ELOISE –

Measured electronic stopping power in $CaWO_4$ and Al_2O_3 at sub-keV in comparison with Geant4 simulation

Holger Kluck · J. Burkhart · M. Stöger-Pollach
holger.kluck@oeaw.ac.at

VIEWS24, Vienna (Austria), 26 April 2024

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS
FWF Der Wissenschaftsfonds.

- What is ELOISE?
  – Verifying Geant4 simulation in $CaWO_4$ and Al_2O_3 at sub-keV energies
  this talk: electron energy loss

- How to get reference data
  – Electron Energy Loss Spectroscopy (EELS) of $CaWO_4$ and Al_2O_3

- Comparing data and simulation
  – Geant4 10.6.3 "out of the box"

- Connecting data and simulation
  – Deduce electronic stopping powers as input to future simulations

- Summary & Outlook

Der Wissenschaftsfonds.

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

[HK, SciPost Phys. Proc., 12 (2023) 64, arXiv:2212.12634]

What is ELOISE?

R**el**iable Backgr**o**und S**i**mulation at **S**ub-keV **E**nergies

ELOISE: Motivation

CRESST

Cryogenic **Rare Event Search**
with Superconducting Thermometers

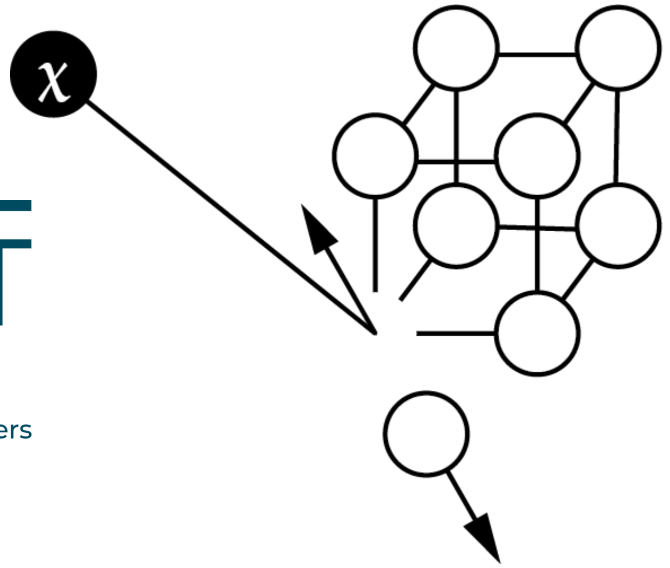
nucleus
EXPERIMENT

- $CaWO_4$ 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
  → a *reliable* background model is crucial

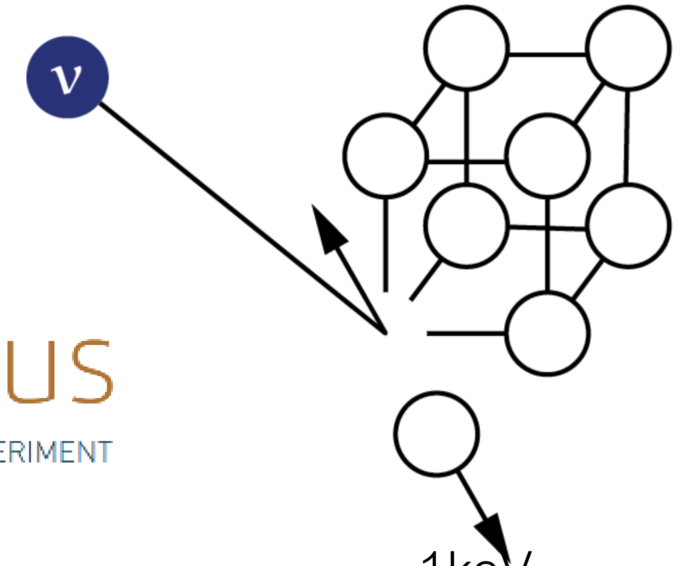
ELOISE: Energy Scale

DM — elastic scattering

ν — CEνNS



CRESST
Cryogenic **Rare Event Search** with Superconducting Thermometers



nucleus EXPERIMENT

Table 1: The maximal recoil energies caused by CEνNS with a neutrino of 2 MeV kinetic energy ($E_{\mathrm{rec},\nu}$) and by elastic scattering with a 2 GeV/c^2-DM particle with a velocity of 220 m s^{-1} ($E_{\mathrm{rec,DM}}$) and the minimal displacement energies (E_{dis}) for $CaWO_4$ [8] and Al_2O_3 in case of Al [9].

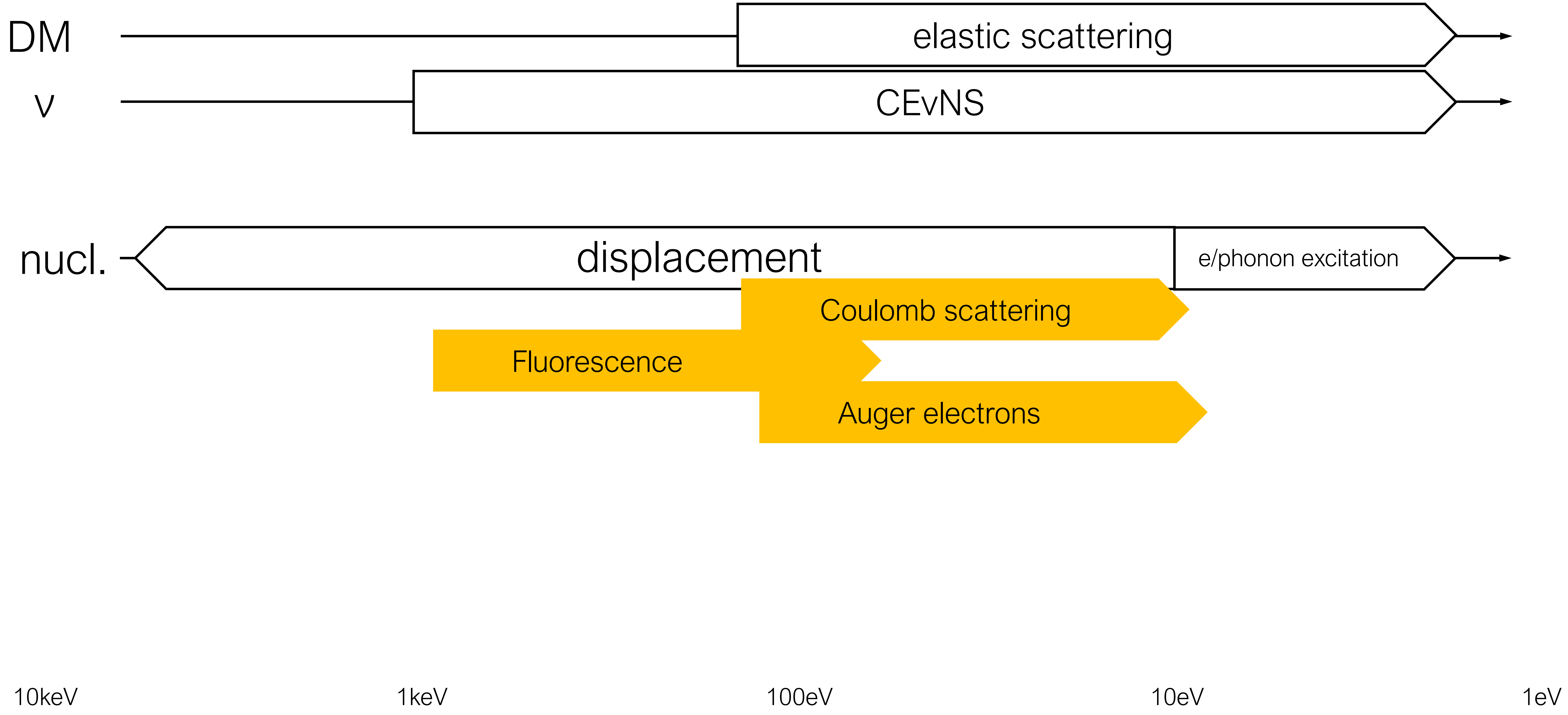
	$_{8}$O	$_{13}$Al	$_{20}$Ca	$_{74}$W
$E_{\mathrm{rec,DM}}$/eV	106.4	69.2	48.6	11.5
$E_{\mathrm{rec},\nu}$/eV	499.9	296.5	199.5	43.5
E_{dis}/eV	20	47.5	24	196

