

Geant4 simulations of sub-keV electron energy loss in CaWO_4 and Al_2O_3 by ELOISE

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- What is ELOISE?
 - validate Geant4 simulation for CaWO_4 and Al_2O_3 at sub-keV energies
 - focus of his talk:* energy loss by electron ionisation
- The reference data
 - Electron Energy Loss Spectroscopy of CaWO_4 and Al_2O_3
- The comparison
 - Geant4 10.6.3 “out of the box”
- Outlook & Summary

What is ELOISE?

Reliable Background Simulation at Sub-keV Energies
(for CaWO_4 and Al_2O_3)



Der Wissenschaftsfonds.

ELOISE is founded by the Austrian science fund (FWF) under grant number P34778-N

[\[HK, SciPost Phys. Proc. 12 \(2023\) 064\]](#)

ELOISE: Motivation



- CaWO_4 and Al_2O_3 are prominent targets for rare event searches:
 - CRESST searching for Dark Matter induced nuclear recoils
 - NUCLEUS searching for Coherent Elastic Neutrino-Nucleus Scattering (CEvNS)
- In both cases the signal is *rare* compared to the background and measured down to $\text{O}(10 \text{ eV})$
→ a *reliable* background model at *sub-keV* is crucial

ELOISE: Energy Scale

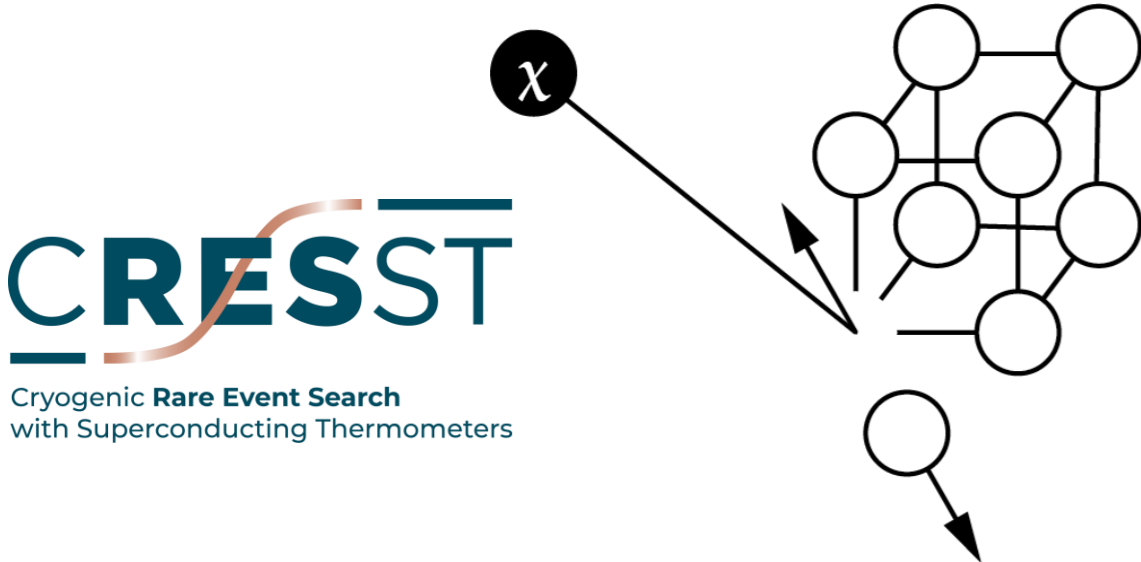
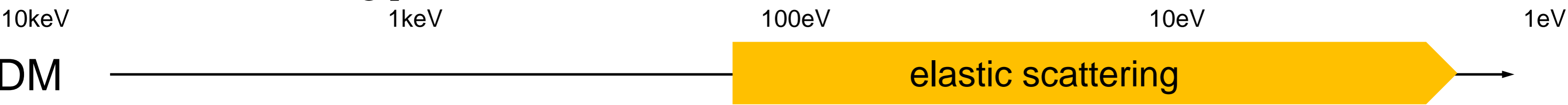
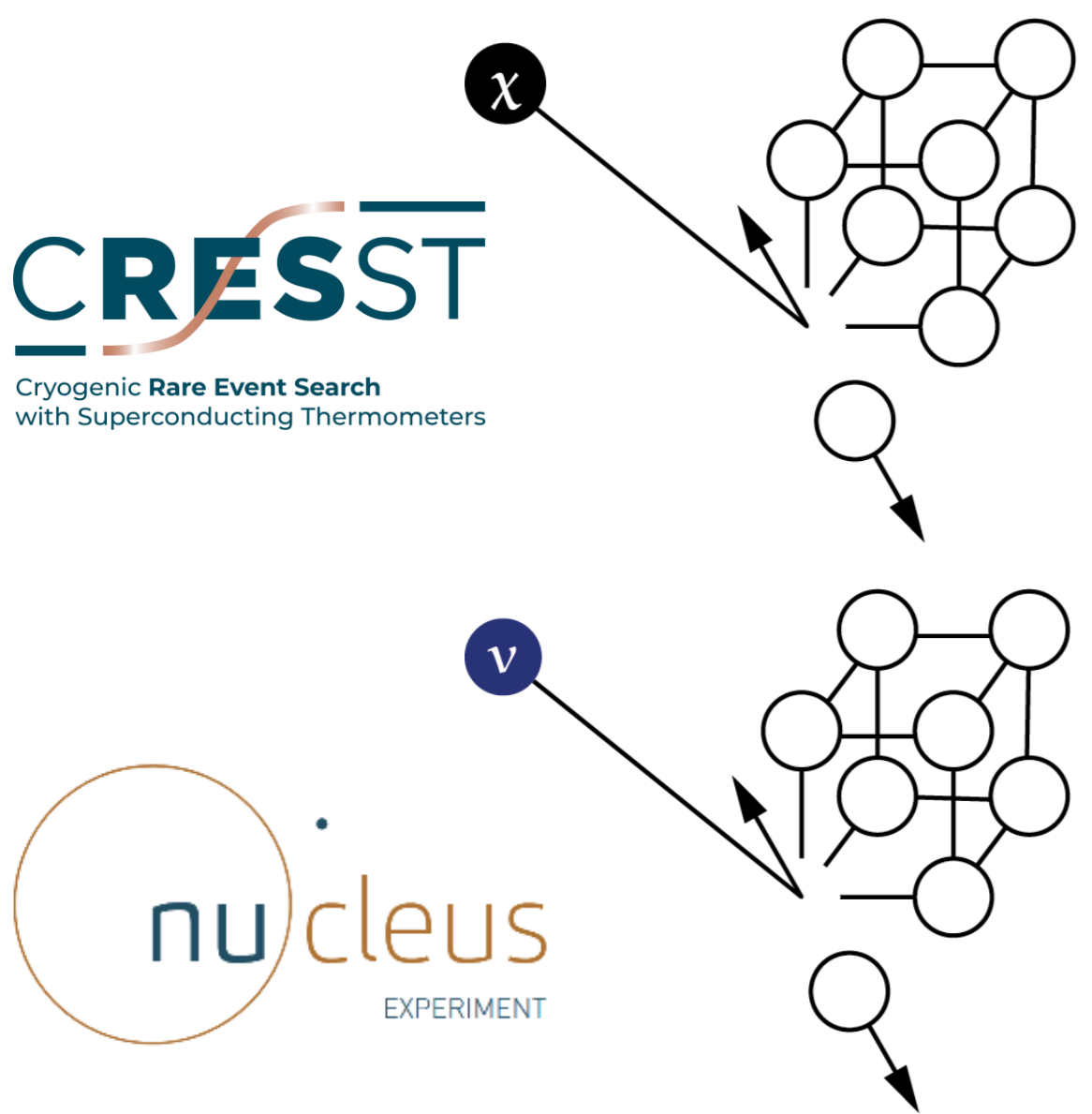
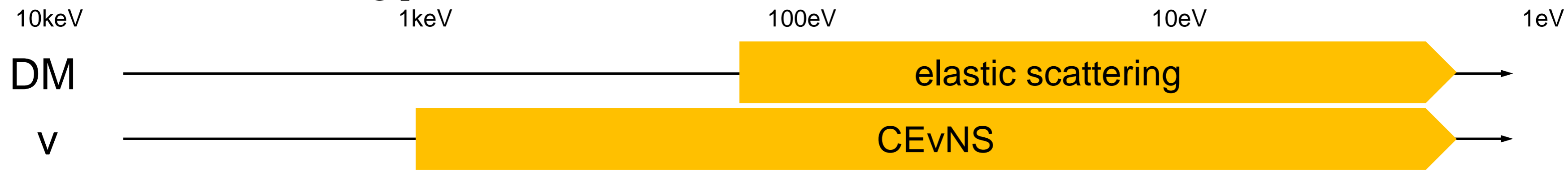


Table 1: The maximal recoil energies caused by CE ν NS with a neutrino of 2 MeV kinetic energy ($E_{\text{rec},\nu}$) and by elastic scattering with a 2 GeV/c²-DM particle with a velocity of 220 m s⁻¹ ($E_{\text{rec,DM}}$) and the minimal displacement energies (E_{dis}) for CaWO₄ [8] and Al₂O₃ in case of Al [9].

	⁸ O	¹³ Al	²⁰ Ca	⁷⁴ W
$E_{\text{rec,DM}}/\text{eV}$	106.4	69.2	48.6	11.5
$E_{\text{rec},\nu}/\text{eV}$	499.9	296.5	199.5	43.5
E_{dis}/eV	20	47.5	24	196

[HK, SciPost Phys. Proc. 12 (2023) 064]

ELOISE: Energy Scale



CRESST
Cryogenic Rare Event Search
with Superconducting Thermometers

nucleus
EXPERIMENT

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ELOISE: Interactions of Interest

