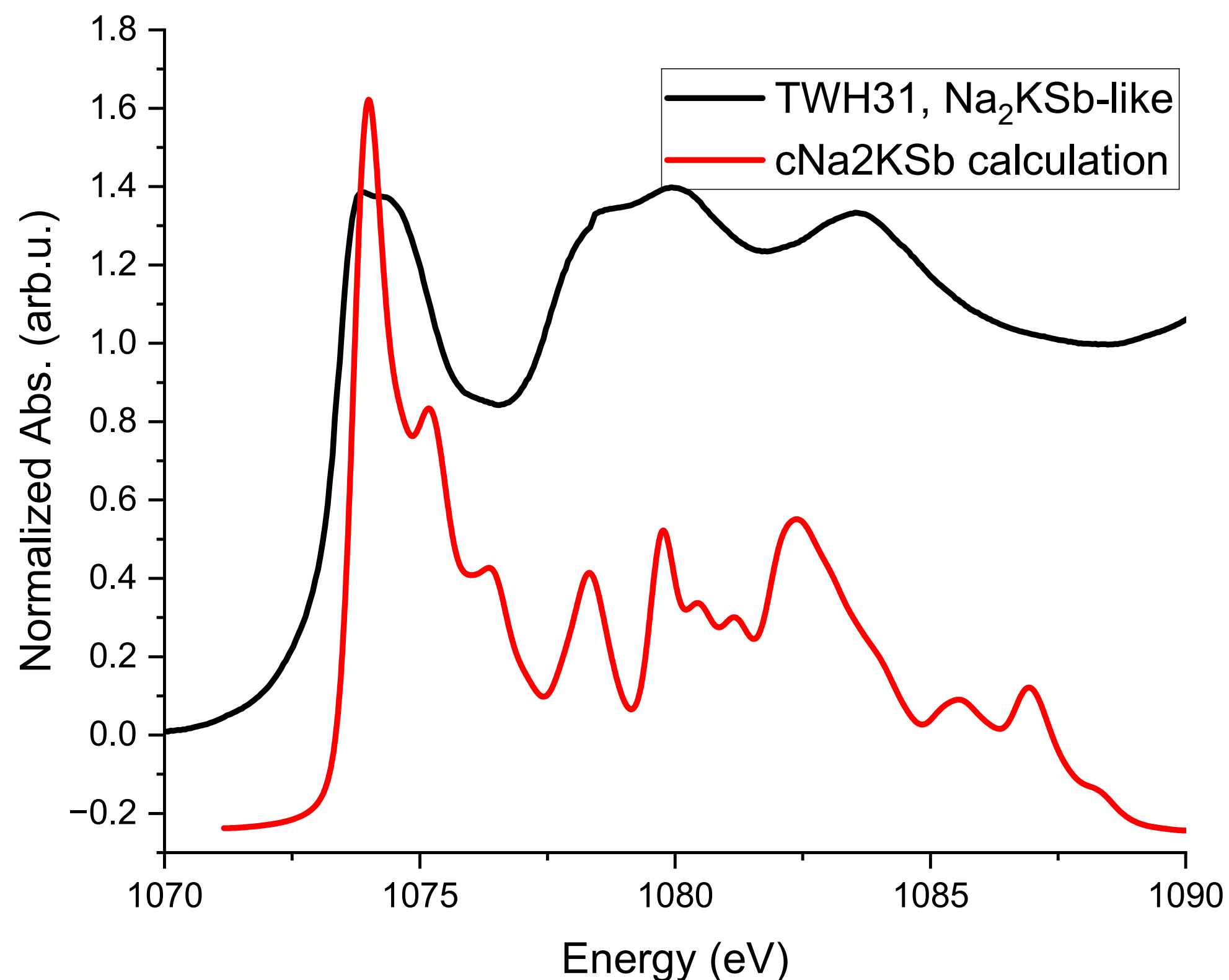


- K^+ $L_{2,3}$ -edge (295 – 305 eV)
main transition:
 $2p^6 3d^0 \rightarrow 2p^5 3d^1$
- **MPD $\approx$ 2 nm**
- **Strong difference between the Na_2KSb sample and the others**
- **Crystal structure effect?**