[HK2023]

→ Physics at the sub-keV scale

10keV 1keV 100eV 10eV 1eV

ELOISE: Interactions of Interest



ELOISE: Interactions of Interest

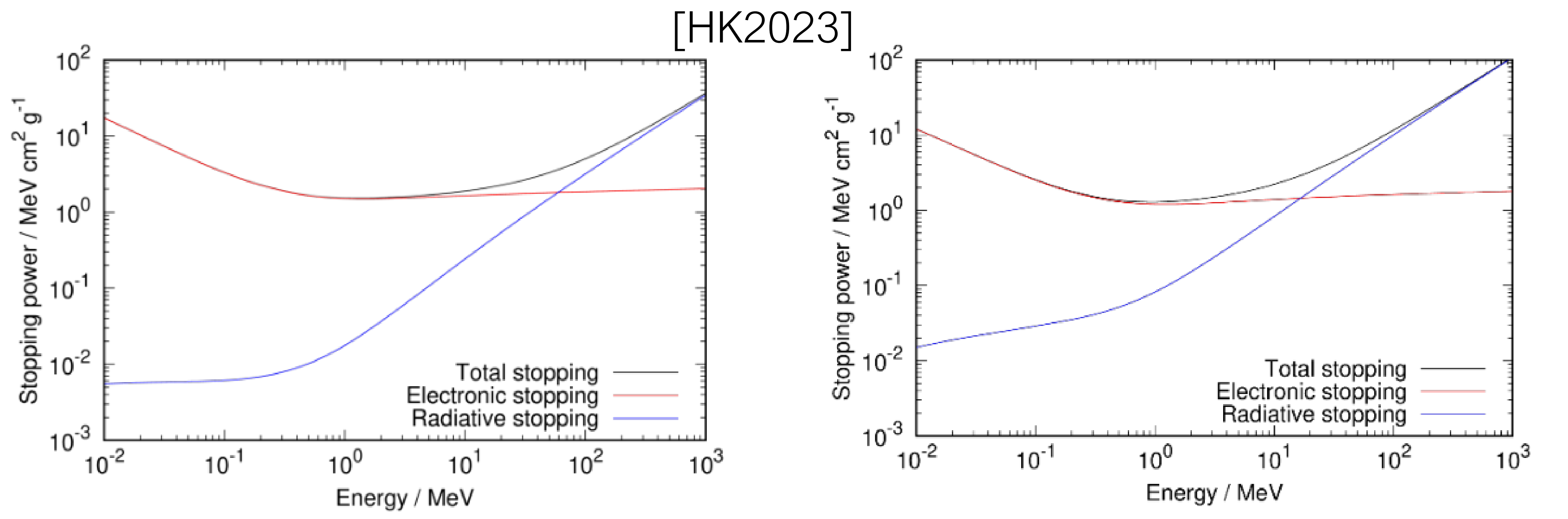
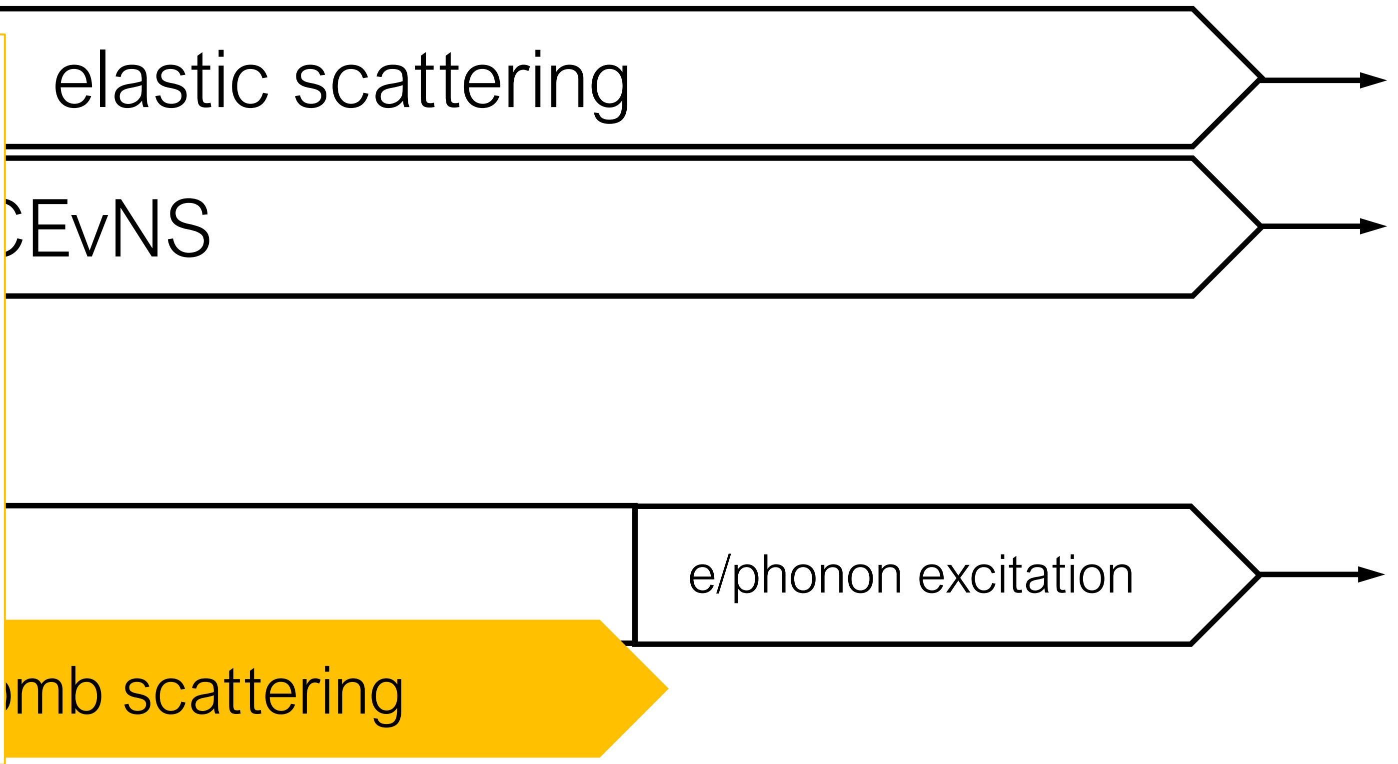
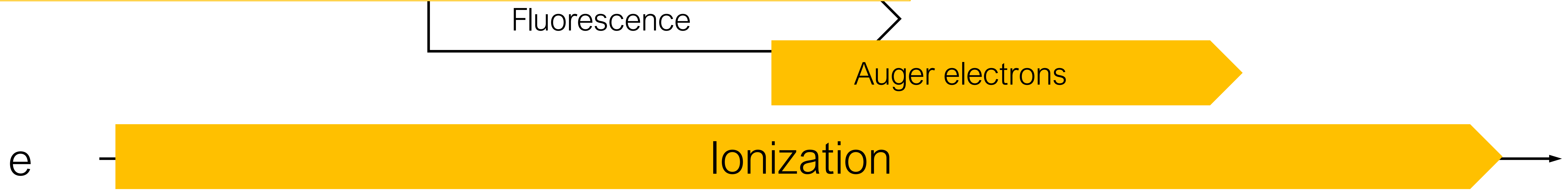