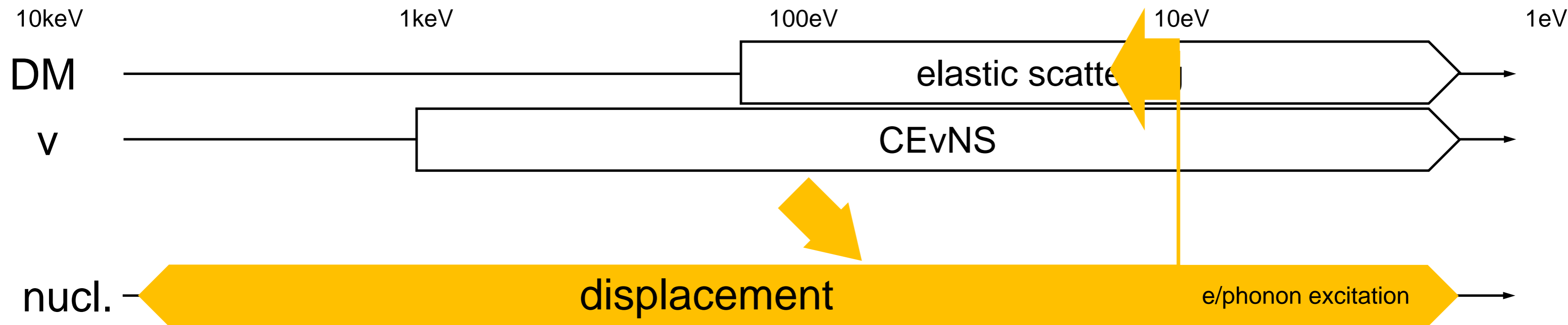


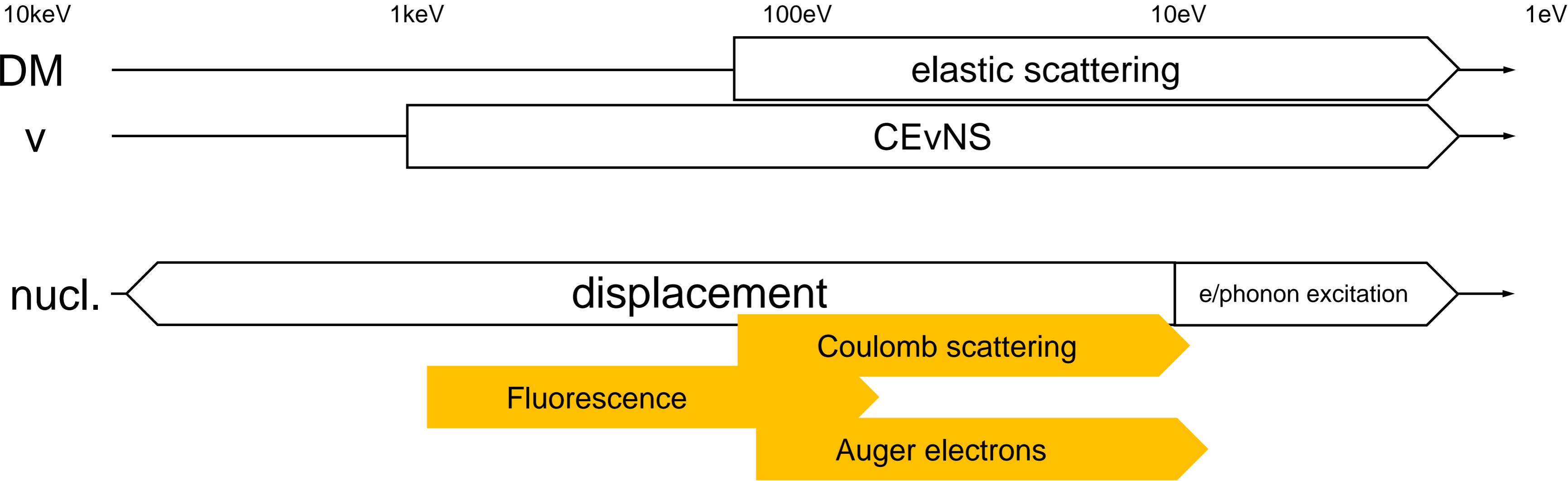
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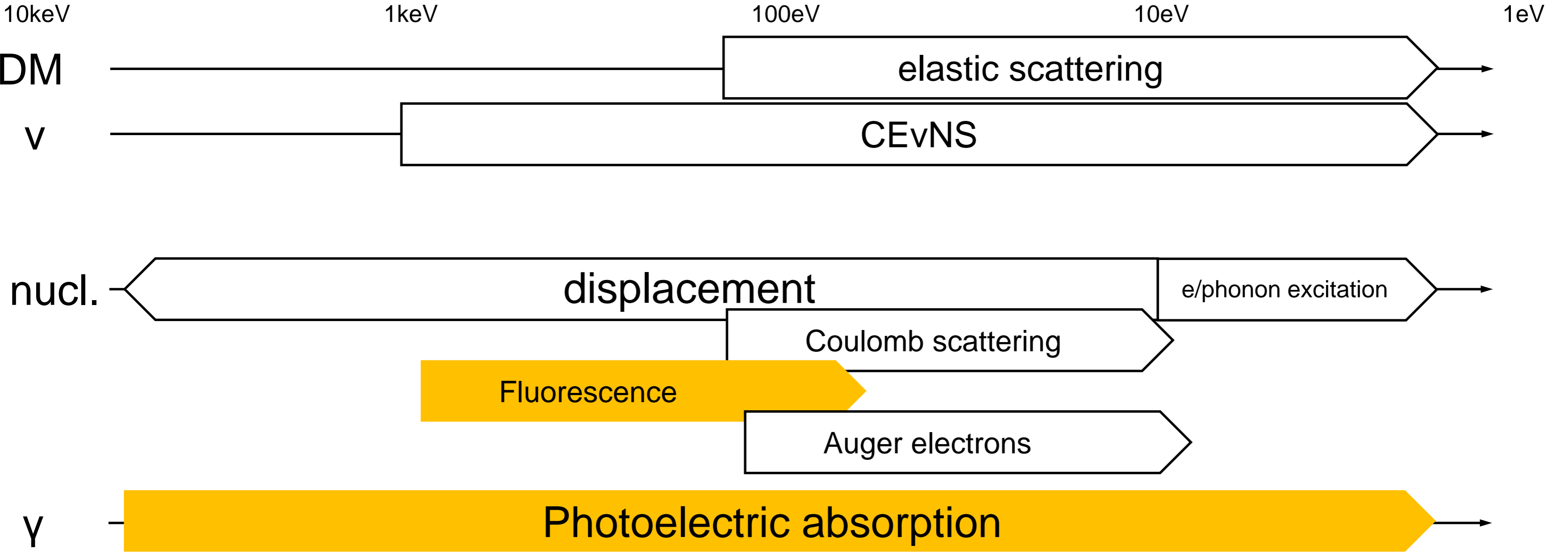
[HK, SciPost Phys. Proc. 12 (2023) 064]

? Breakdown of free atom approach

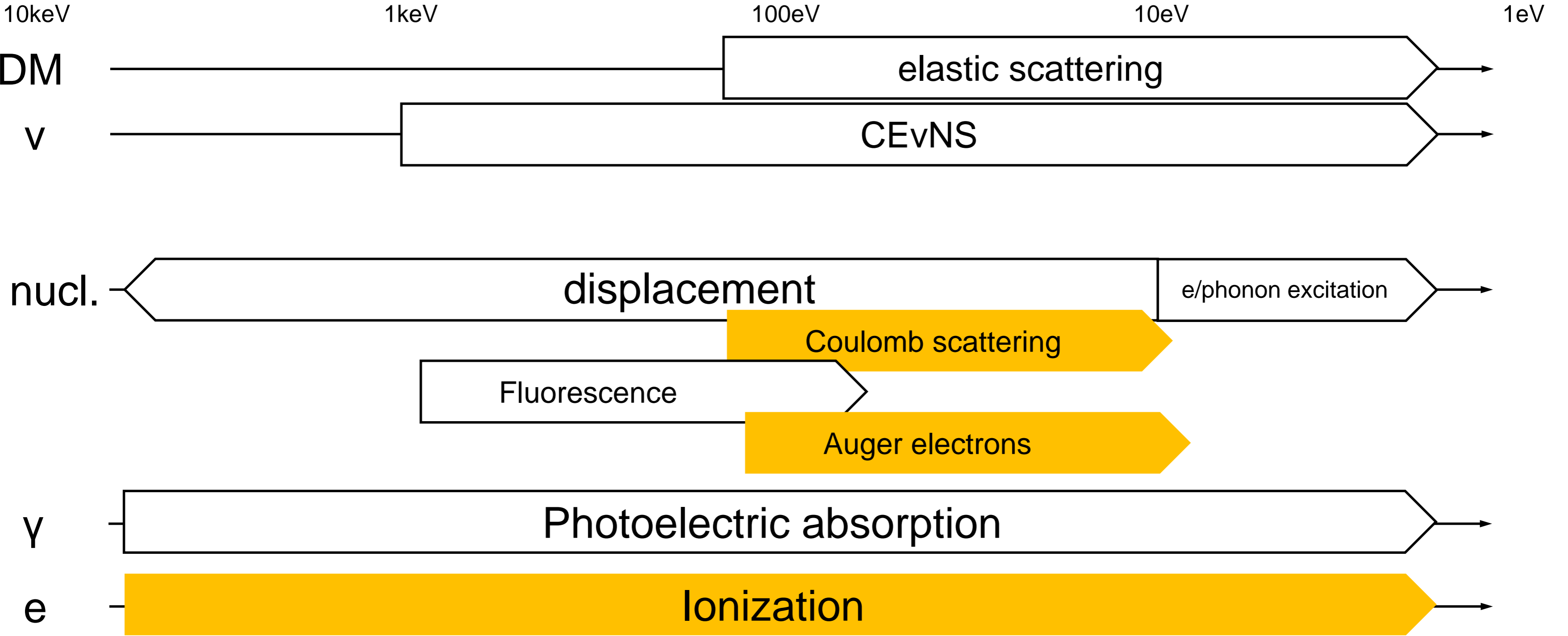
ELOISE: Interactions of Interest



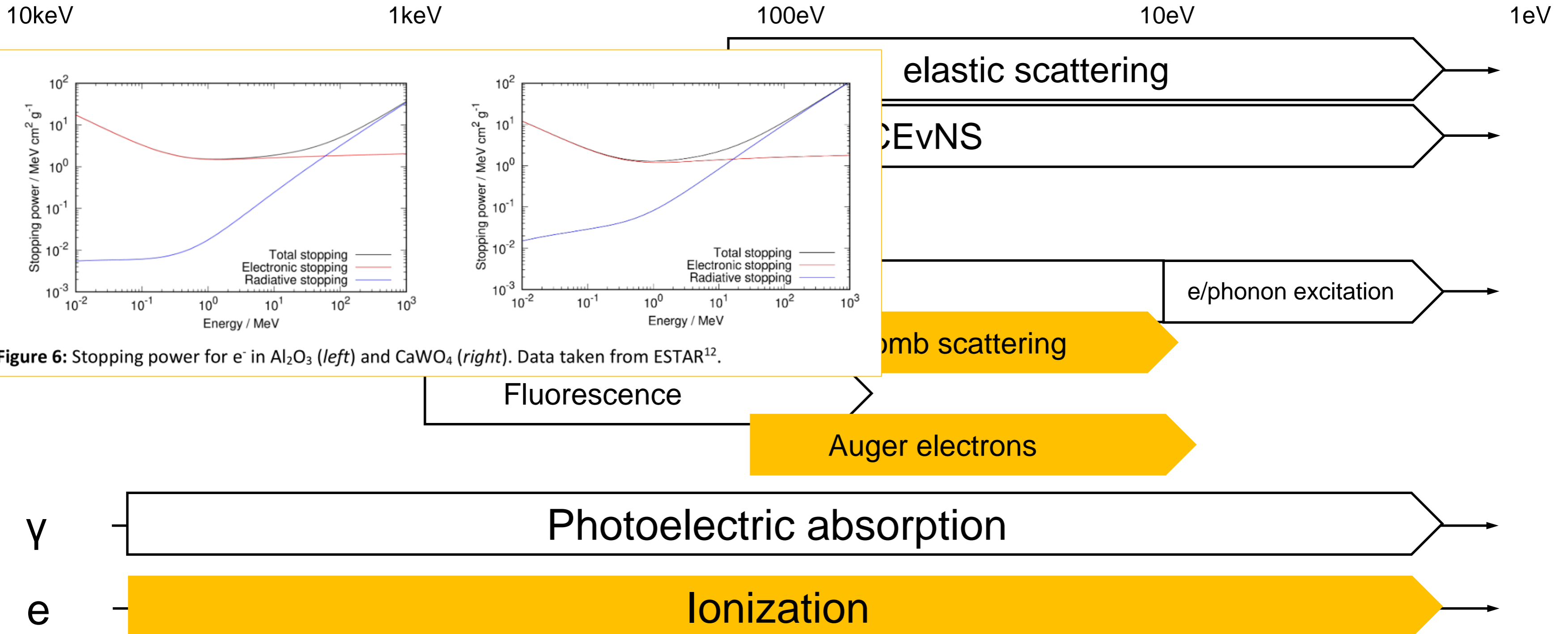
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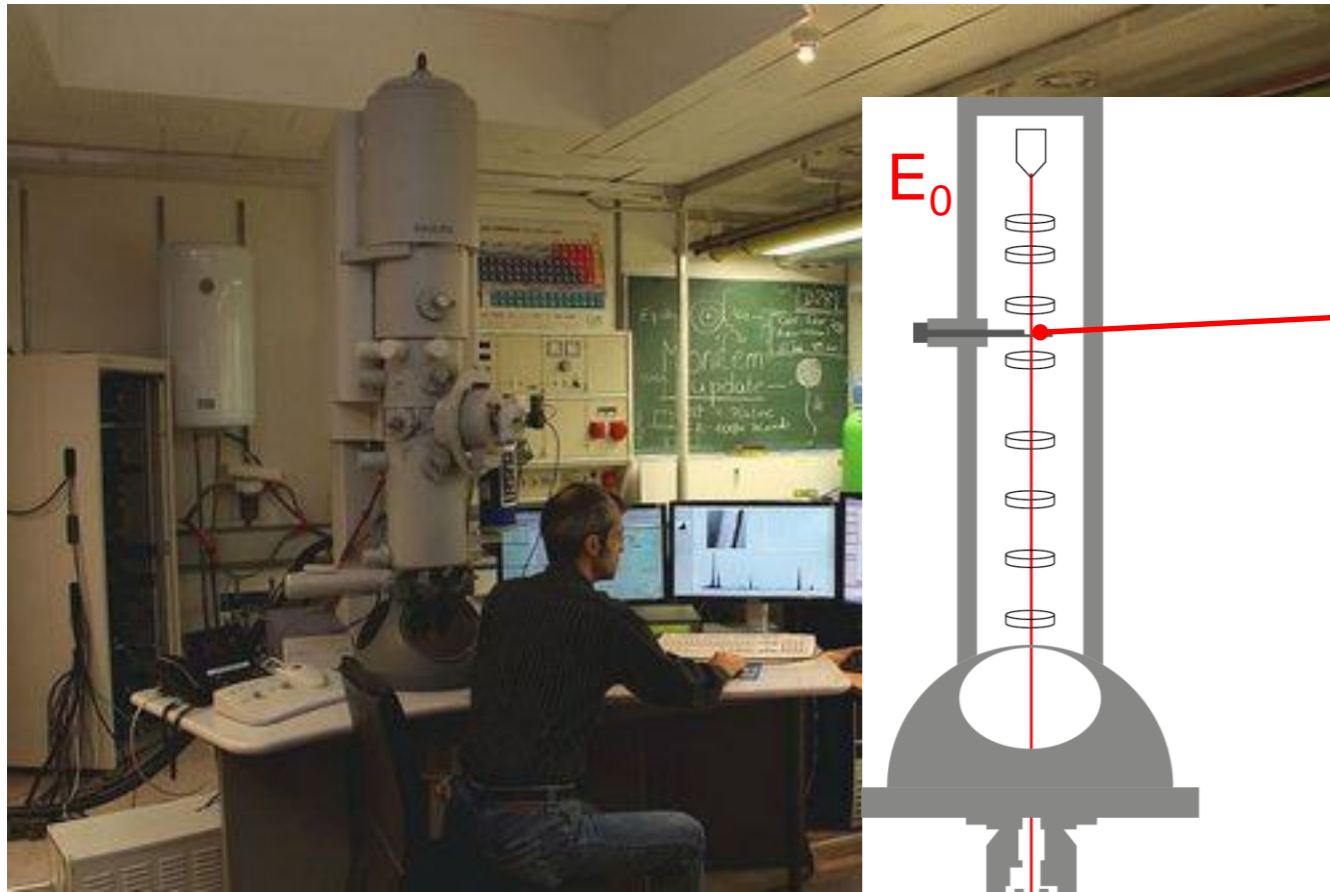