$L_{2,3}$ -edge measurements



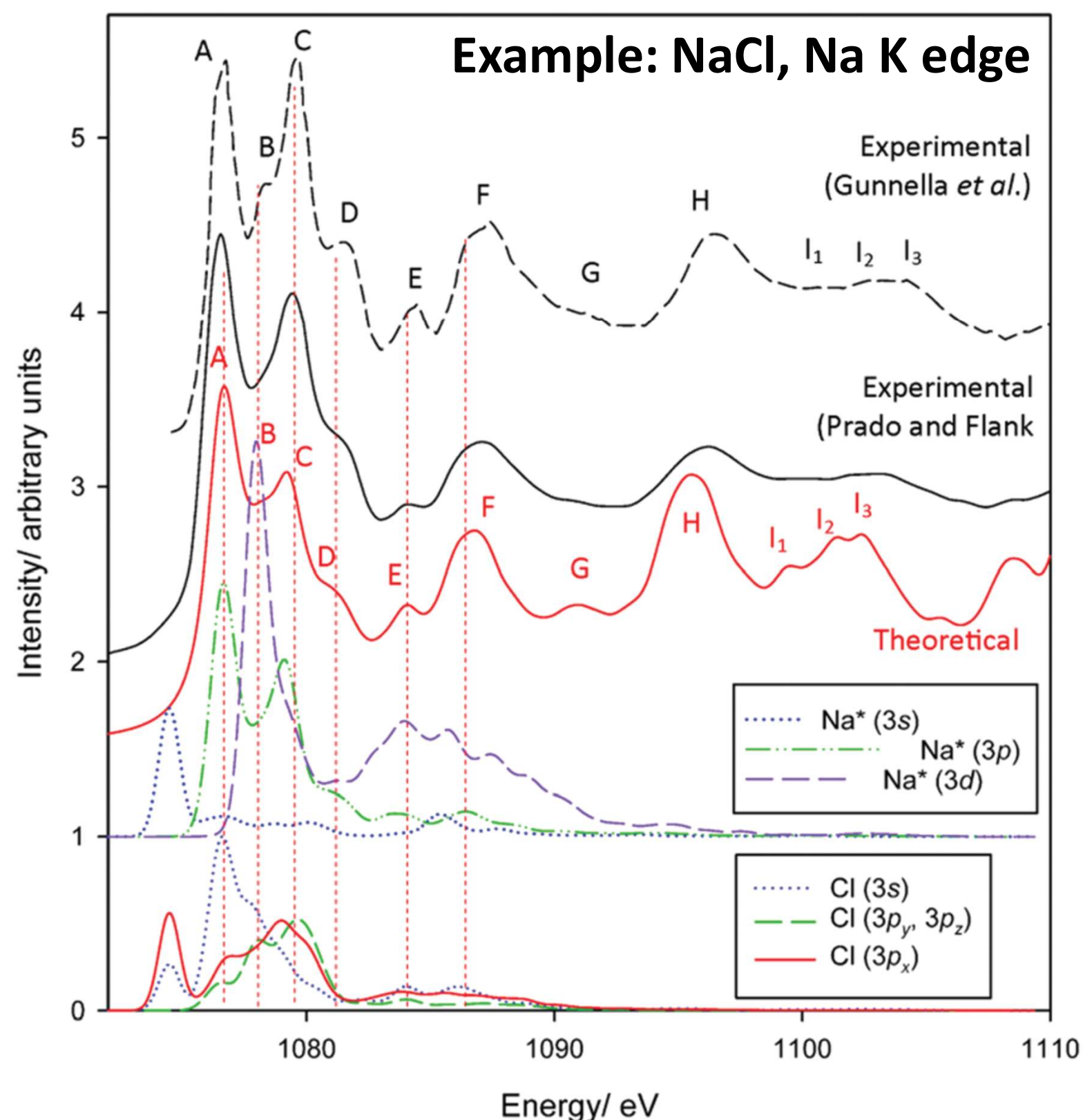
DFT calculations + EXCITE

FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

Conclusions and future work

- Experimental results:
 - **Complete XPS characterization of Na-K-Sb samples with different probing depth**
 - **First XAS characterization of Na-K-Sb photocathodes at many relevant absorption edges**
- Next steps:
 - **Multi-layer modeling of oxidized Na-K-Sb to reproduce depth dependent XPS (SESSA)**
 - **Comparison of XAS spectra with DFT and multiplet calculations (coll. FSU)**