Figure 6: Stopping power for e⁻ in Al_2O_3 (*left*) and $CaWO_4$ (*right*). Data taken from ESTAR[12].





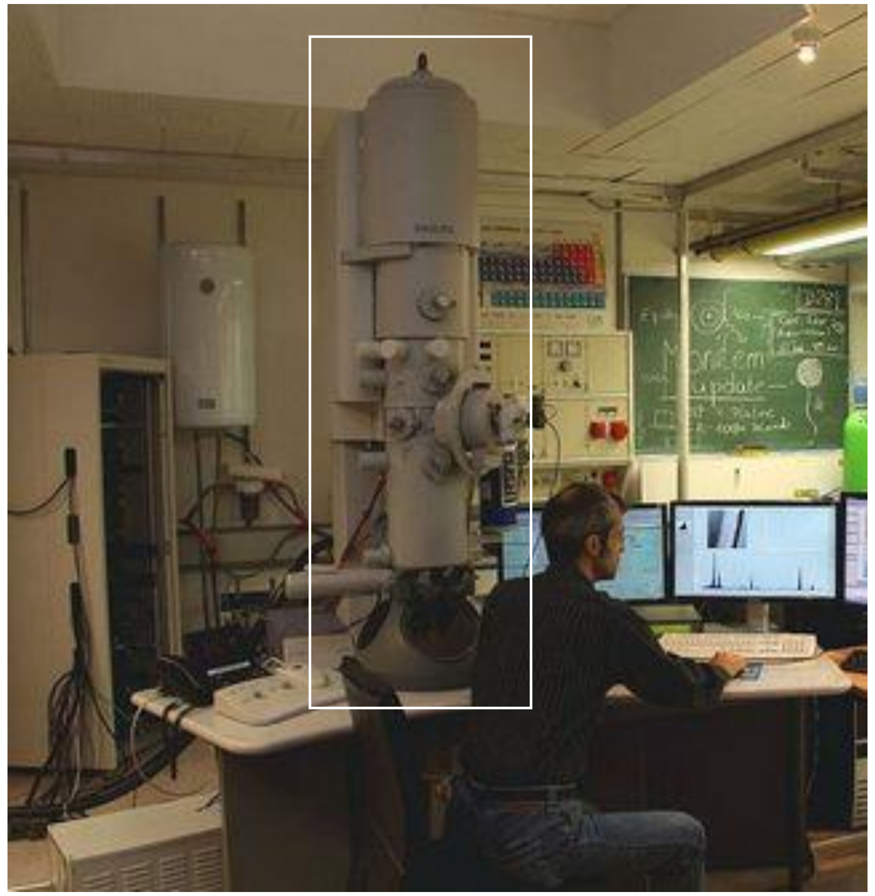
➔No reference data below 1 keV

10keV 1keV 100eV 10eV 1eV

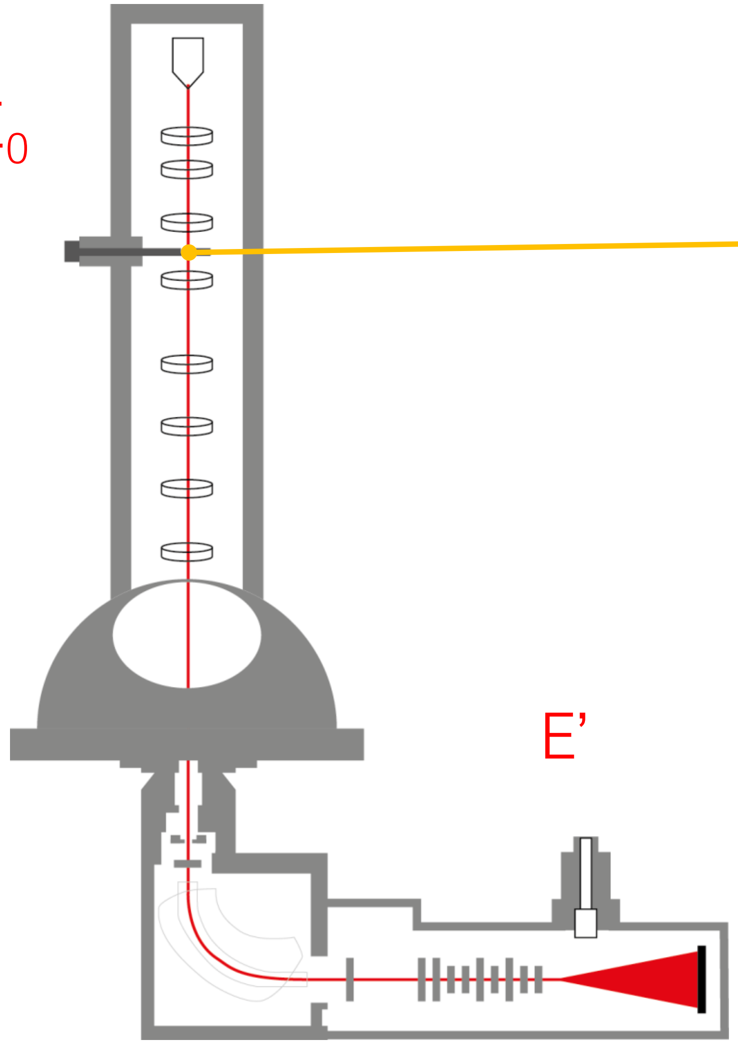
How to get reference data

EELS of $CaWO_4$ and Al_2O_3

Reference Data: EELS

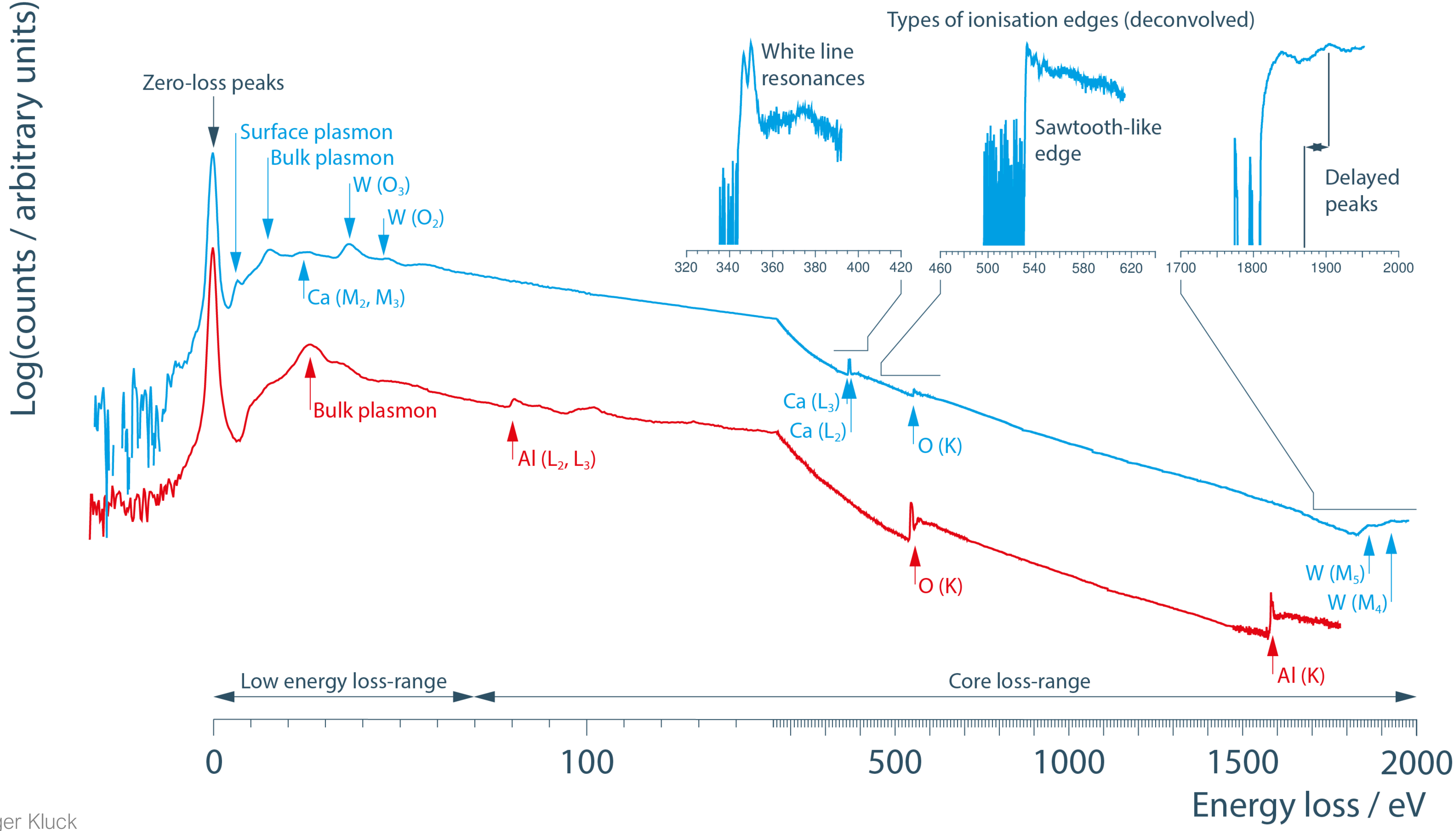


EELS conducted
by M. Stöger-Pollach, TU Wien, USTEM



- Samples of $CaWO_4$, Al_2O_3 provided by NUCLEUS