Reference Data: Electron Energy Loss Spectroscopy of CaWO_4 and Al_2O_3

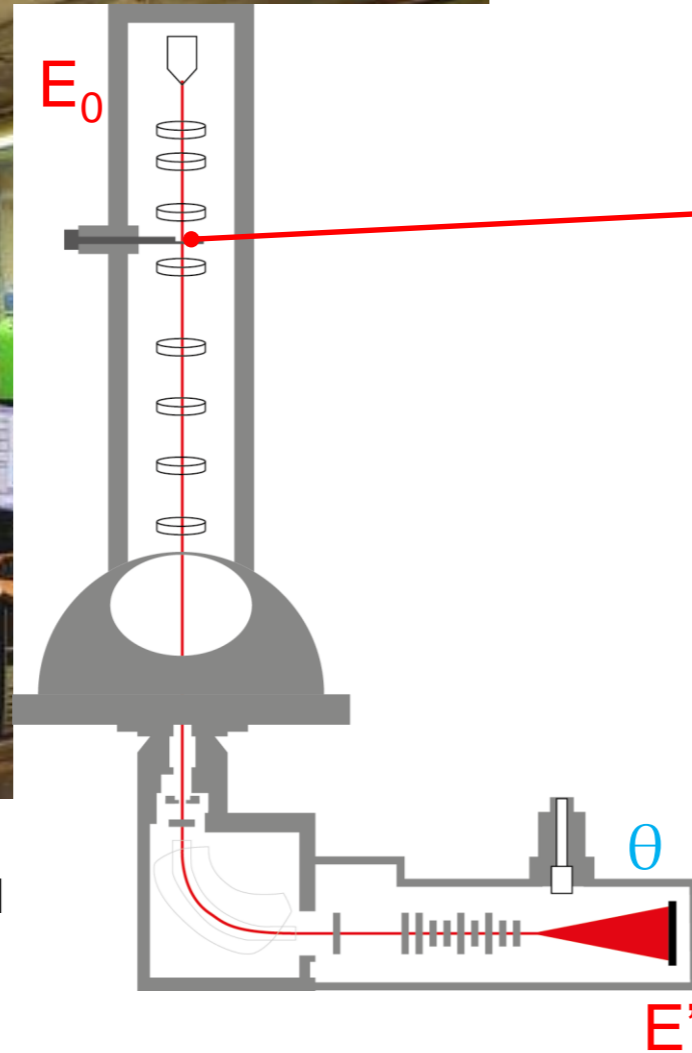
Reference Data: Requirements

- Measurement of reference data has to be *reproducible* in simulation with as few as possible systematic uncertainties
→ keep it *simple*
- Electron Energy Loss Spectroscopy (EELS) on thin samples
 - Simple geometry:
“free floating” cuboid of $\text{CaWO}_4/\text{Al}_2\text{O}_3$ in vacuum
 - Simple interactions:
only *single* e^- interactions

Reference Data: EELS

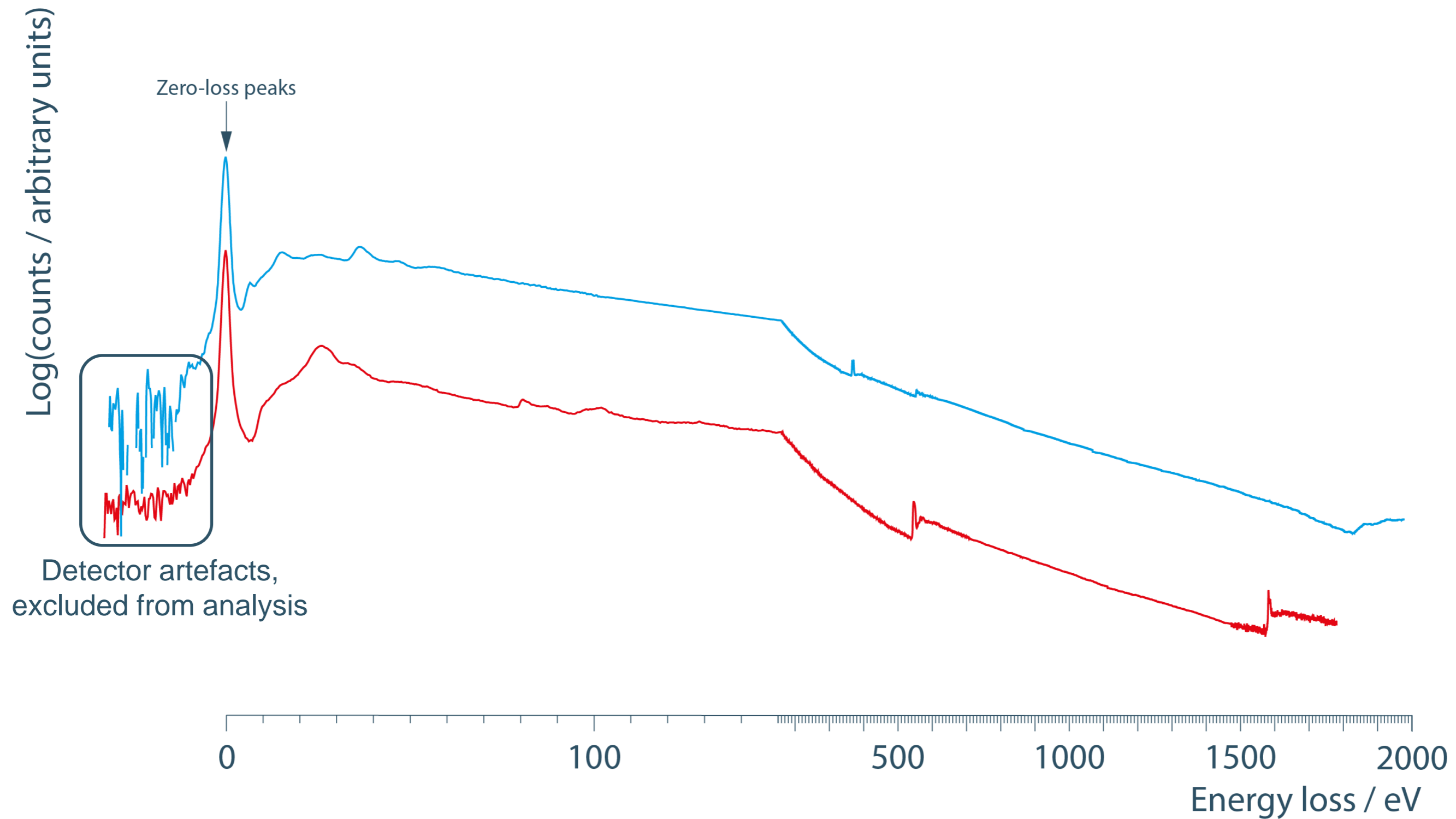


EELS conducted
by M. Stöger-Pollach, TU Wien, USTEM

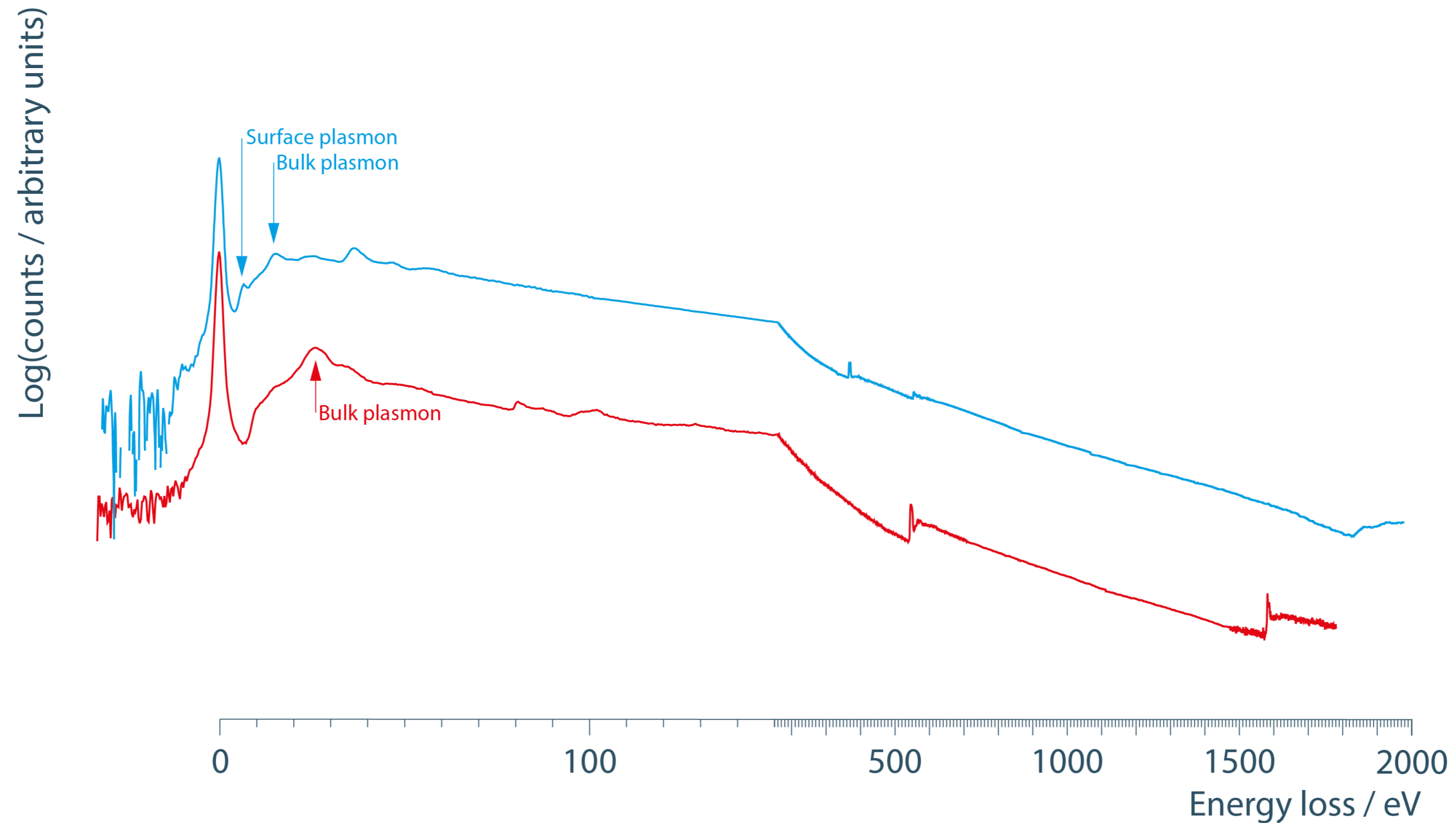


- CaWO_4 , Al_2O_3 samples provided by NUCLEUS
- Only *single* e^- interactions
→ *thin* target (~ 105 nm)
- Well established method:
Electron Energy Loss Spectroscopy (EELS)
→ monochromatic e^- ($E_0 = 200$ keV)
→ collection angle $\theta = 28$ mrad
→ energy loss: $E_0 - E'$