 - **Comparison of XPS valence band spectra (not shown) with DFT calculation (coll. FSU)**
- Focus on:
 - **Sample degradation during the measurements**
 - diagnostic tests performed during beamtime
 - **Lack of literature references for Sb L-edge and for alkali oxides K and L edges**
 - reference spectra of Sb, Na-Sb, K-Sb collected

K-edge measurements



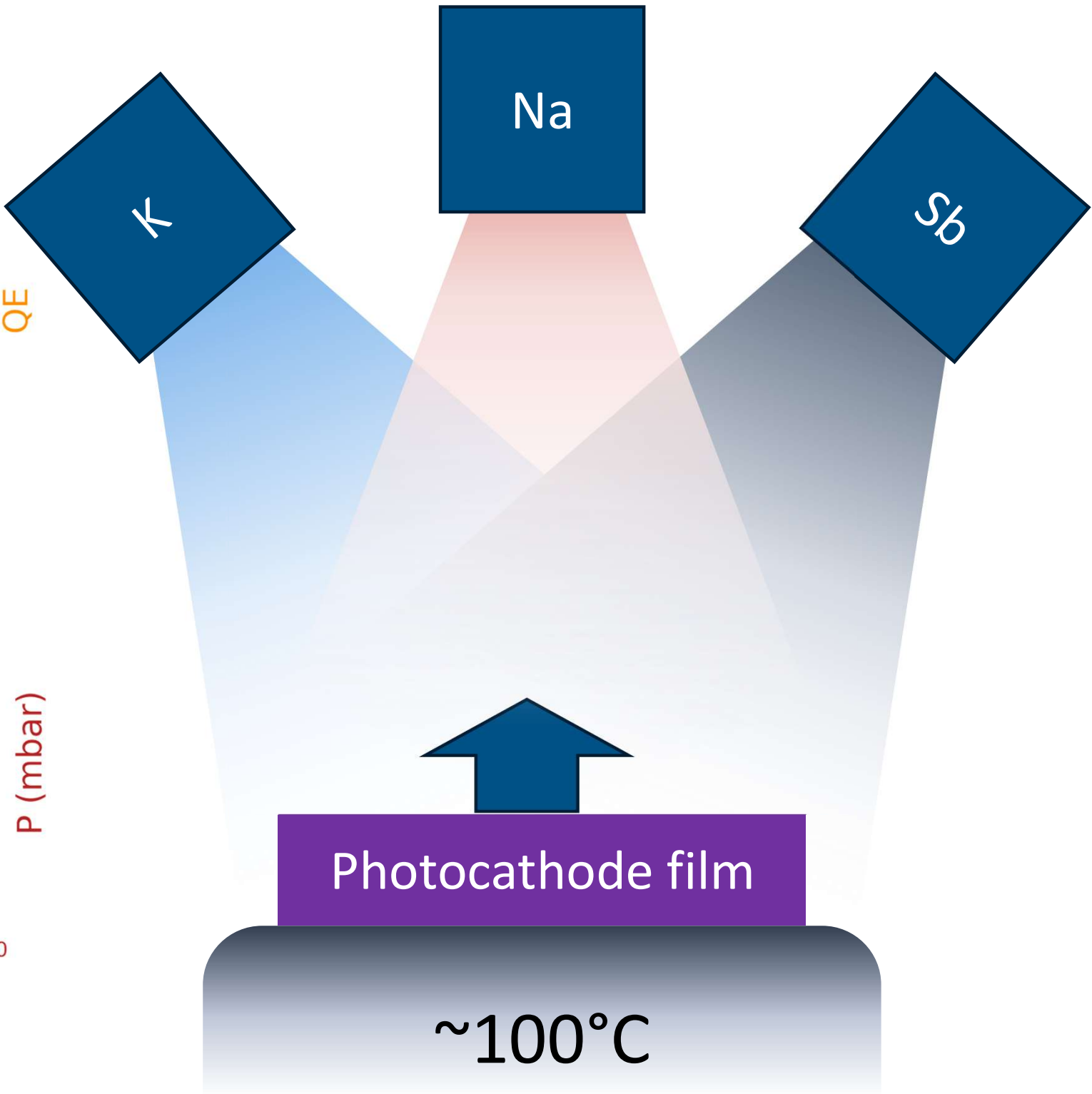
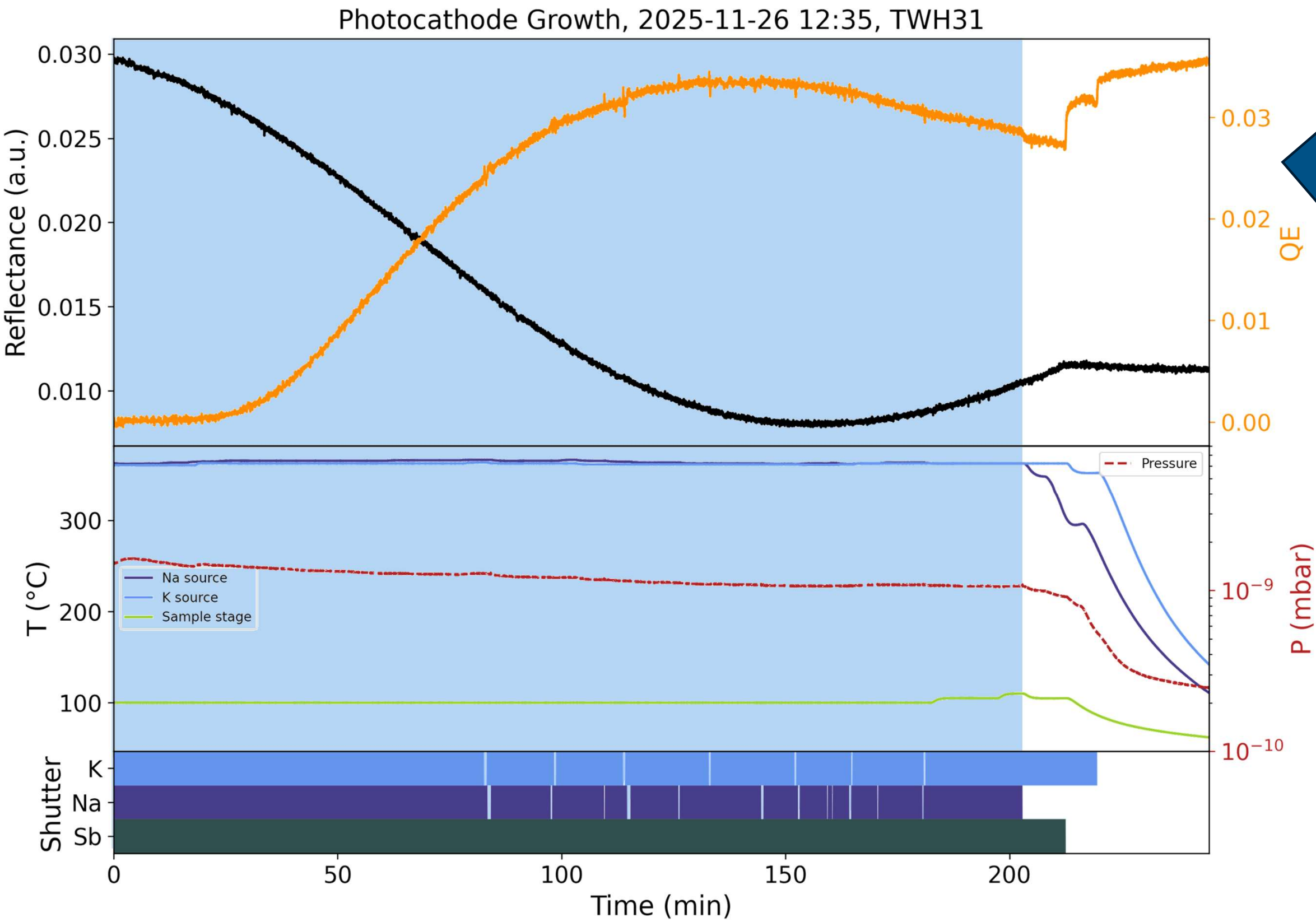
- **K-edge spectral features reproduce the ones of the DOS of the material**
- **Features corresponds to both Na and Cl states (p-DOS)**
- **Reflects hybridization of metal and ligand ions**