- Only *single* e^- interactions
  → *thin* target
  - Disk with ∅=3mm and h=
  - 77 nm for $CaWO_4$
  - 57 nm for Al_2O_3
- Monochromatic e^- (E_0=200 keV)
- Well established method:
  Electron Energy Loss Spectroscopy (EELS)
  →Energy loss: E_0-E'

EELS of $CaWO_4$ and Al_2O_3



Comparing data and simulation

Qualitative comparison of the EELS measurement with “out of the box” Geant4 simulations

Physics Setting

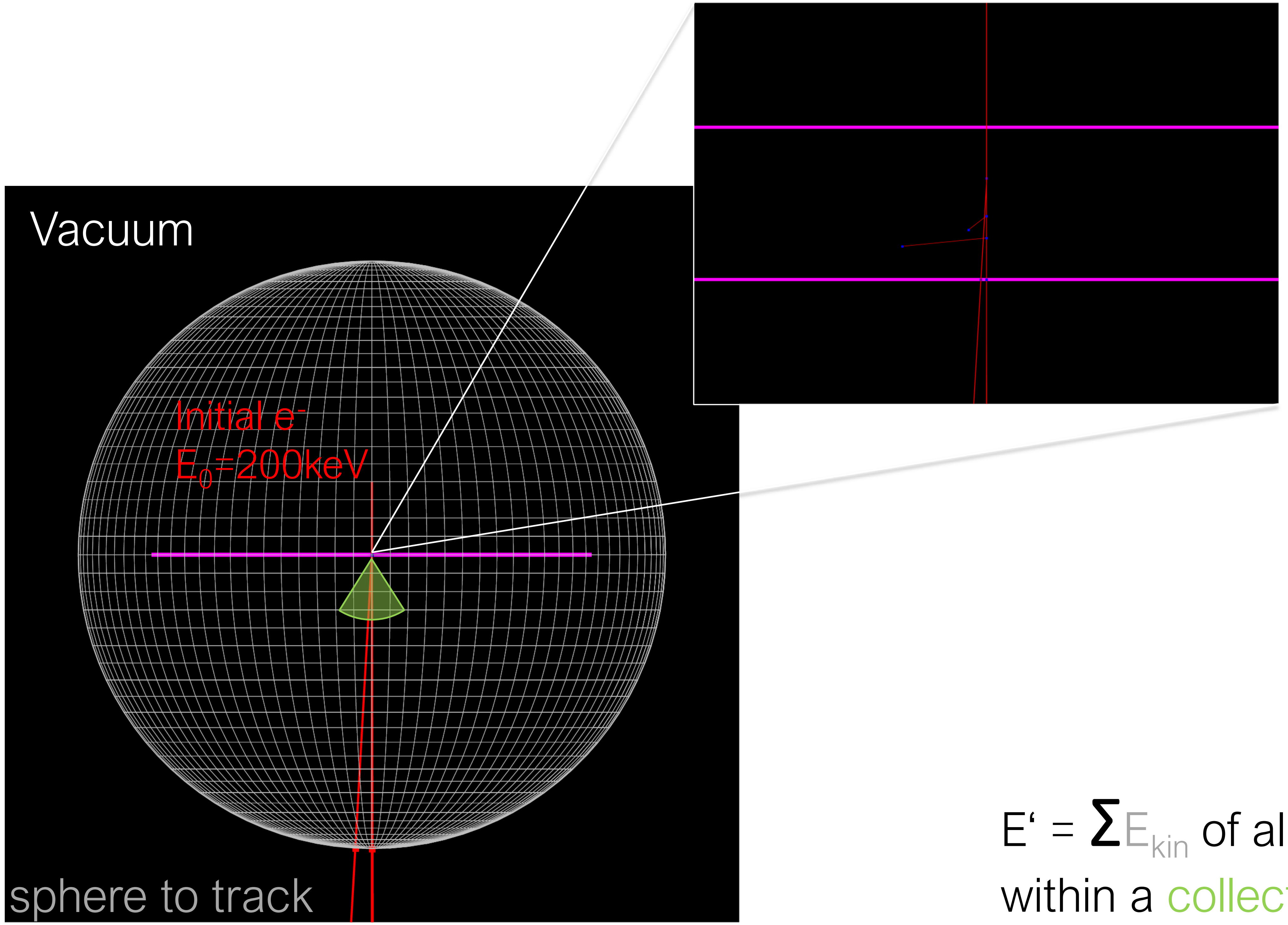
Used as „standard configuration“:

- Geant4 10.6.3
- `Shielding` physics list with
  - `G4EmStandardPhysics_option4` for EM physics
  - Enable atomic de-excitation
  - Track e^- down to 1 eV
  - Range cut of 500 nm

```
/process/em/fluo true
/process/em/auger true
/process/em/augerCascade true
/process/em/pixe true
/process/em/deexcitationIgnoreCut true
/process/em/lowestElectronEnergy 1 eV
/run/setCut 500. nm
/run/setCutForAGivenParticle proton  0. nm
/cuts/setLowEdge 1. eV
```

- *No* tuning on physics processes/models

Implemented Setup

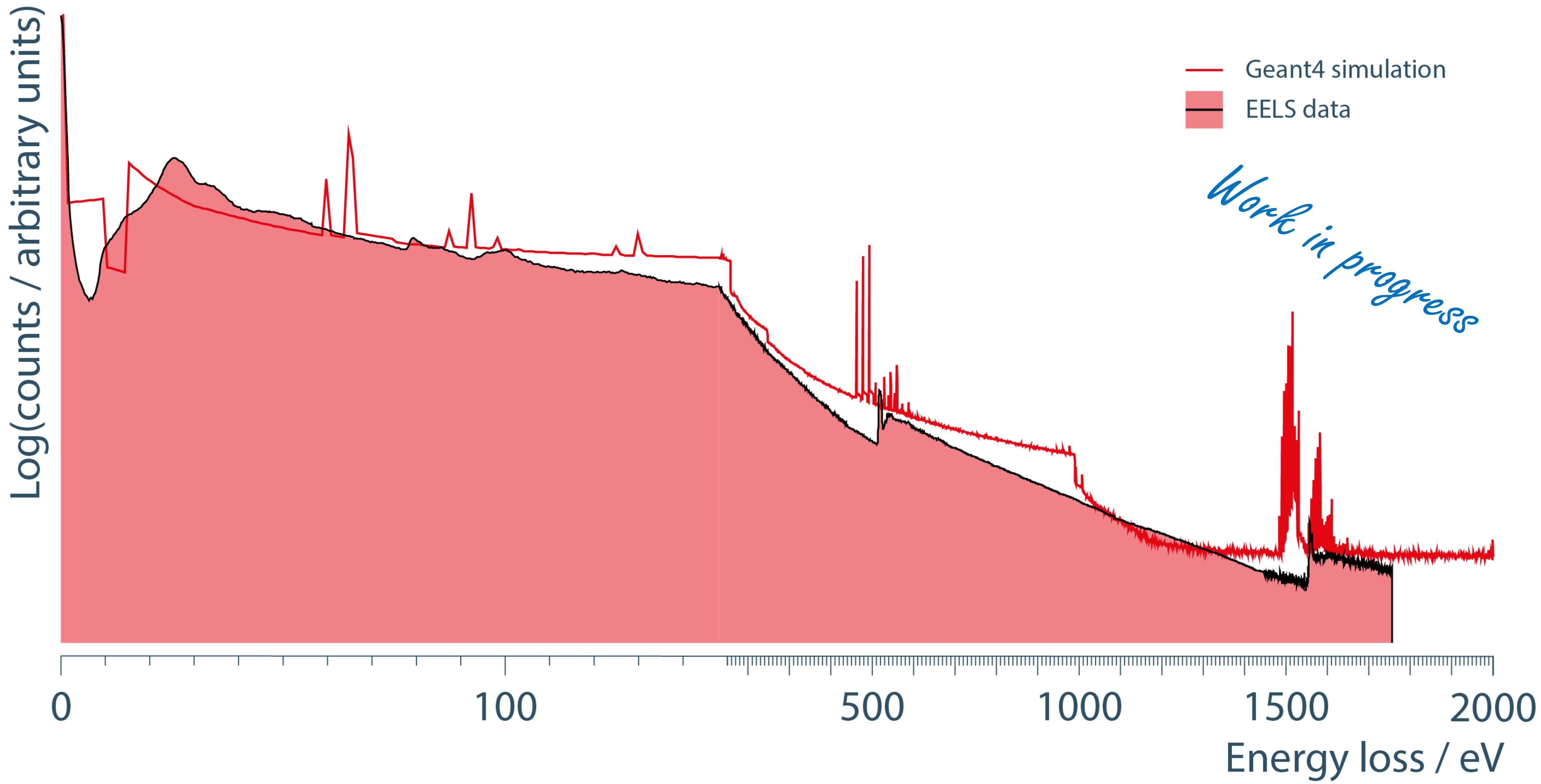


„Ghost“ sphere to track transmitted e^- → get E_{kin}

Target: disk of ∅=3mm and h=
77 nm for G4_CALCIUM_TUNGSTATE
57 nm for G4_ALUMINUM_OXIDE

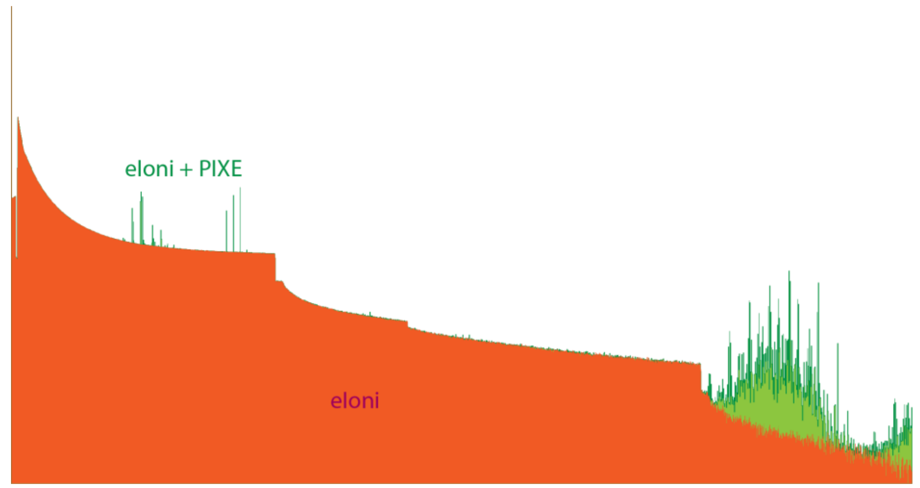
$E' = \sum E_{kin}$ of all transmitted e^-
within a collection angle/2=14 mrad
→$\Delta E = E_0 - E'$