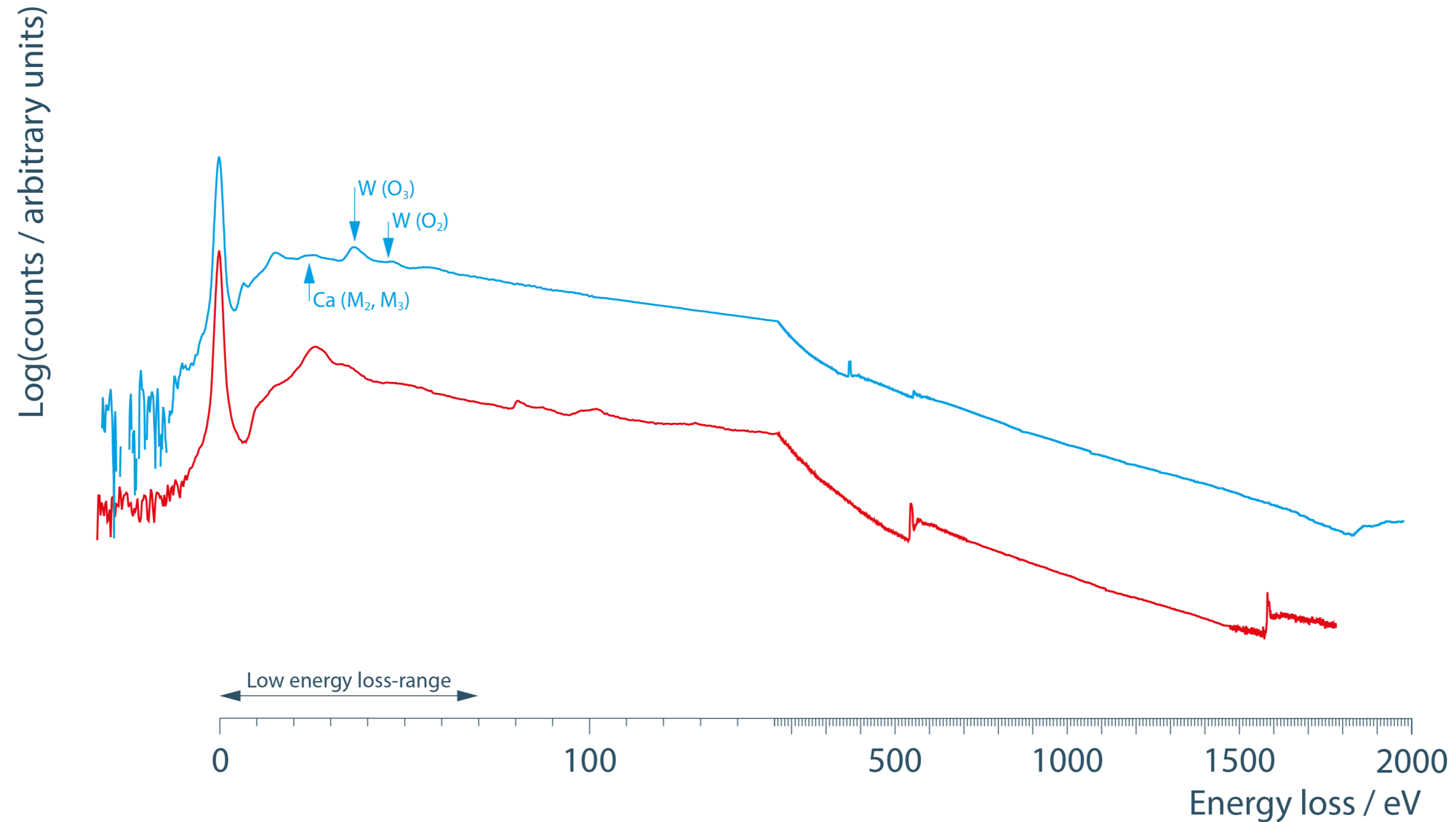
EELS of CaWO_4 and Al_2O_3



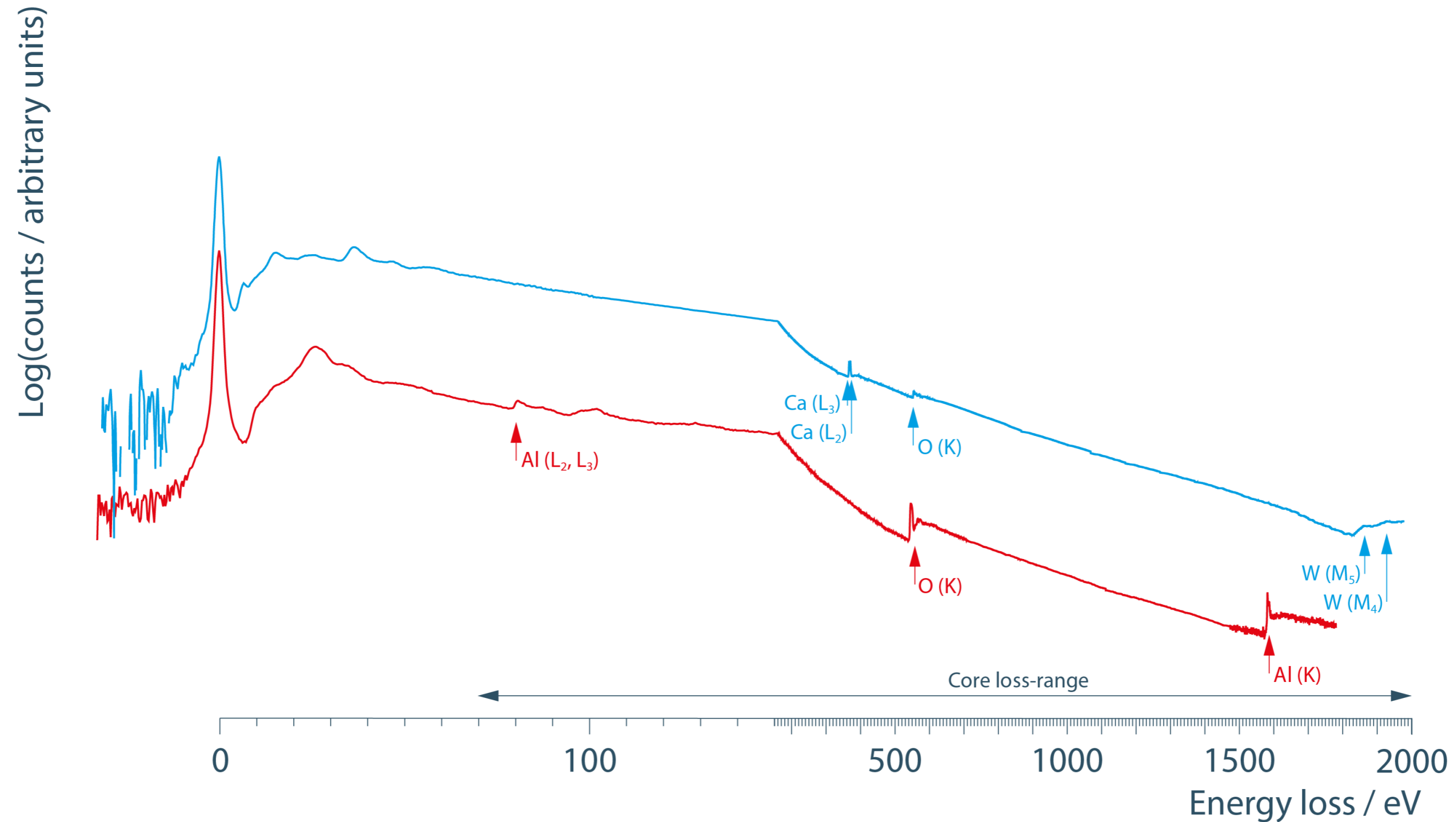
EELS of CaWO_4 and Al_2O_3 - Collective Excitations



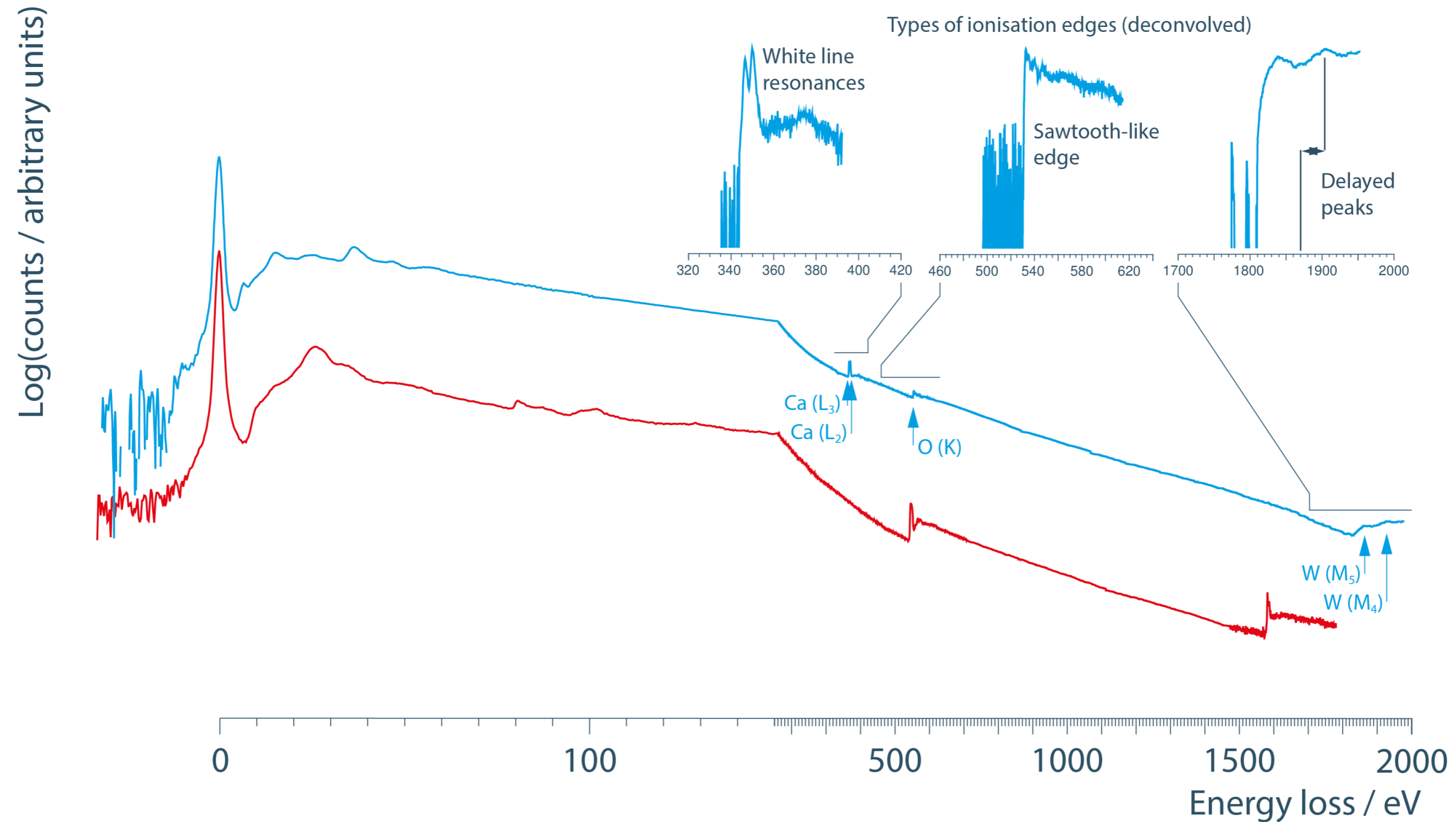
EELS of CaWO_4 and Al_2O_3 – Ionisation on Outer Shell e^-



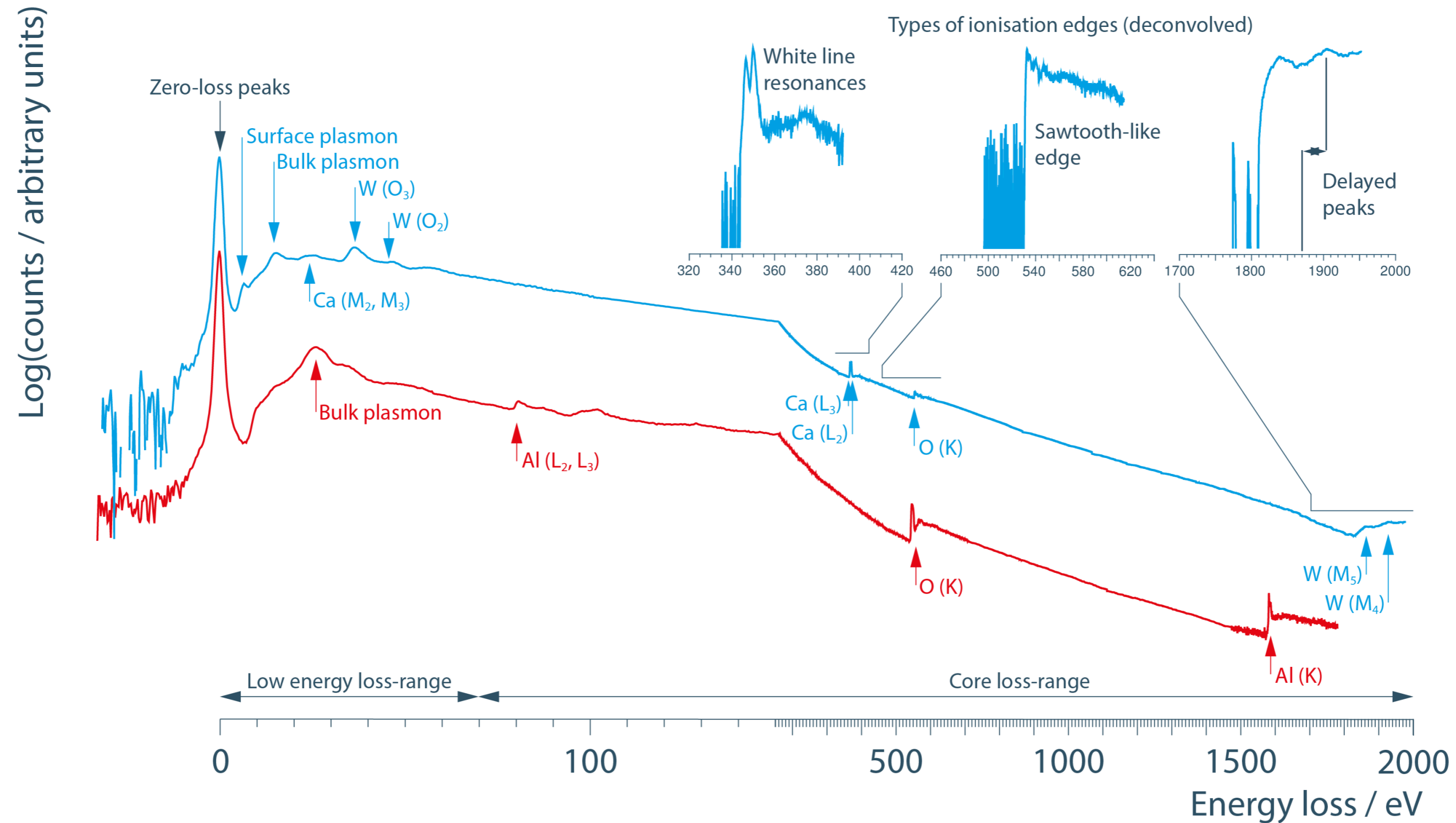
EELS of CaWO_4 and Al_2O_3 – Ionisation on Core Shell e^-