G.J. McIntosh, A. Chan Phys. Chem. Chem. Phys. (2018) 20 (37): 24033–24044.

Triple-evaporation growth at HZB

Dube et al., J. Appl. Phys. 138 (2025) 045704.

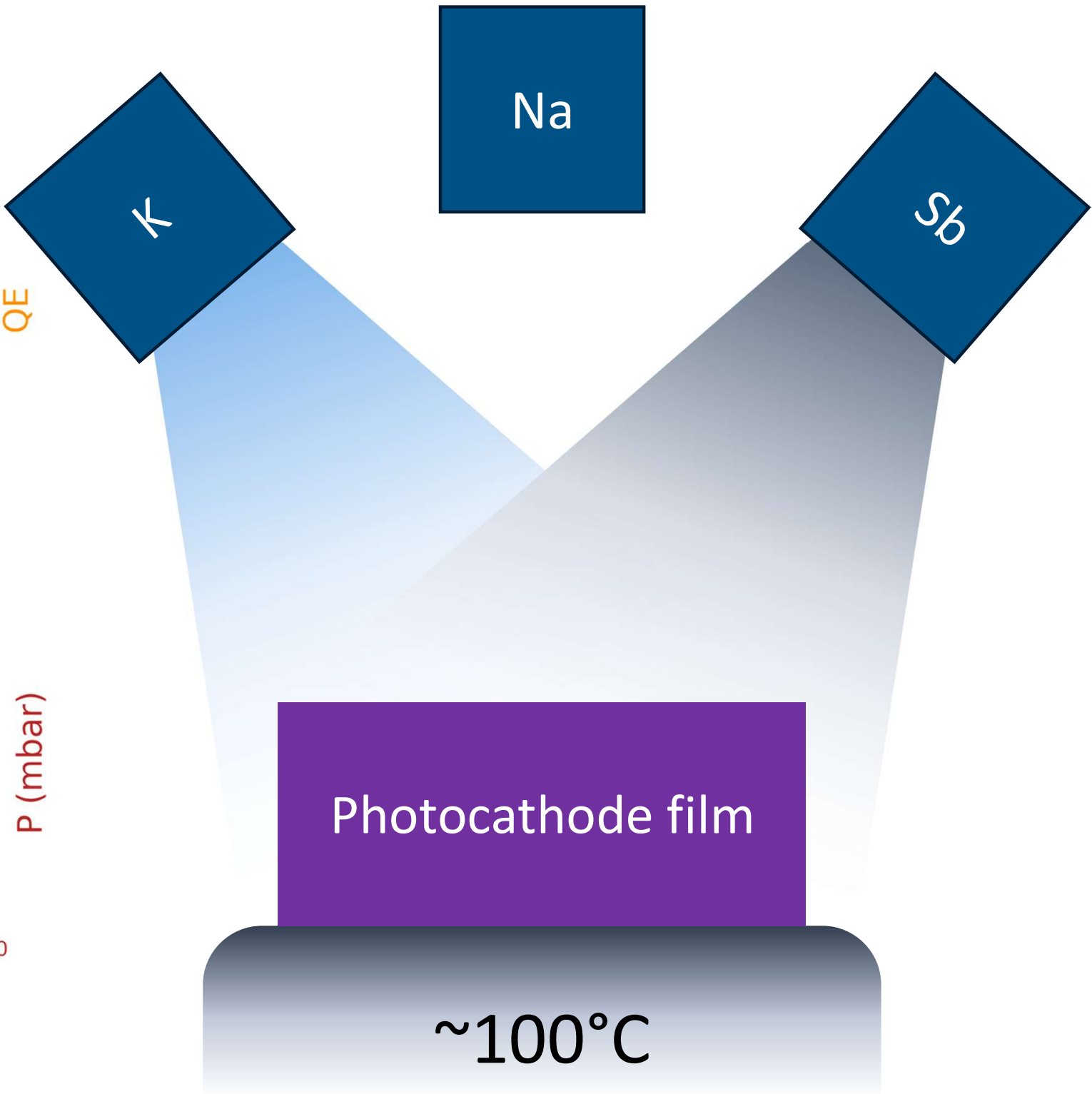
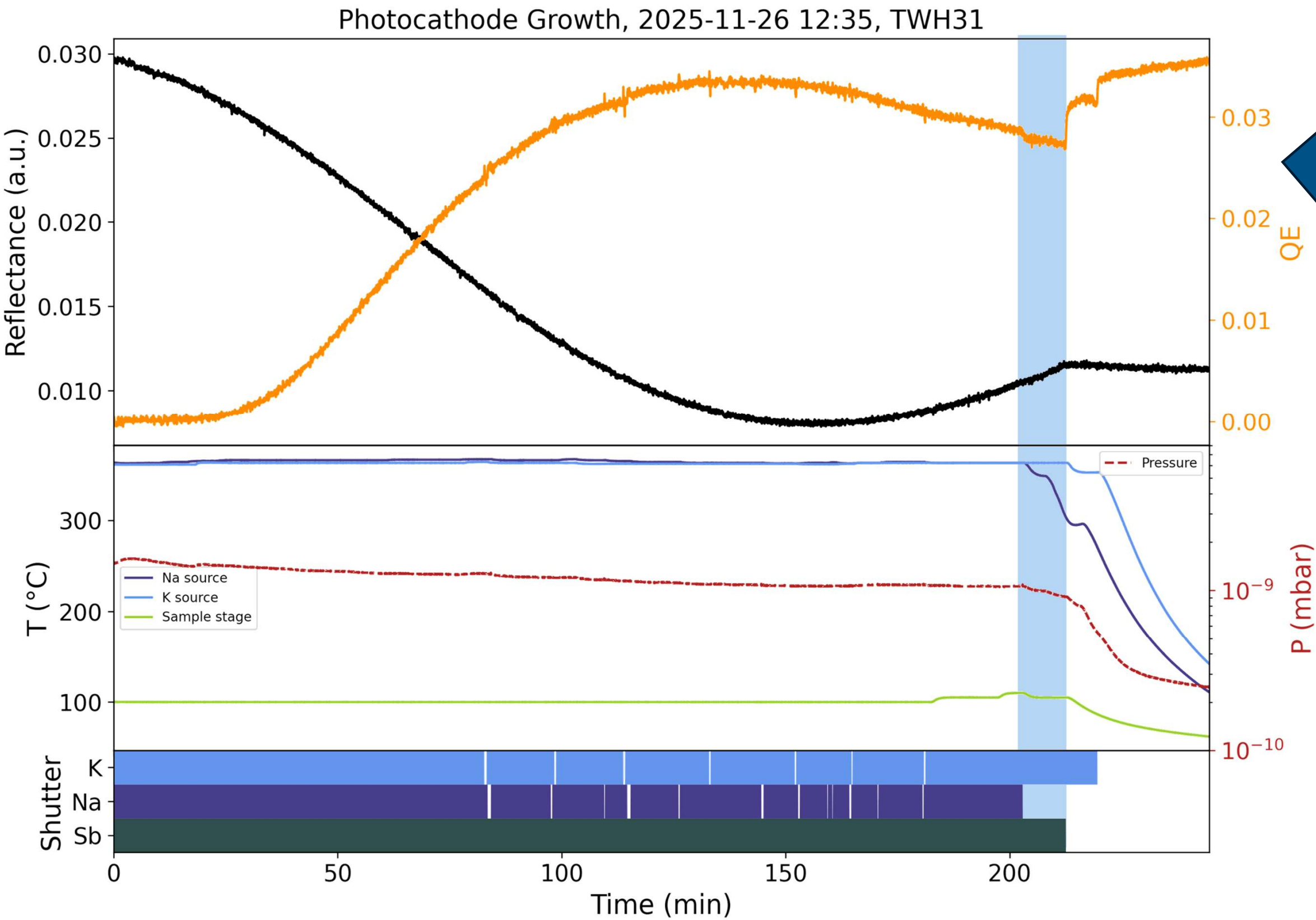
Wang, C. et al., J. of Phys. D: Applied Physics 59.7 (2026) 075102.