Comparison Geant4 vs EELS for Al_2O_3

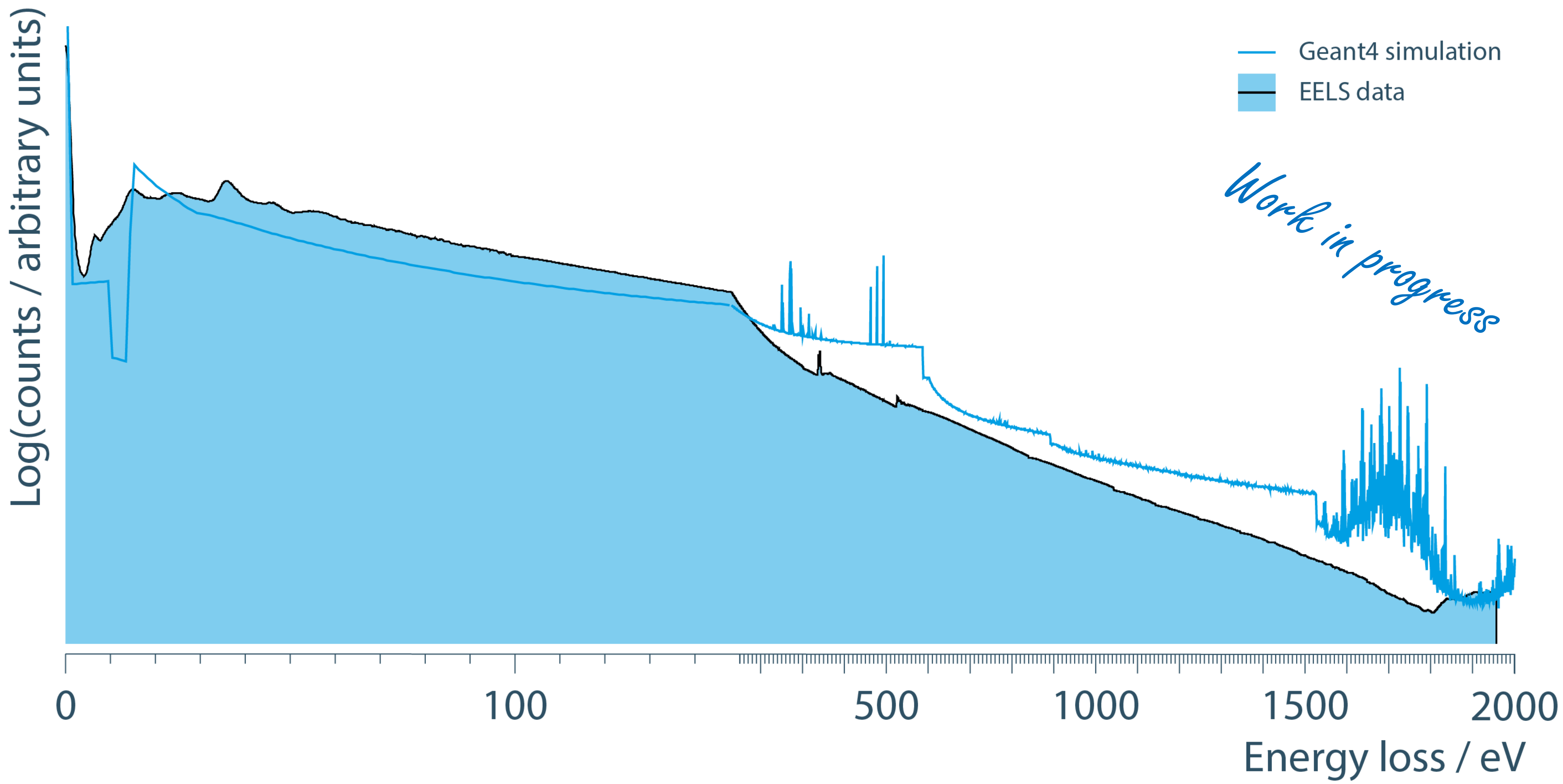


Simulation normalized to measured counts in [0,2keV]

- Overall trend is roughly matching
- Not matching for edges (`eIoni`) and peaks (`PIXE`)
- Artefact E<15eV



Comparison Geant4 vs EELS for $CaWO_4$



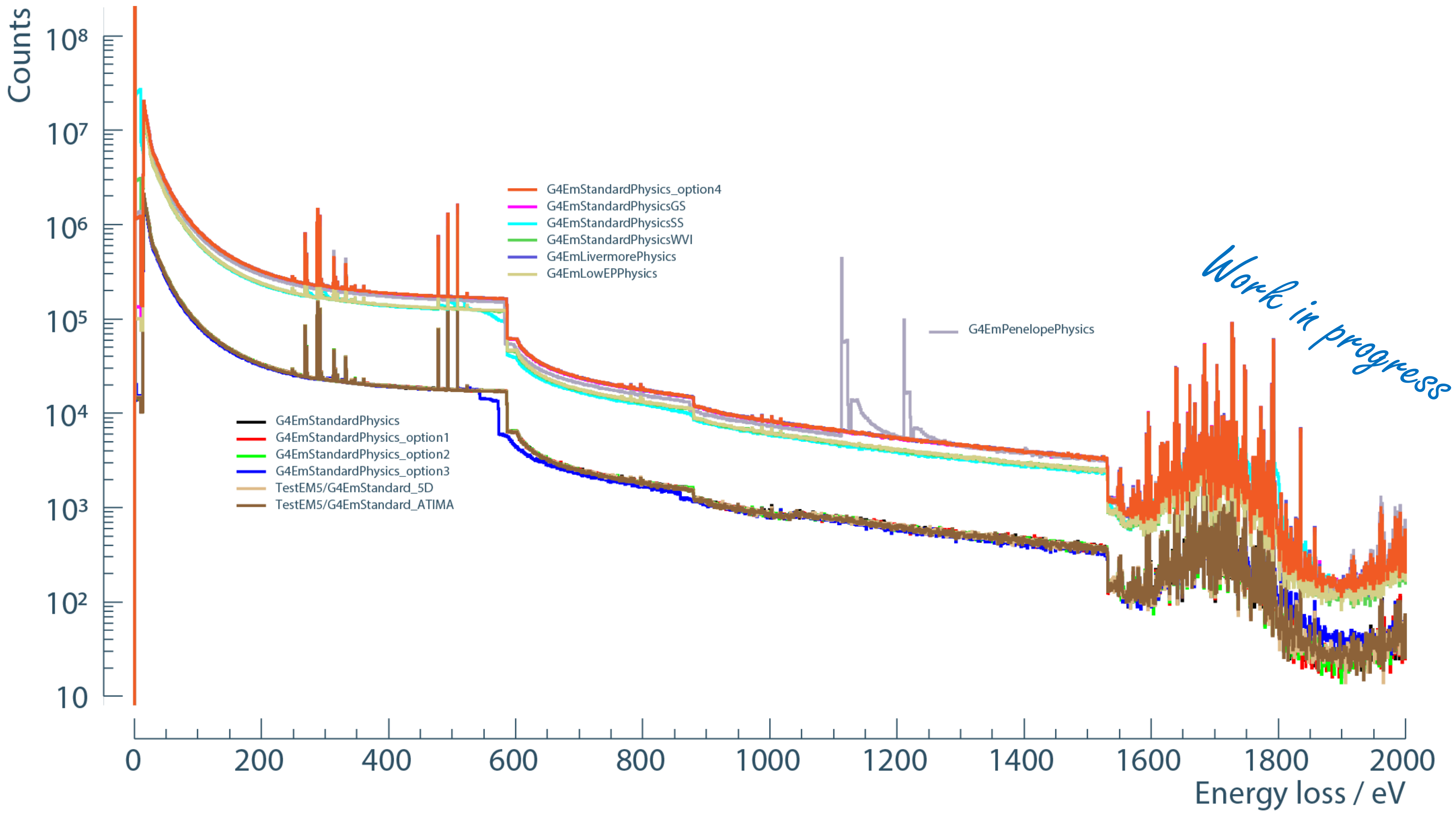
Simulation normalized to measured counts in [0,2keV]