EELS of CaWO_4 and Al_2O_3 – Diverse Spectral Features



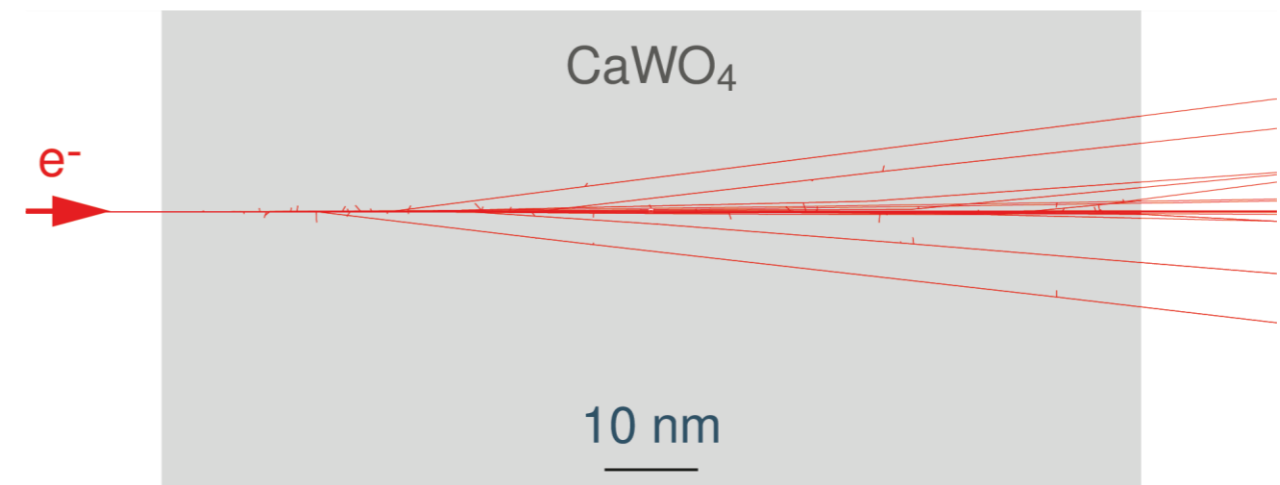
EELS of CaWO_4 and Al_2O_3 – Complex Sub-keV Spectra



Qualitative Comparison with Geant4

Qualitative Comparison with Geant4

- Work in progress!
- Use Geant4 10.6.3 (called from the ImpCRESST simulation code [1]), applicability limit ~ 250 eV*
- Here: physics not tuned / **out of the box** G4EmStandardPhysics_option4**



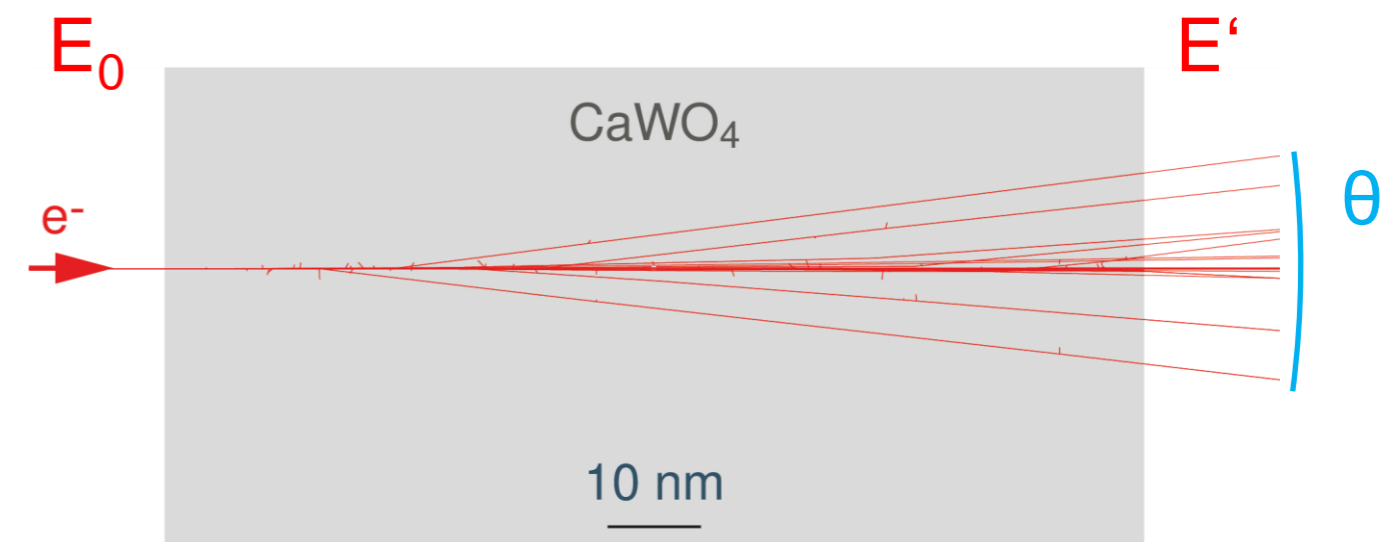
* For Livermore models [\[Livermore low-energy electromagnetic models\]](#)

** "G4EmStandardPhysics_option4, containing the most accurate models from the Standard and Low Energy Electromagnetic physics working groups" [\[Geant4, Book For Application Developers, rev7.1\]](#)

[1] [\[A.H Abdelhameed, HK, et al. \(CRESST Collaboration\), Eur.Phys.J. C79 \(2019\) 881\]](#)

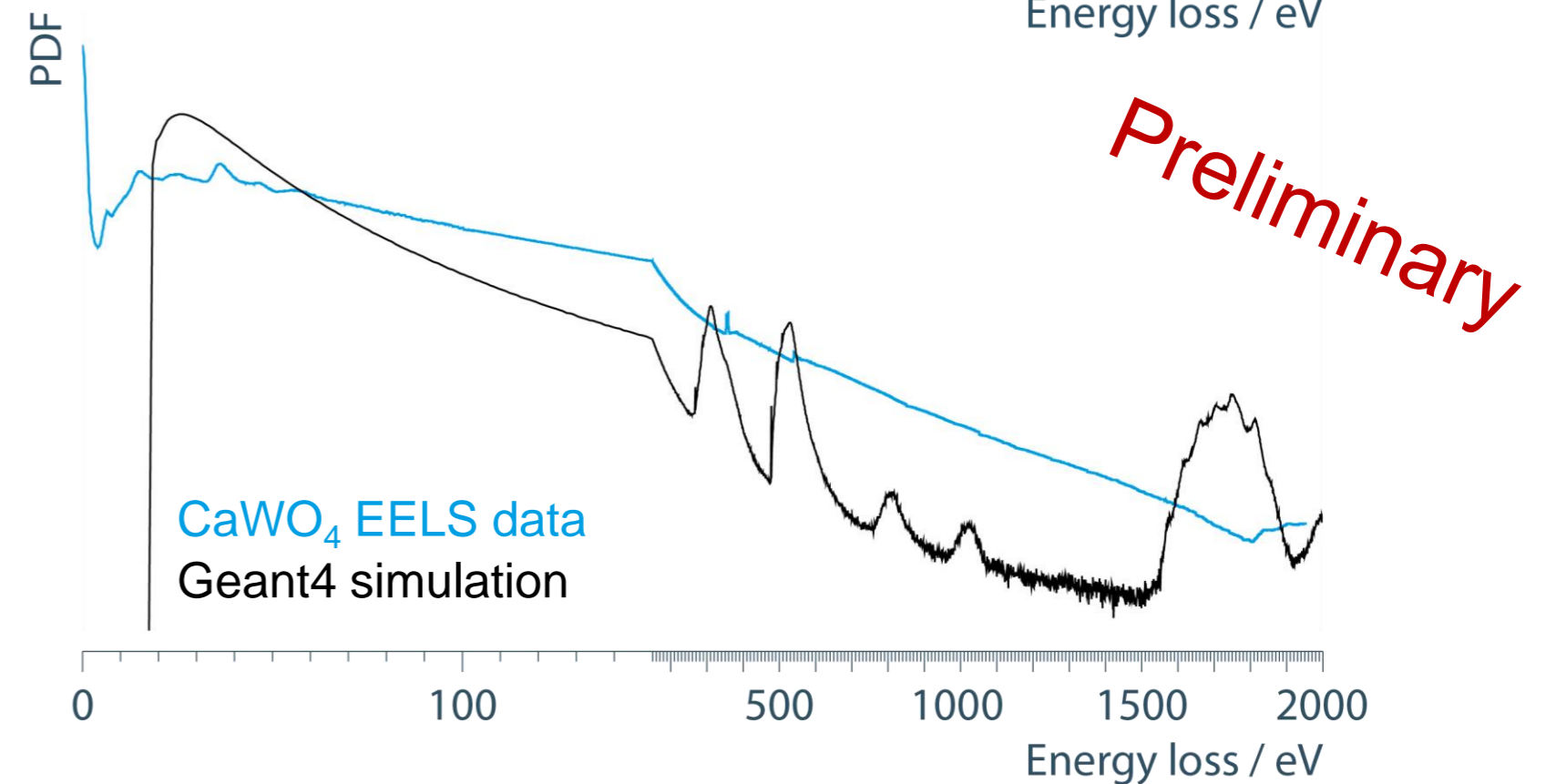
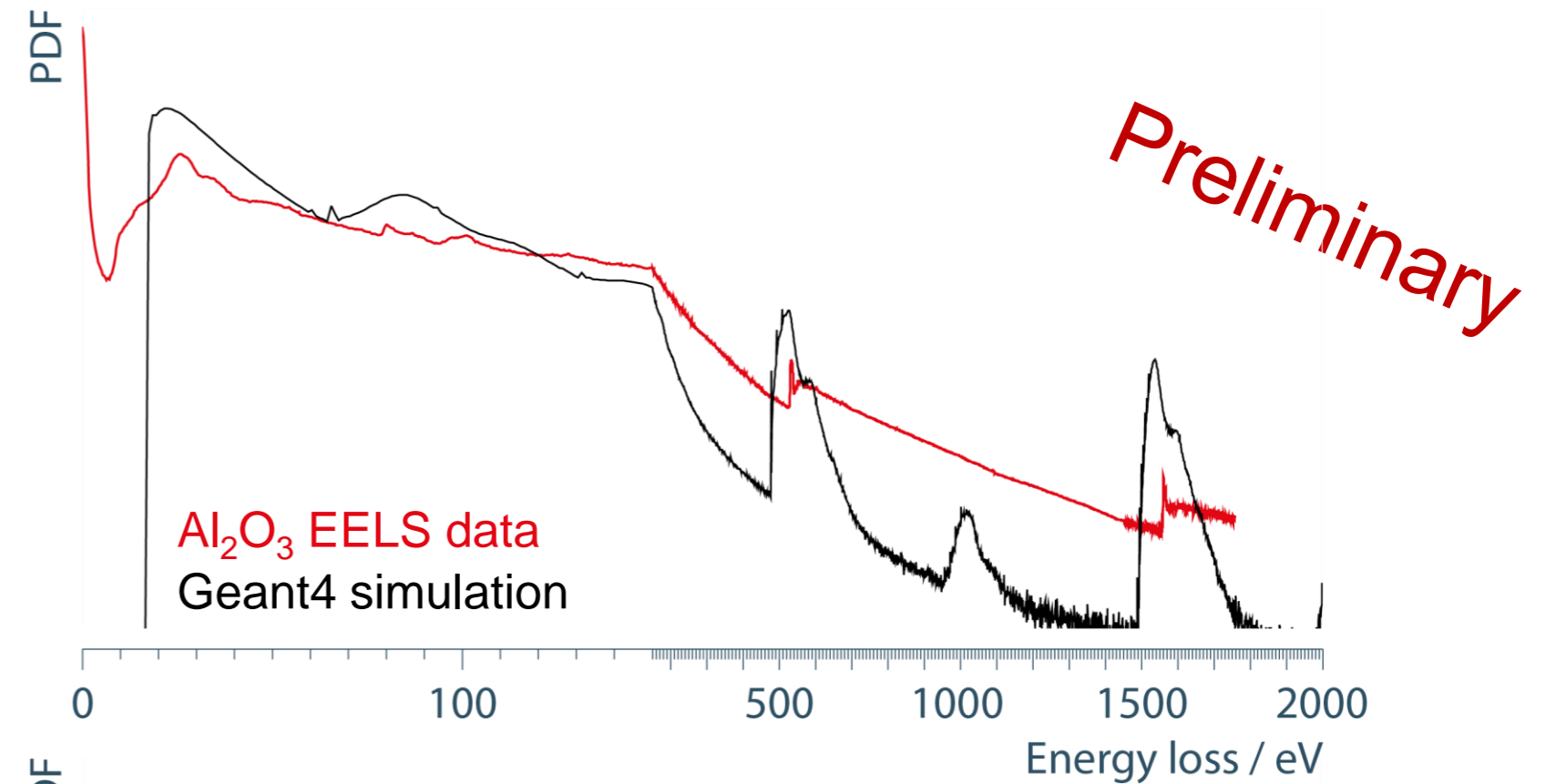
Qualitative Comparison with Geant4