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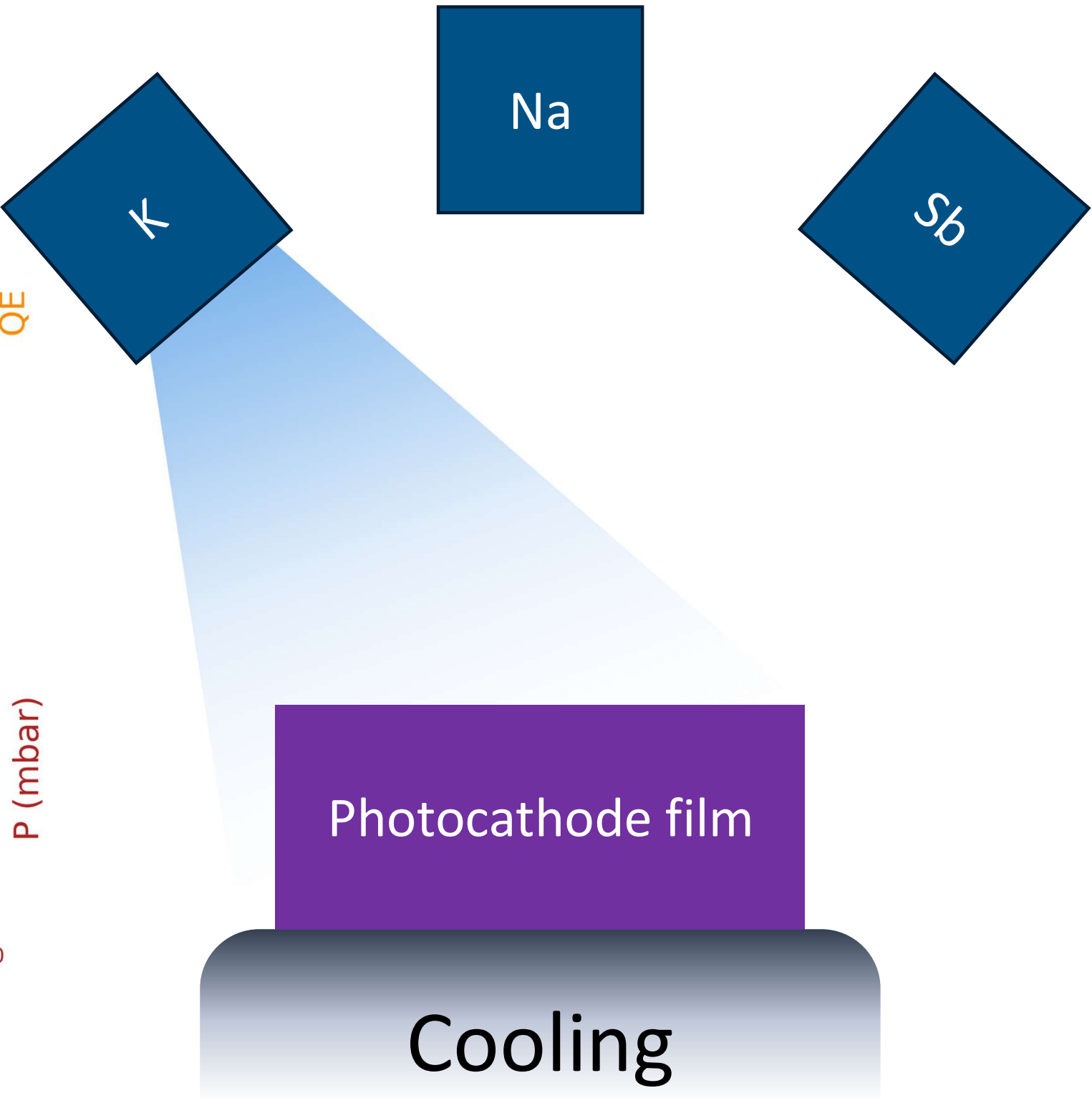
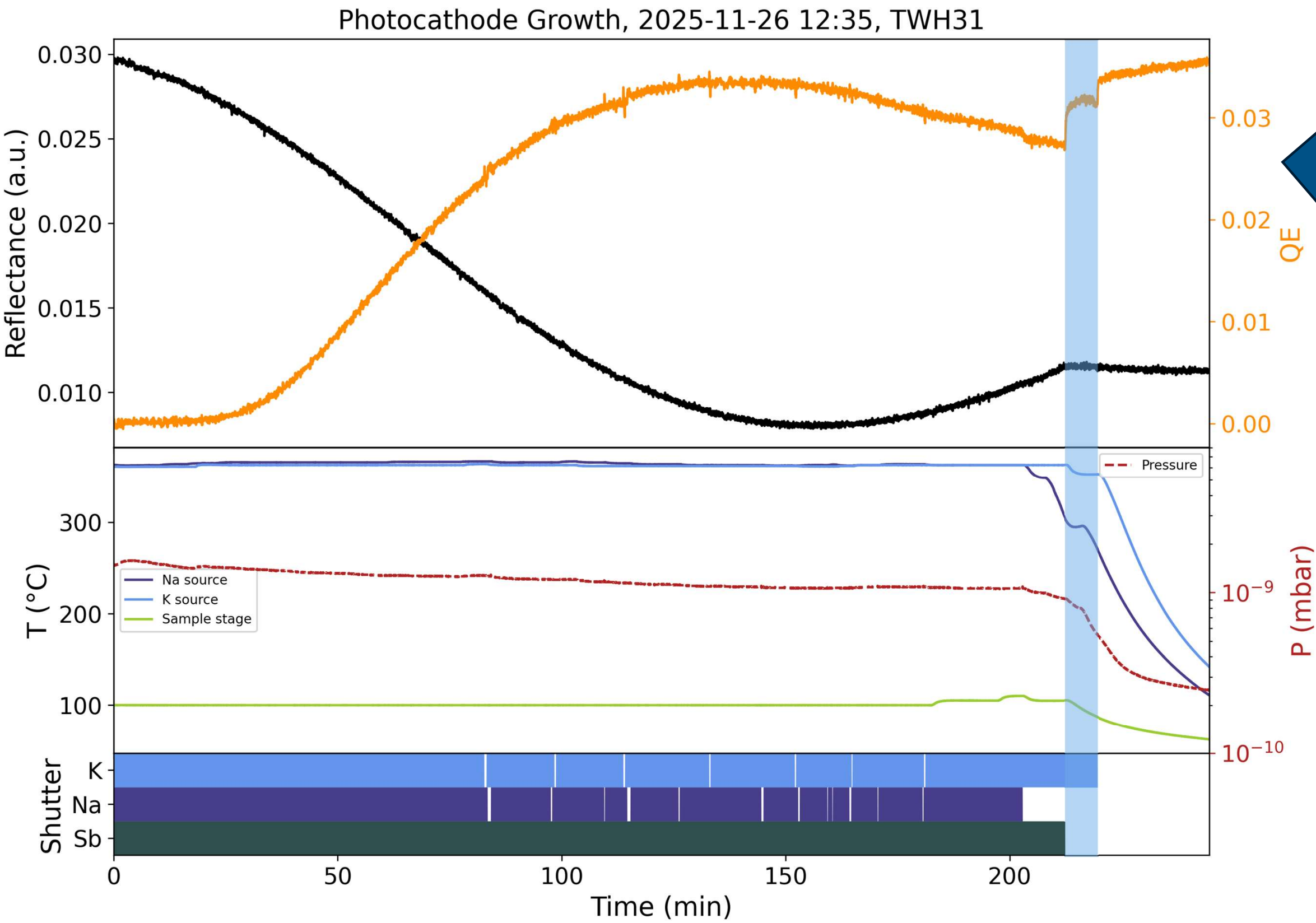
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