- Same findings as for Al_2O_3

→ Needs further study

→ Check if improvement is possible with
  - Different EM physics constructor
  - Different EM process settings

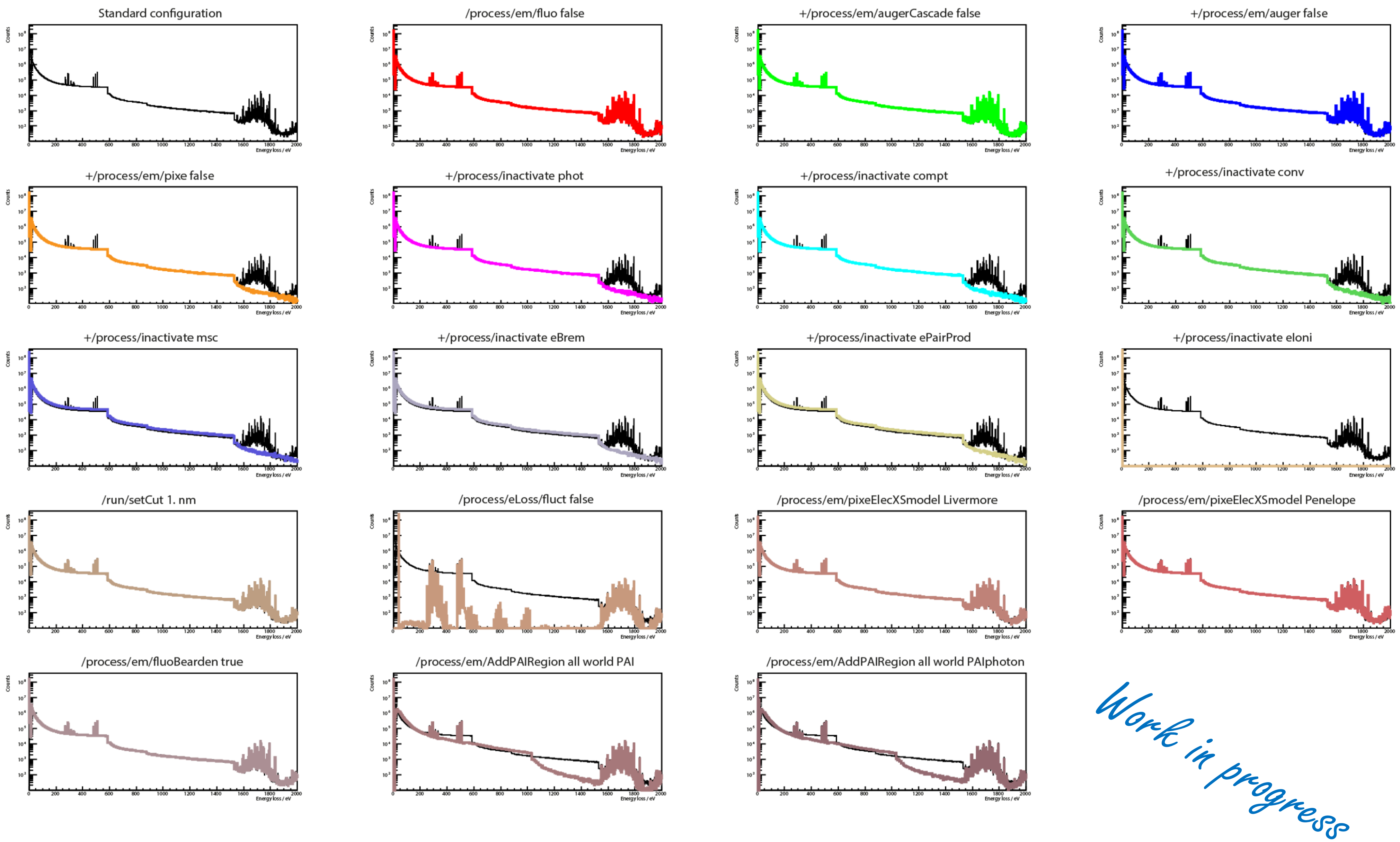
Impact of EM Physics Constructors ($CaWO_4$)



- 2 groups of EM physics constructors, differ by ~10 in absolute count yields
  → no consistent correlation with eIoni-models (Livermore vs Möller-Bhabha)
- With the exception of `G4EmPenelopePhyiscs`, no strong differences in spectral features

→ No obvious improvment

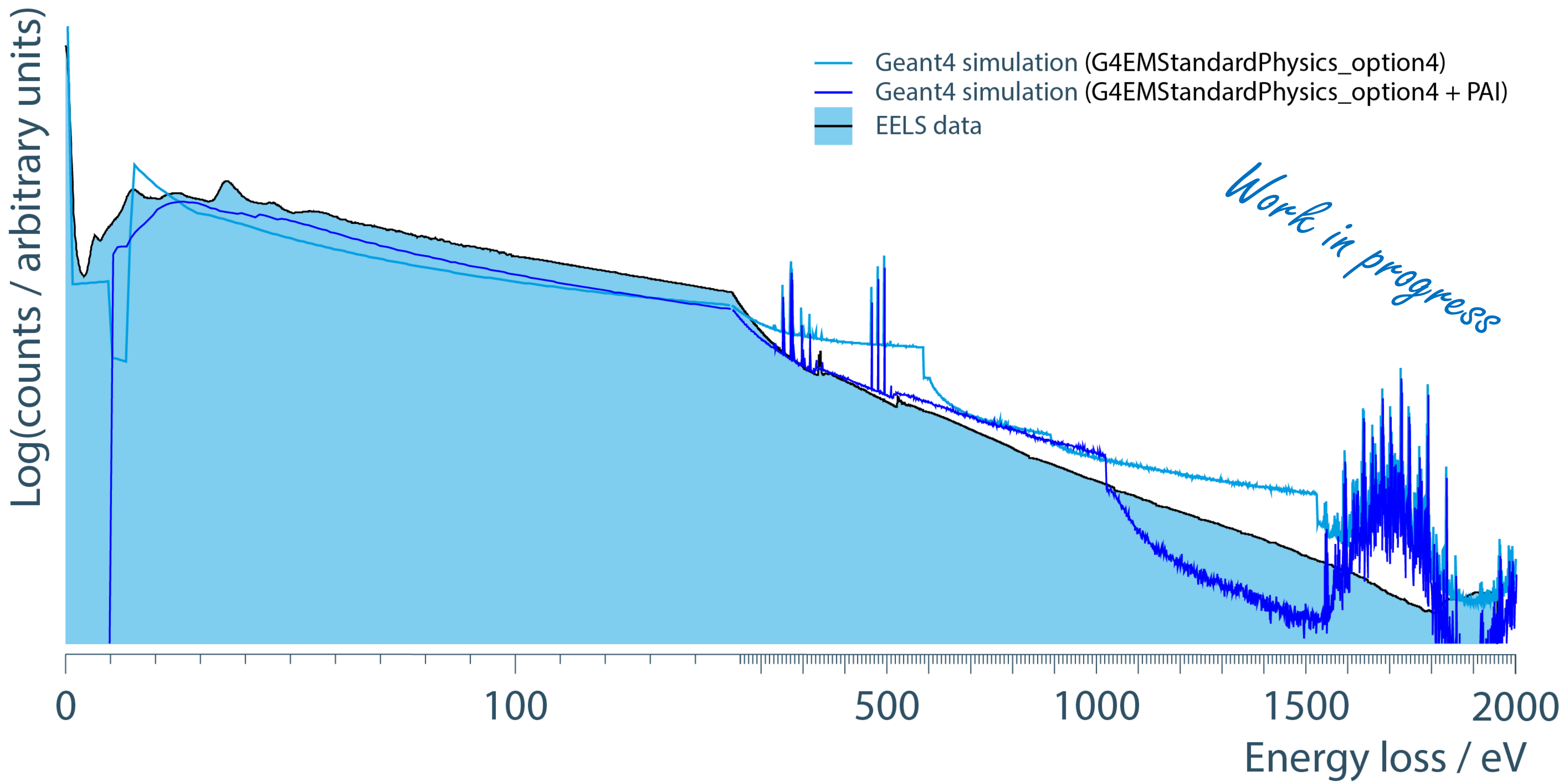
Impact of EM Process Settings ($CaWO_4$)