- Work in progress!
- Use Geant4 10.6.3 (called from the ImpCRESST simulation code), applicability limit ~ 250 eV
- Here: physics not tuned / **out of the box** G4EmStandardPhysics_option4
- Shoot e^- ($E_0=200\text{keV}$) through 105 nm of CaWO_4 / Al_2O_3
→ Record energy loss $E_0 - E'$
if $\theta \leq 28$ mrad



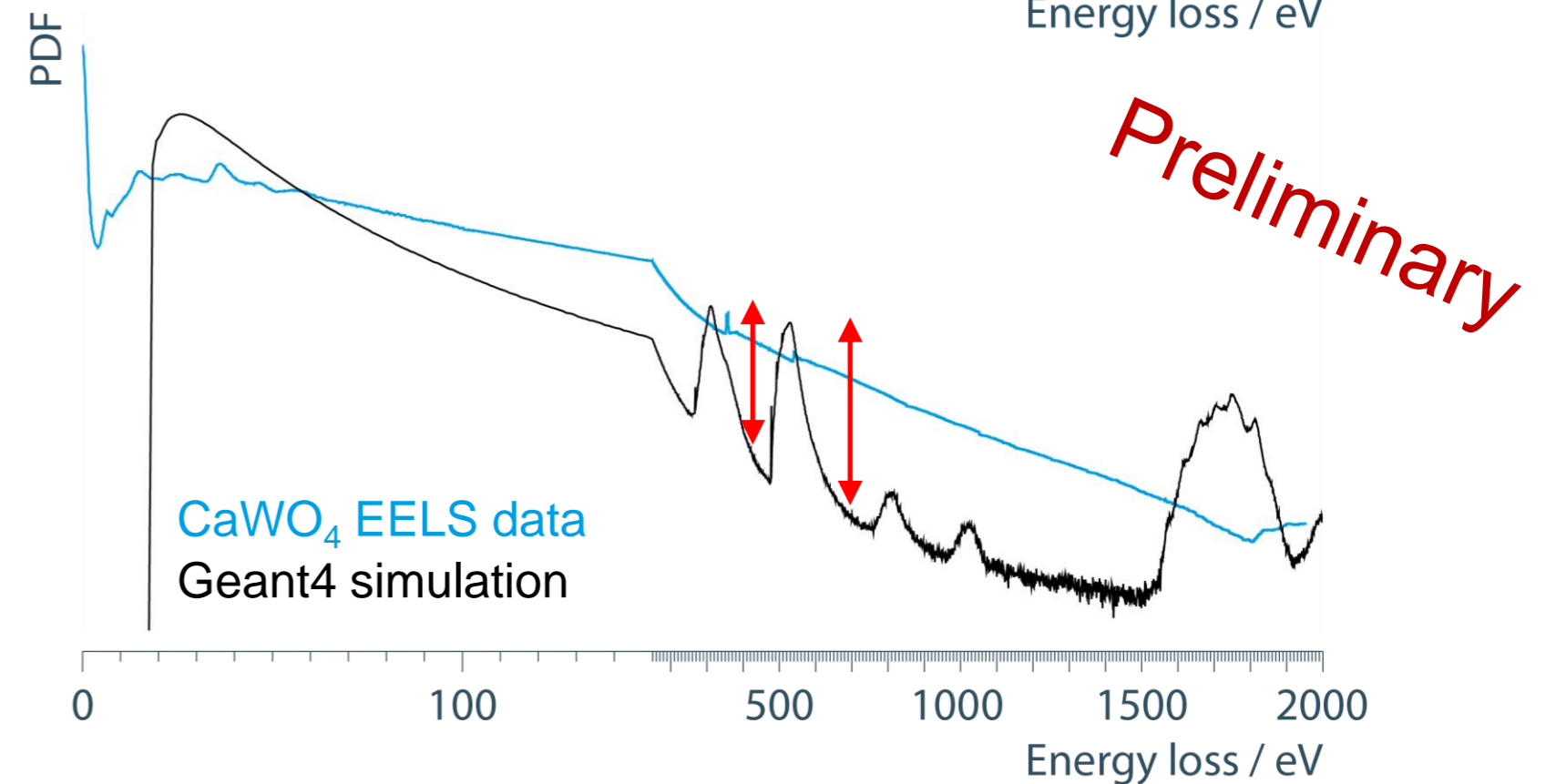
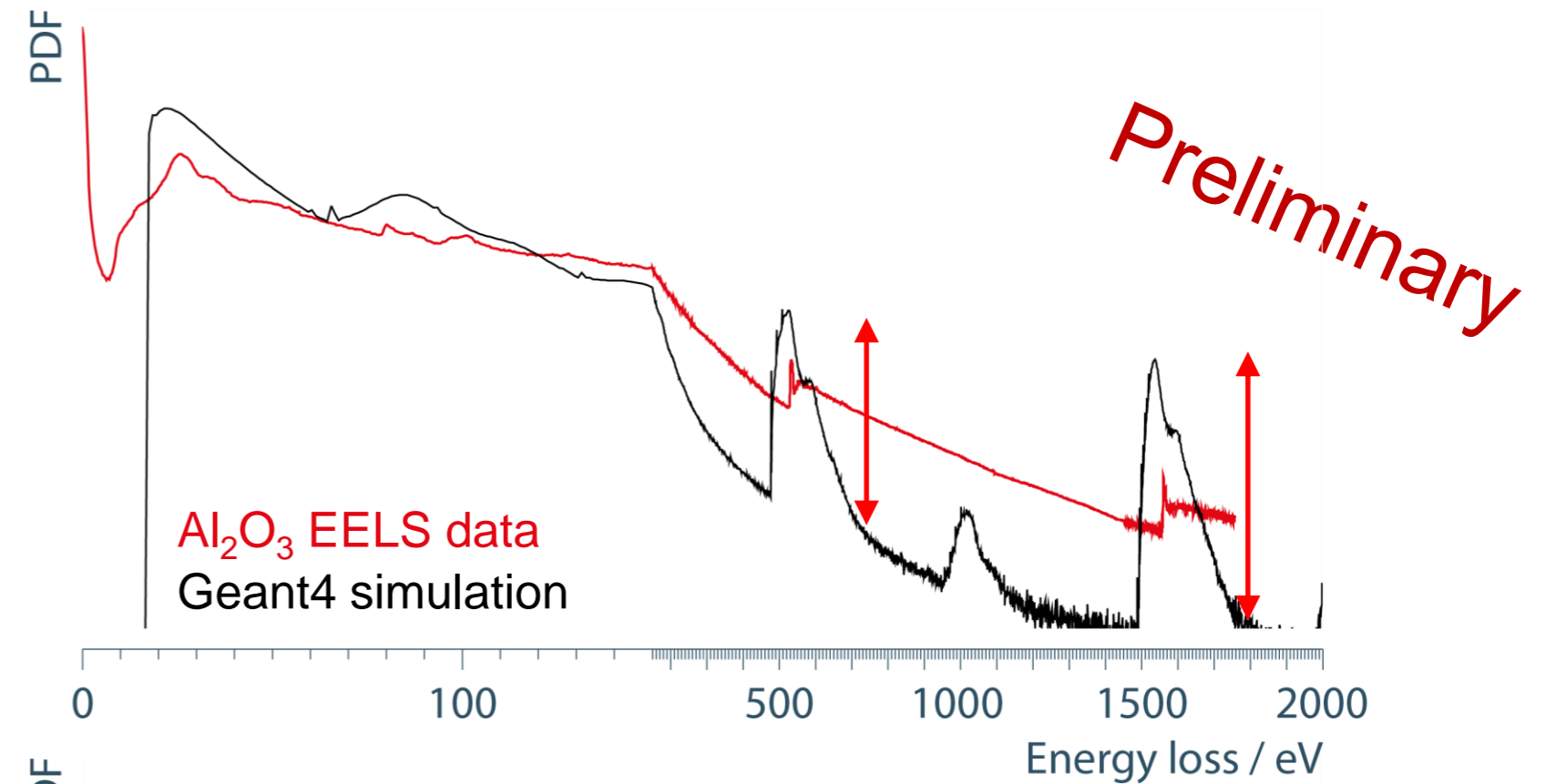
Qualitative Comparison with Geant4

- Work in progress!
- Comparing empirical PDFs



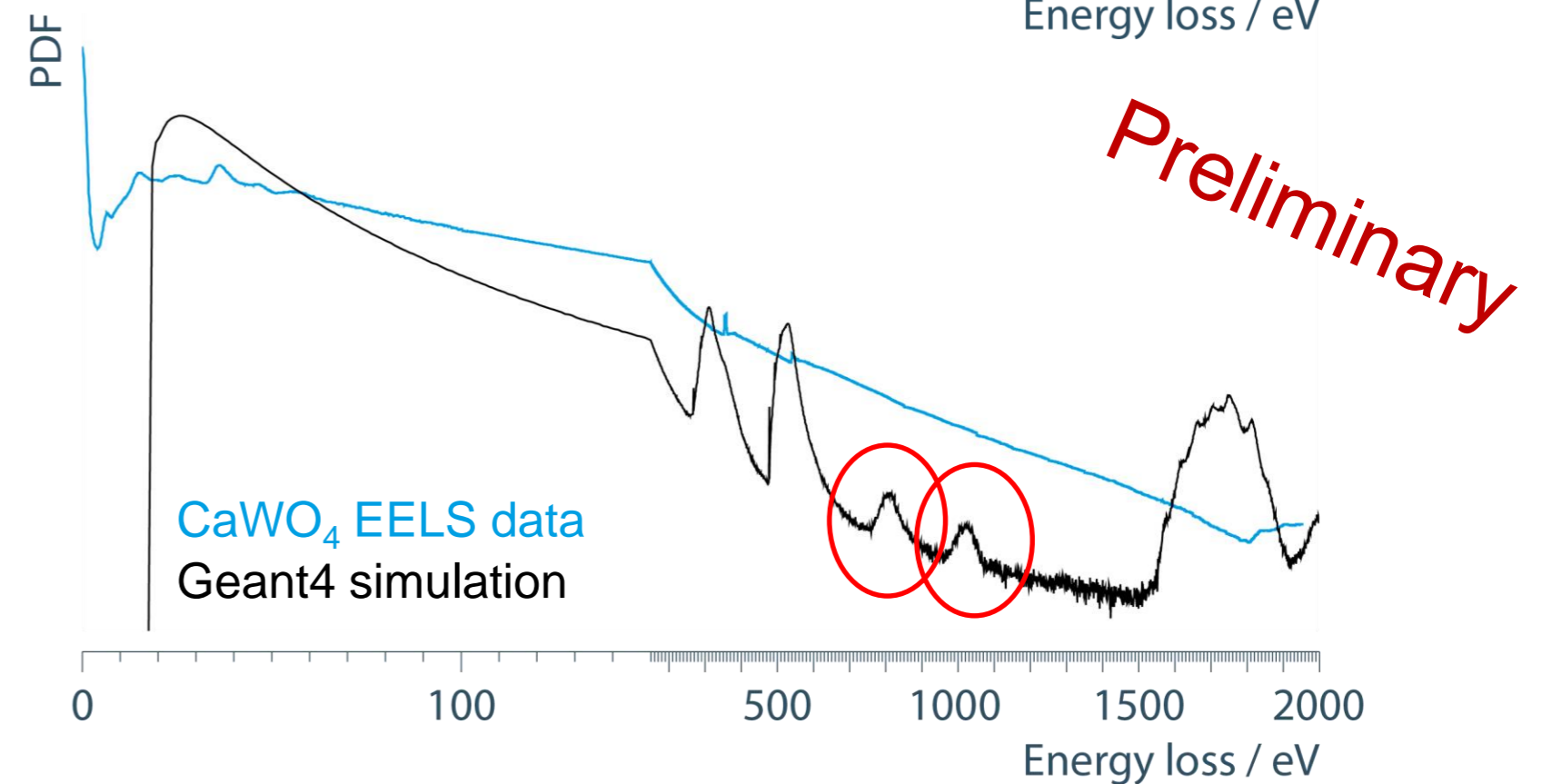
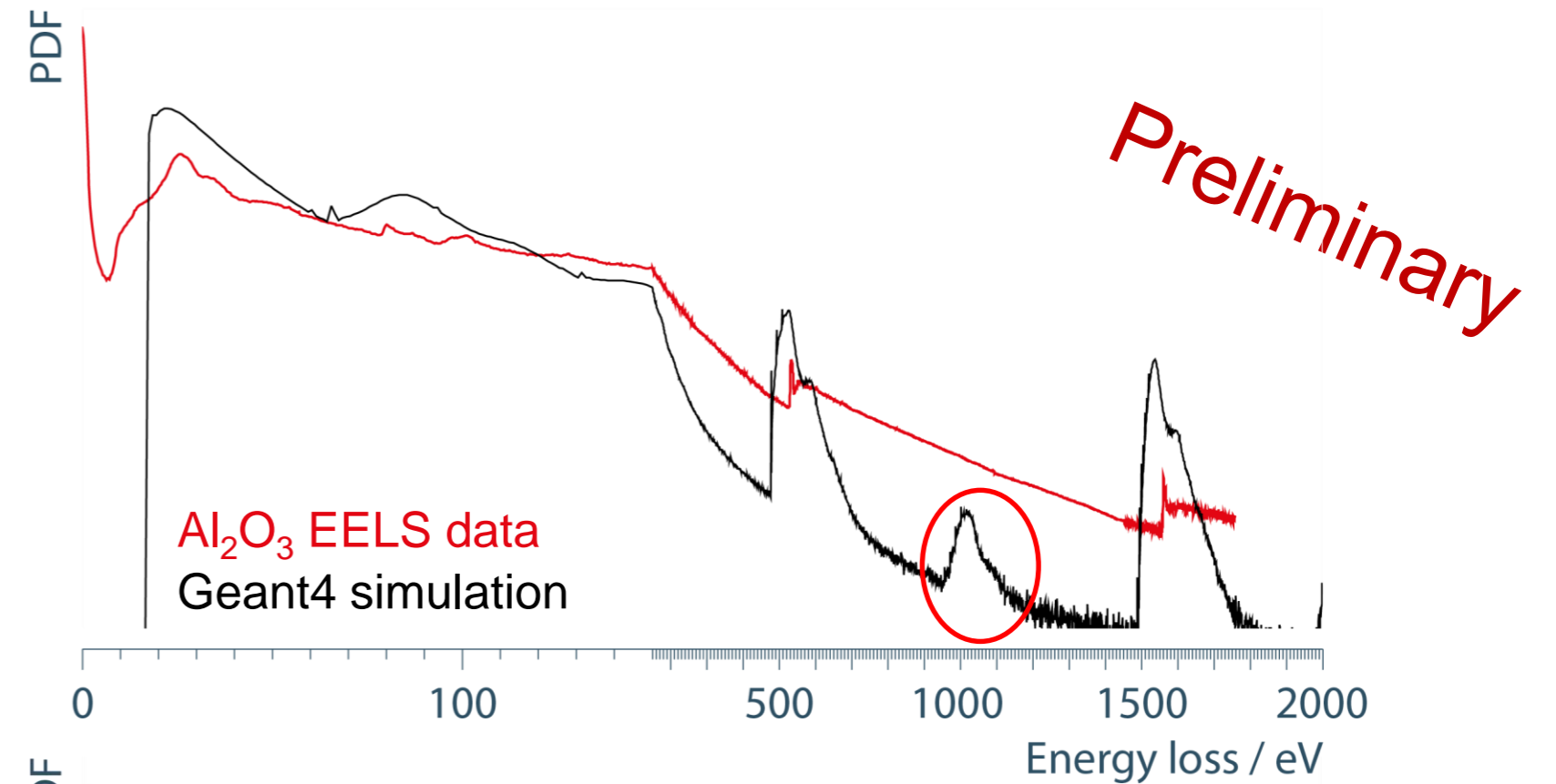
Qualitative Comparison with Geant4