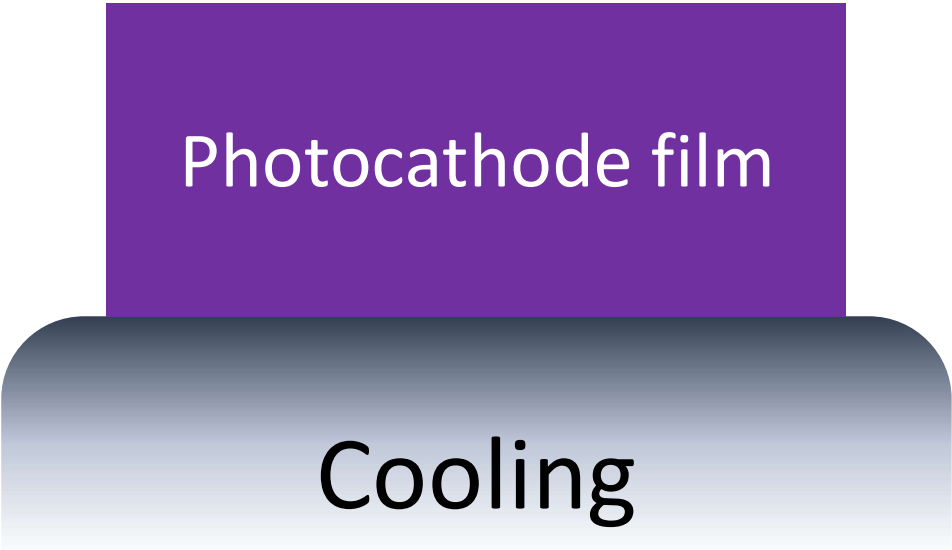
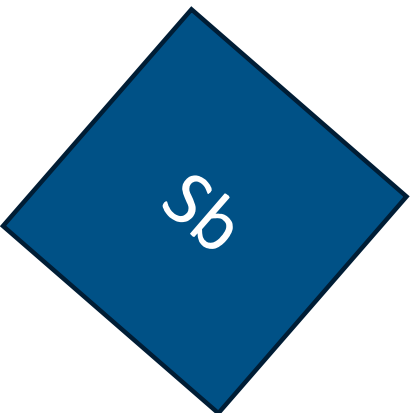
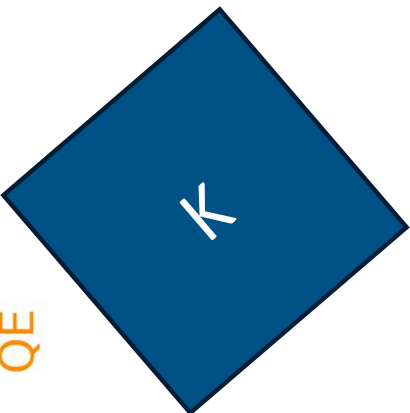
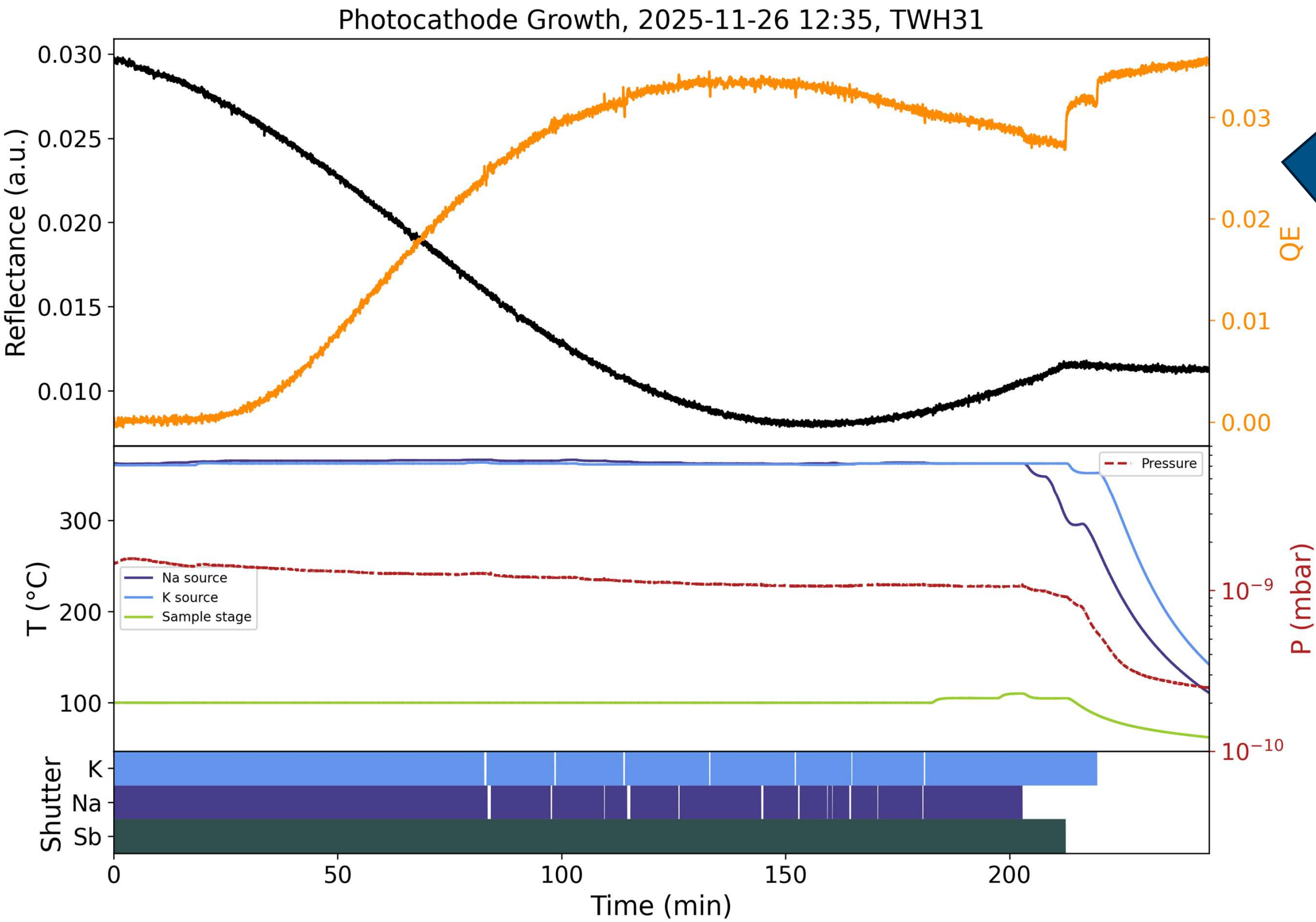
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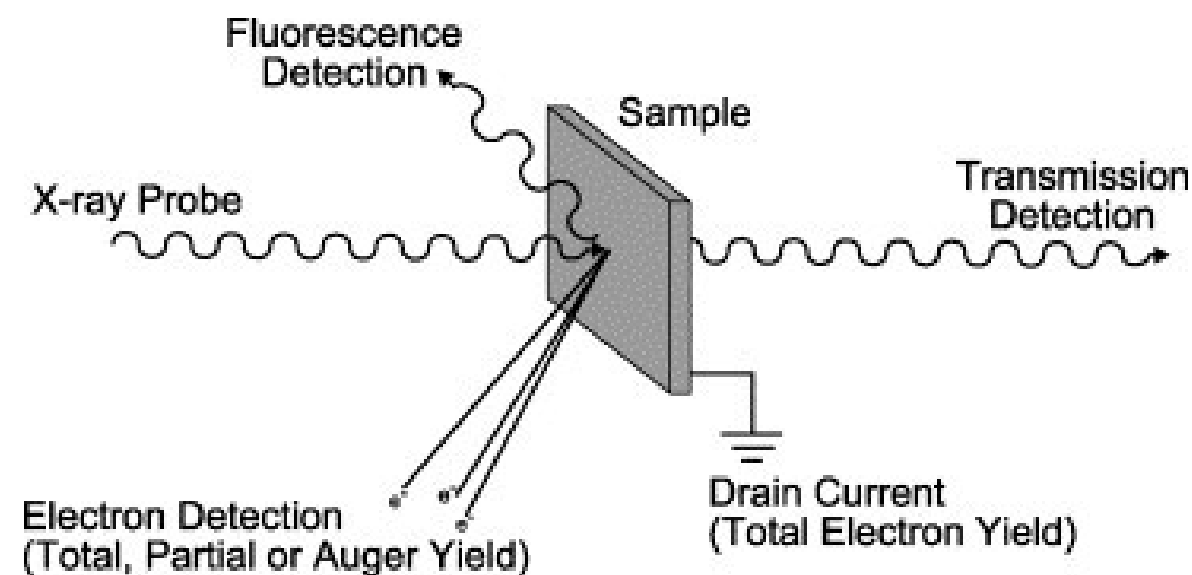
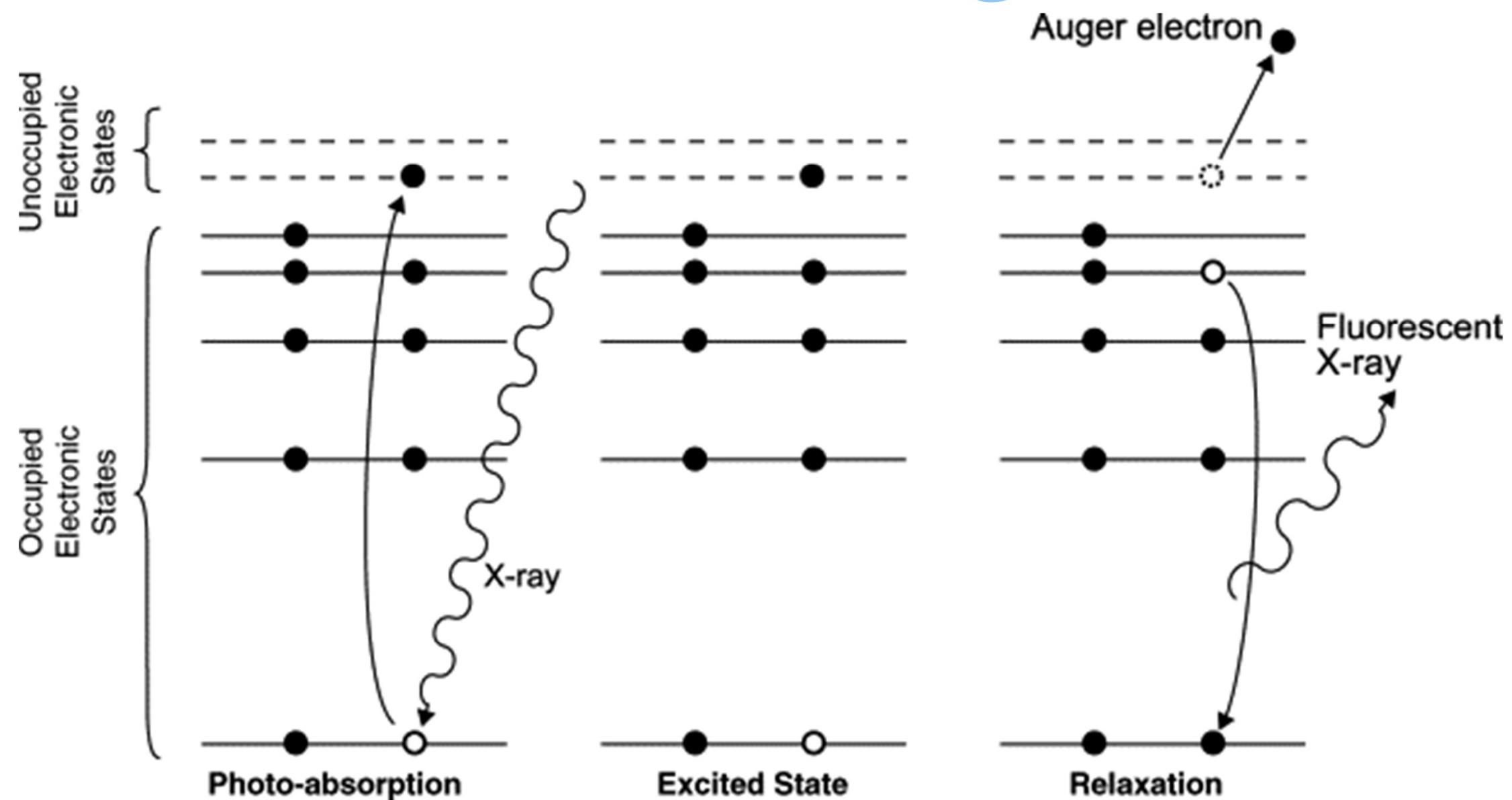
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Near-edge fine structure in XAS