- Work in progress!
- Comparing empirical PDFs
- **S/B** too high in Geant4



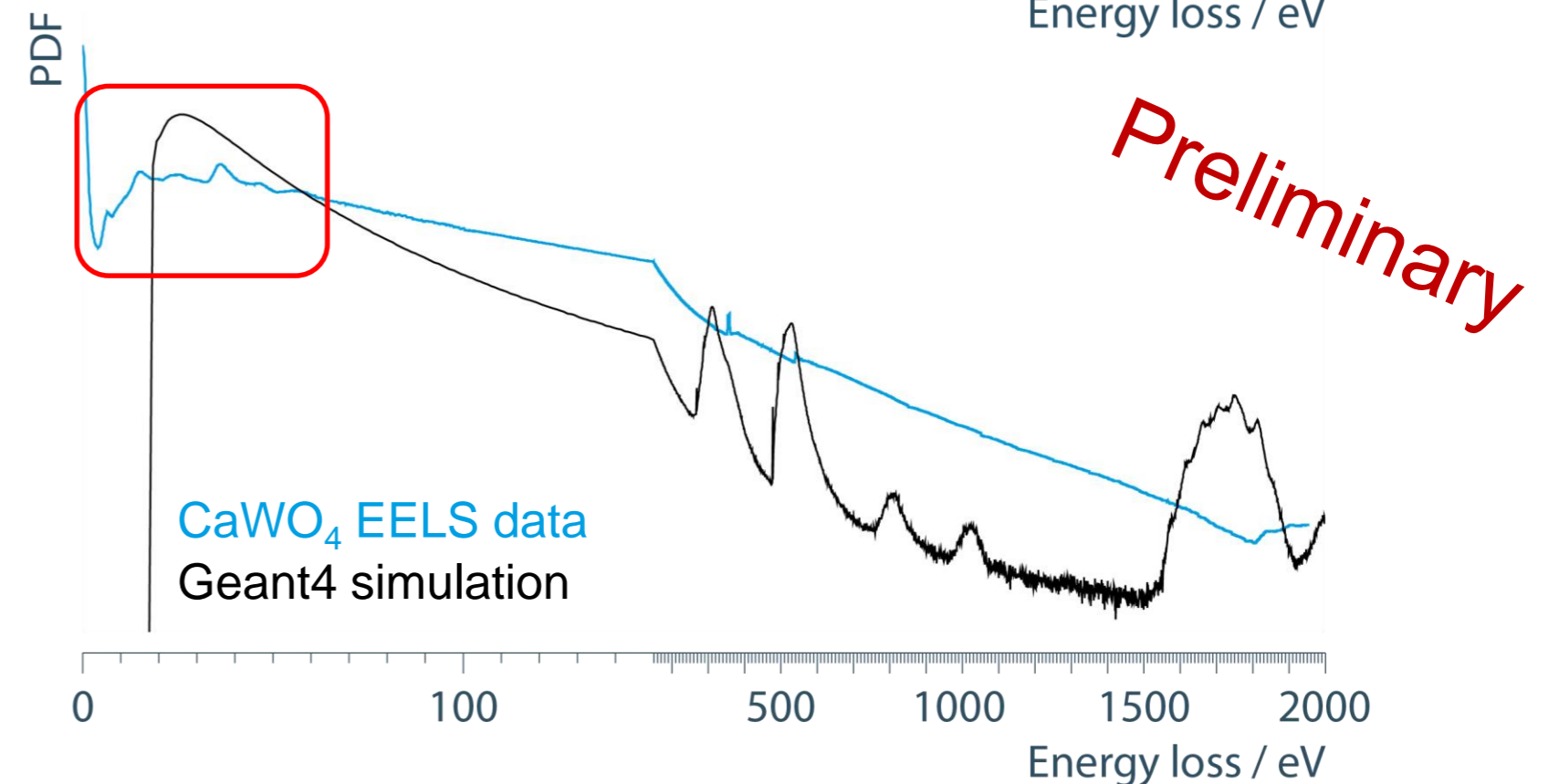
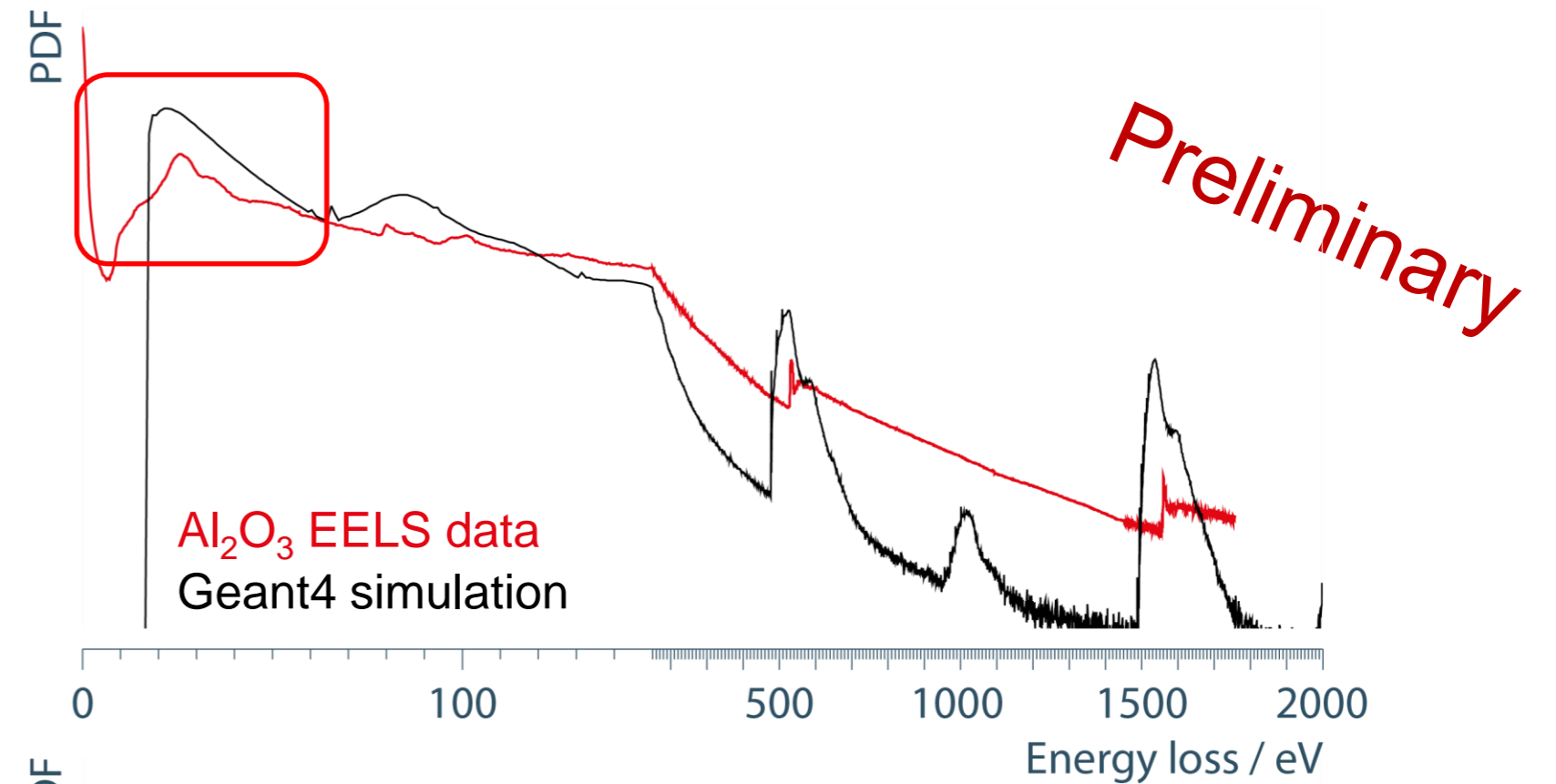
Qualitative Comparison with Geant4

- Work in progress!
- Comparing empirical PDFs
- **S/B** too high in Geant4
→ **Multiple interactions visible**