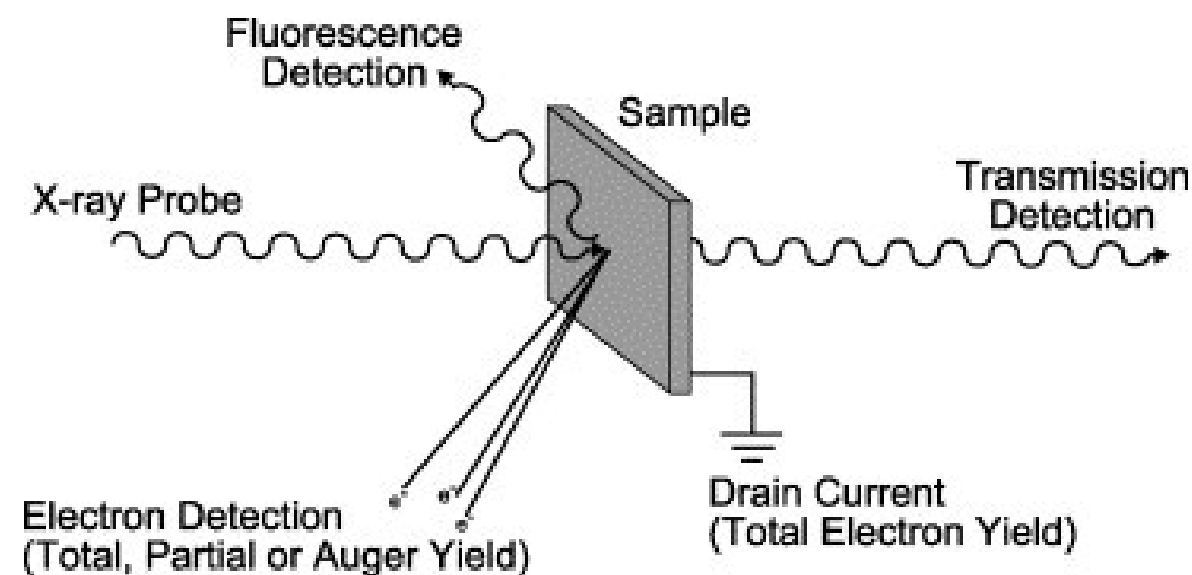
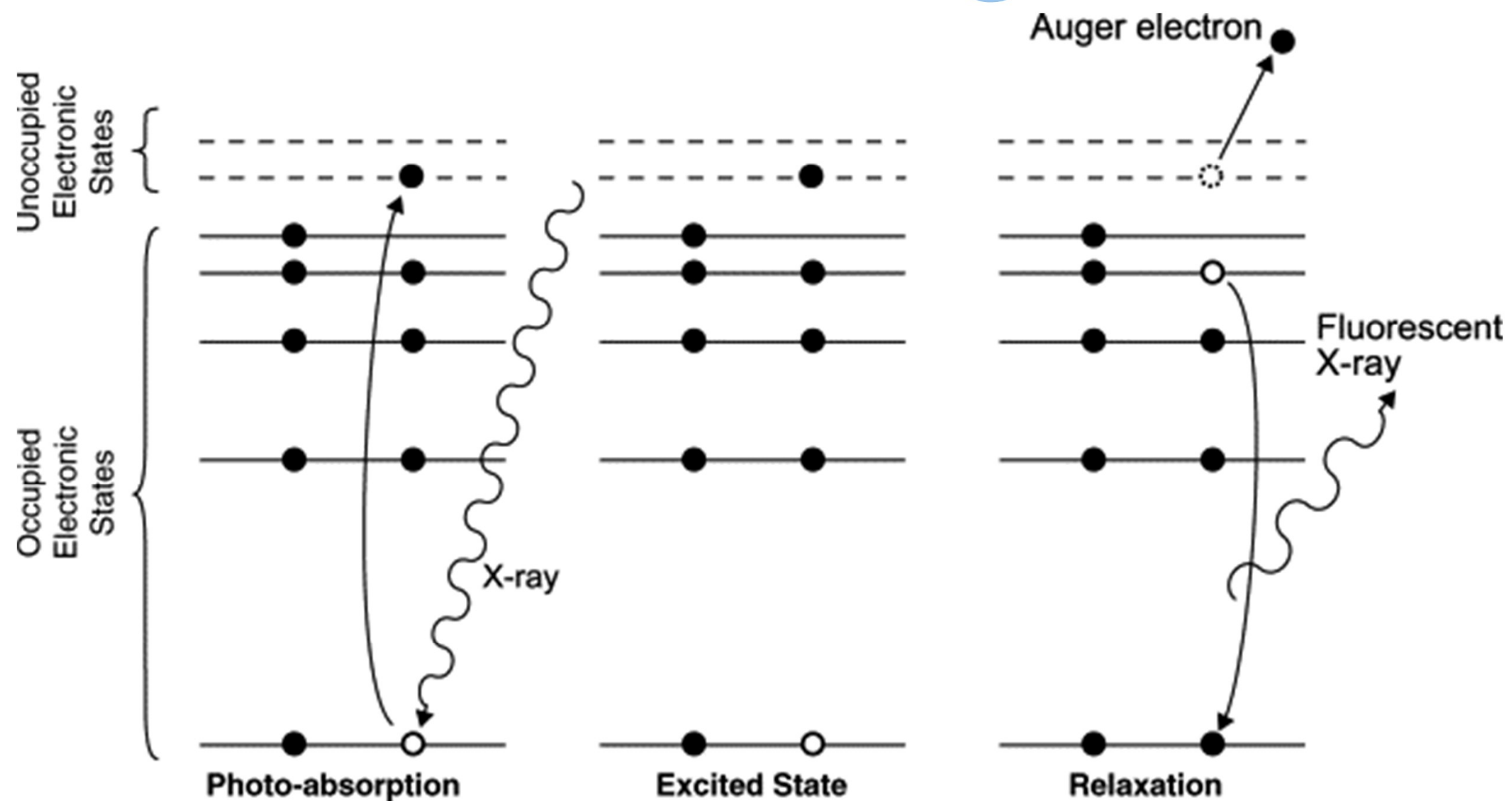


K-edge

Resonant absorption from 1s state

- **Na⁺** K-edge (1070 – 1100 eV)
main transition:
 $1s^2 3p^0 \rightarrow 1s^1 3p^1$
- **K⁺** K-edge (3605 – 3625 eV)
main transition:
 $1s^2 4p^0 \rightarrow 1s^1 4p^1$

Near-edge fine structure in XAS



$L_{2,3}$ -edge

Resonant absorption from 2p state

- K^+ $L_{2,3}$ -edge (295 – 325 eV)
main transition:
 $2p^6 3d^0 \rightarrow 2p^5 3d^1$
- Sb^{3-} $L_{2,3}$ -edge (4125, 4370 eV)
 $2p^6 6s^0 \rightarrow 2p^5 6s^1$

Other measured edges:

Sb L_1 edge (2s state)

Sb $M_{4,5}$ edge (3d states)

Preliminary results on Na-K-Sb (TWH31)