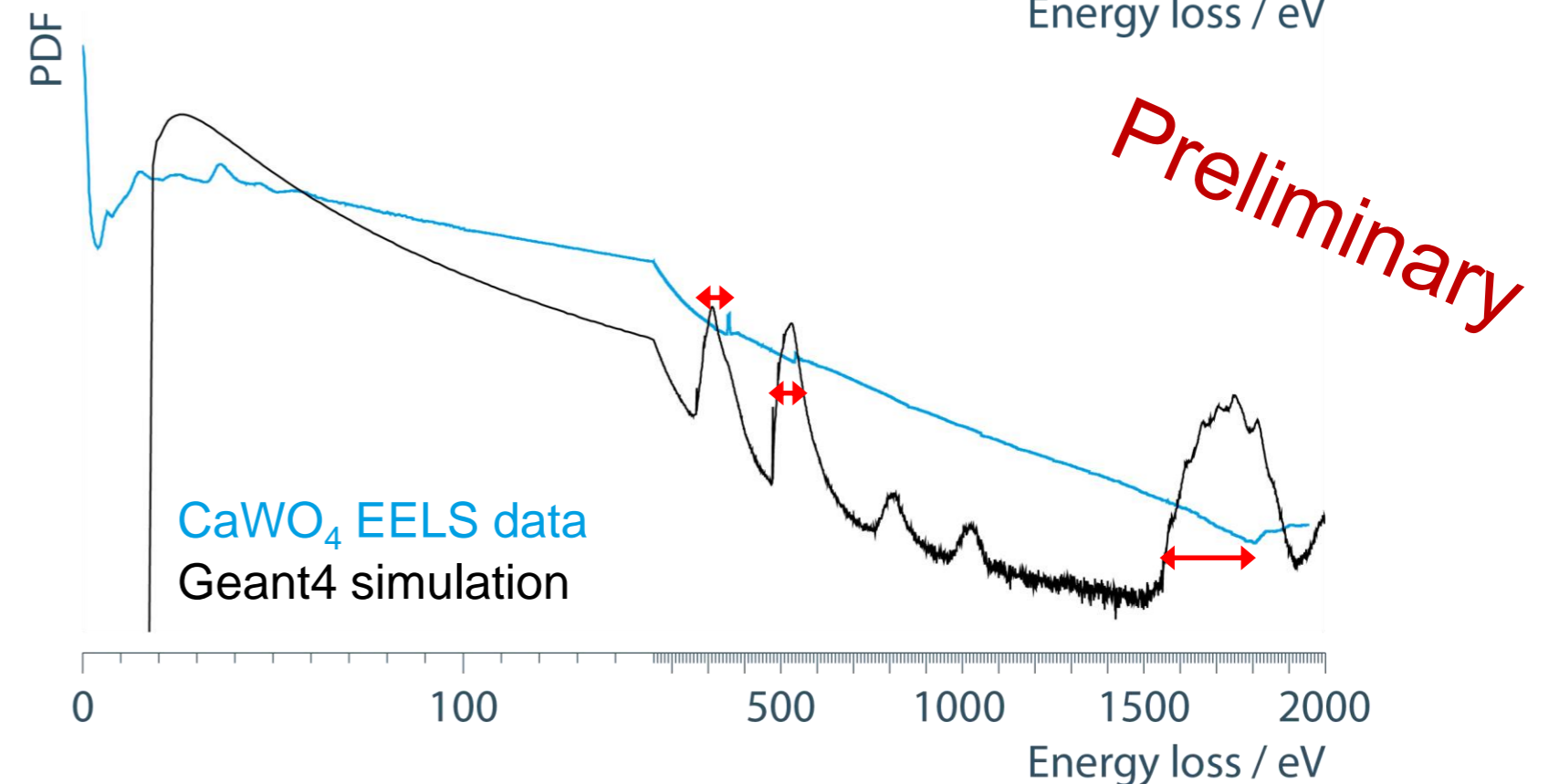
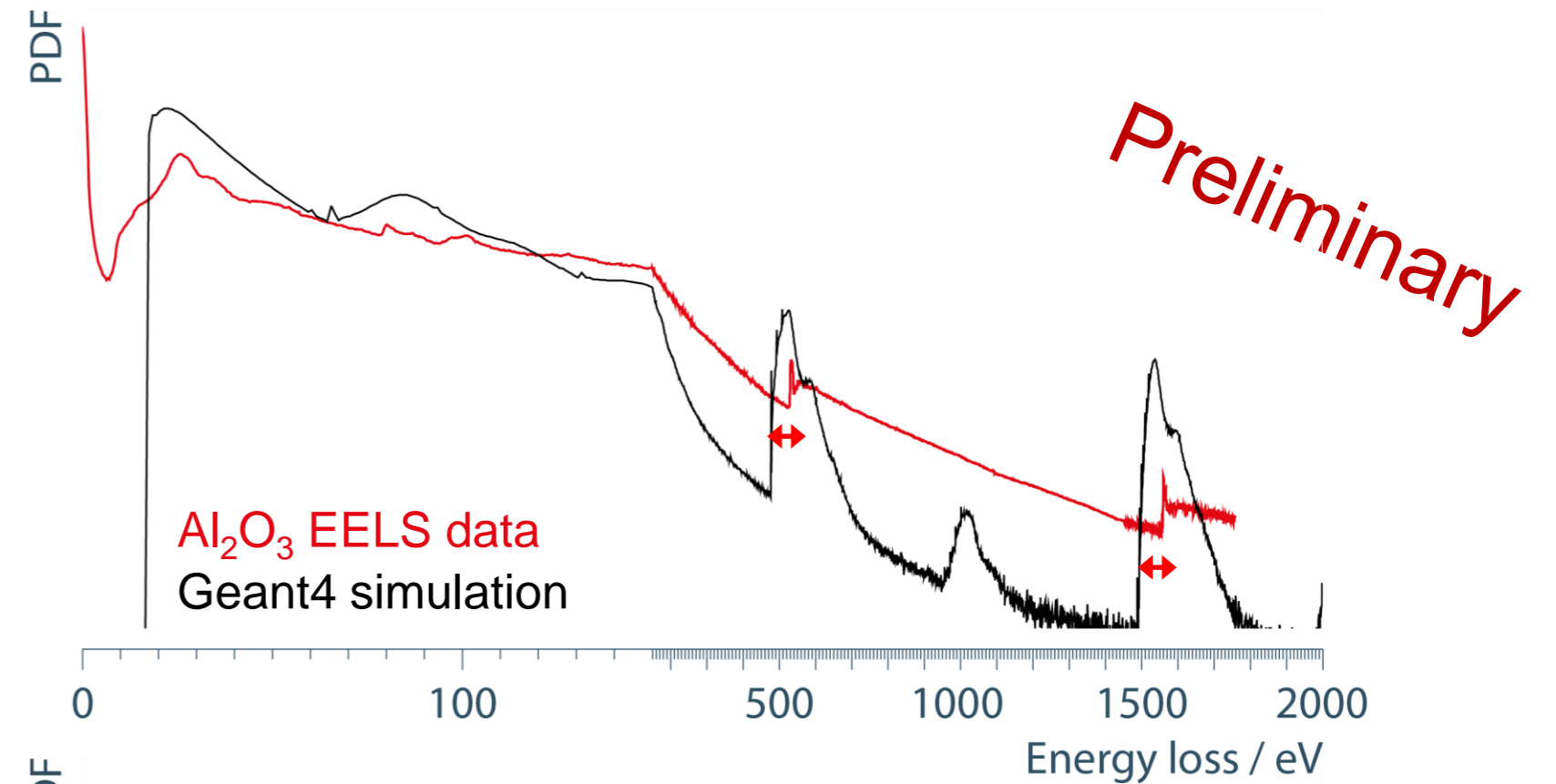
Qualitative Comparison with Geant4

- Work in progress!
- Comparing empirical PDFs
- **S/B** too high in Geant4
- **Spectral features** in low energy loss-ranges **are missing**
Expected as it is below Geant4's applicability limit of 250 eV



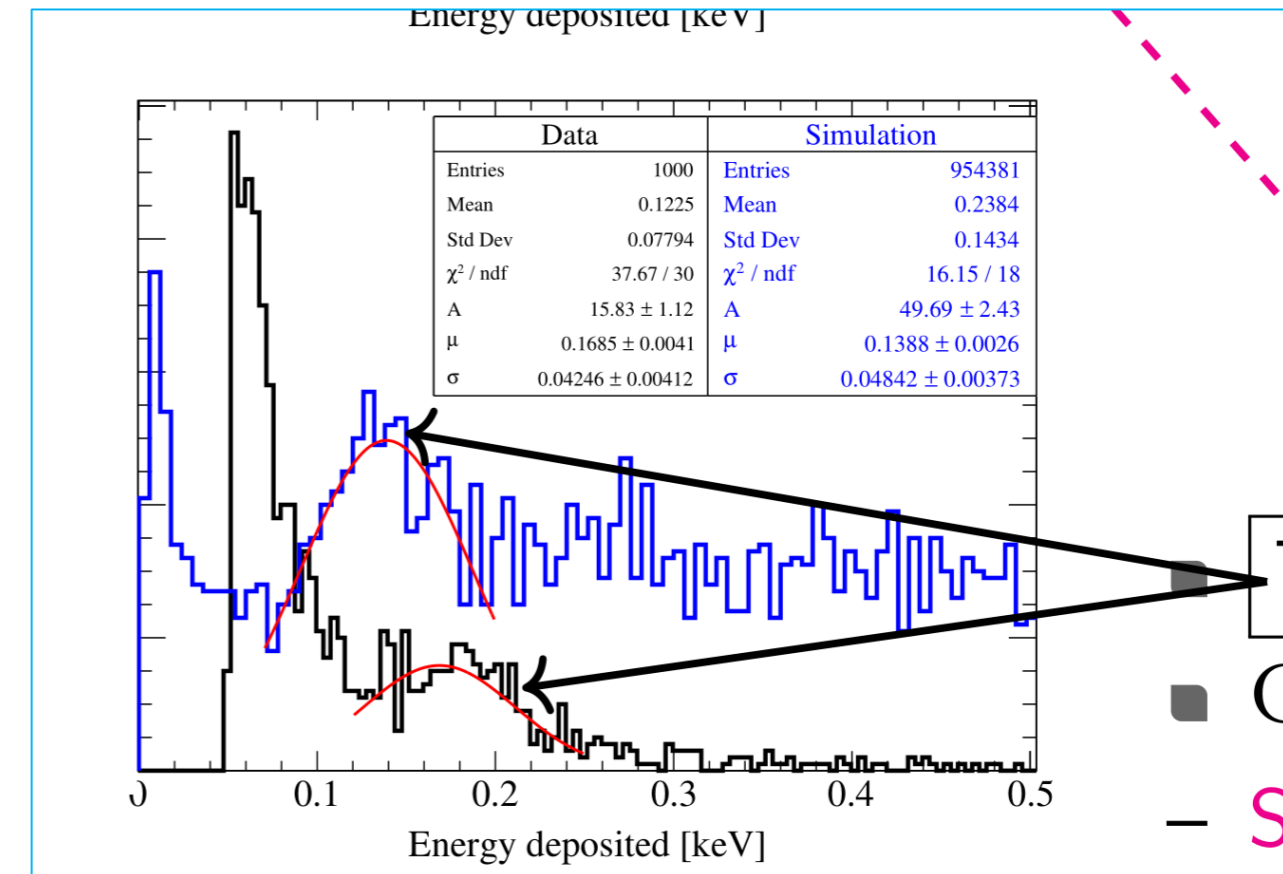
Qualitative Comparison with Geant4

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- **Shape of ionisation edges** in core-loss range differ, **onset differs by up to O(100 eV)**



Qualitative Comparison with Geant4

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[S. Banik (CRESST Collab.), TAUP2023]

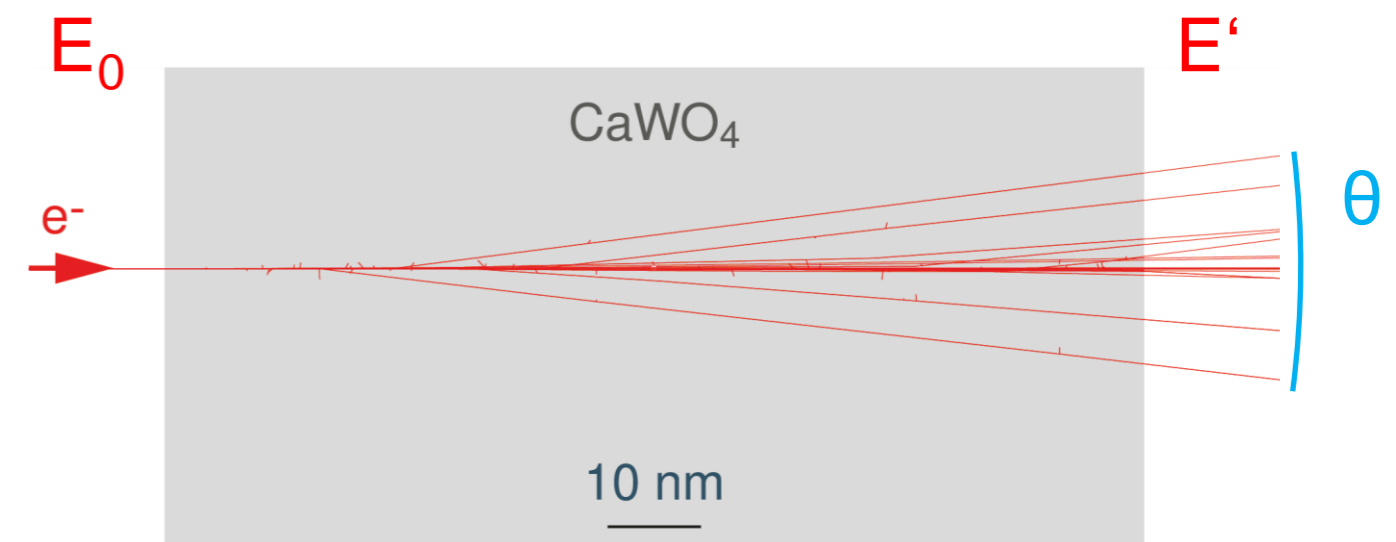
➔ Relevant for high accuracy simulation at sub-keV e.g. of CRESST's ^{55}Fe calibration sources

Outlook: Tuning Geant4

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- Comparing empirical PDFs
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Scattering angle

→ different (elastic) scattering models



Energy loss

→ different ionisation models

Outlook: Tuning Geant4

G4EmStandardPhysics_option4 uses:

- **Penelope** model for **ionisation**
Generalised Oscillation Strength-model fitted to data
- **Goudsmit and Saunderson** model for **elastic scattering**
“Condensed” multiple scatterings into one single step



Alternative:

- **Livermore** model
Data-driven, based on EEDL library
- **Coulomb single-scattering** model

- Studying possibility to use EELS data to develop a data-driven ionisation model for ionisation in the low loss-energy range

Summary and Outlook

Summary

- Rare event searches like CRESST and NUCLEUS have detection threshold of (10 eV) → reliable background simulations at sub-keV are crucial
- Use EELS of Al_2O_3 / CaWO_4 as reference data for validation of Geant4's ionisation model
 - **First Electron Energy Loss spectrum of CaWO_4**
 - **Rich spectral features** on the sub-keV scale → challenging for simulations
- Comparison with Geant4 10.6.3 “out of the box” shows **qualitative differences**:
 - Low loss features are missing, as expected
 - Shapes of core-loss peaks differ, position is **shifted by up to O(100 eV)**

Outlook

- **Tune Geant4**: study alternative physics models and settings
- Extend Geant4: study possibility to develop a **data-driven model for the low loss region**

Discuss Geant4 simulations
for rare event searches at

VIEWS24

Vienna Workshop on Simulations 2024

22-27 April 2024 • Vienna, Austria

<https://indico.cern.ch/e/VIEWS24>

Local organizing committee: Valentyna Mokina • Holger Kluck
• Samir Banik • Jens Burkhardt • Brigitte De Monte

<https://indico.cern.ch/e/VIEWS24>