- Systematic survey of the impact of the process settings on the spectrum
- Compared to standard configuration

- „Interesting" settings:
  - PIXE – but no impact of used PIXE models
  - PAI (Photo Absorption Ionisation) [Apostolakis2000]

Comparison Geant4+PAI vs EELS for $CaWO_4$

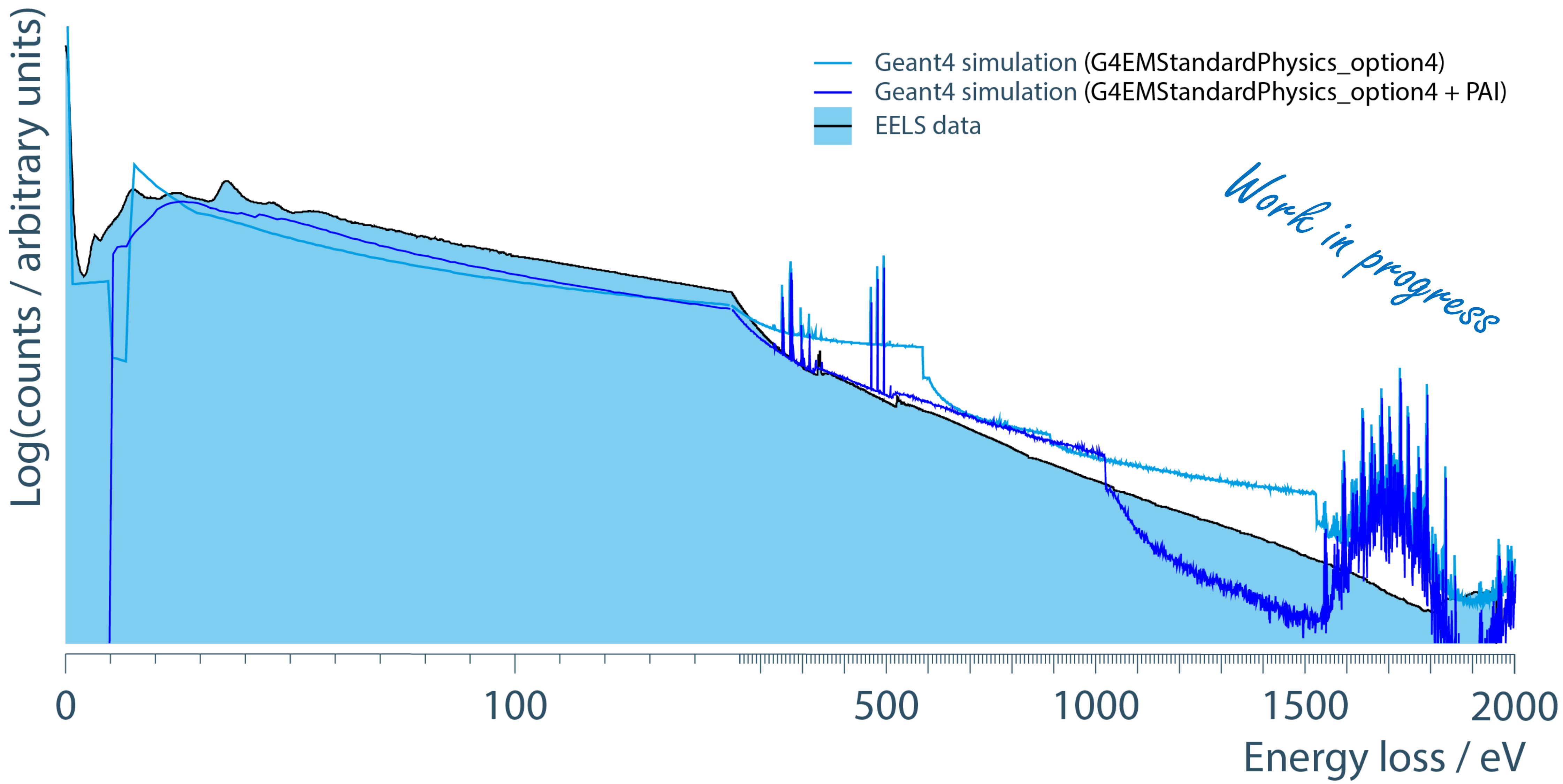


Simulation normalized to measured counts in [0,2keV]

- ~better agreement < 500 eV
- ~same deviation > 500 eV

→ Improvement!?

Comparison of PAI with $CaWO_4$



Simulation normalized to measured counts in [0,2keV]

- ~better agreement < 500 eV
- ~same deviation > 500 eV

→ Improvement!?

- Get even better with MicroElec [Gibaru2021]?
  - $CaWO_4$ and Al_2O_3 are not part of it ☹
  - Possible to extend with tabulated cross sections?

  → Get cross sections from EELS measurement

Connecting data and simulation

Deduce electronic stopping powers from EELS as input to future simulations

Dielectric Function Theory

- The **complex dielectric function**

$$\epsilon(\hbar\omega, \hbar k) = \epsilon_1(\hbar\omega, \hbar k) + i\epsilon_2(\hbar\omega, \hbar k)$$

  gives the response of a target to a swift electromagnetic distortion and it depends on transferred energy $\hbar\omega$ and momentum $\hbar k$

- The **Energy Loss Function (ELF)**

$$ELF = \mathrm{Im}\left[-\frac{1}{\epsilon(\hbar\omega, \hbar k)}\right]$$

  is the electronic excitation spectrum due to inelastic scatterings like ionisation

- The **Optical Energy Loss Function (OELF)**

$$OELF = \mathrm{Im}\left[-\frac{1}{\epsilon(\hbar\omega, 0)}\right]$$

  is the reduced ELF in the optical limit $k \to 0$

➔ EELS → OELF → ELF → differential cross section → stopping power

EELS → OELF

- Deconvolve measured EELS to obtain **single-scattering contribution $\boldsymbol{S}(\hbar\boldsymbol{\omega})$** as function of electron energy loss $E = \hbar\omega$

- It is directly related to OELF [Stöger-Pollach2008]:

$$S(\hbar\omega) = I_0 \frac{t}{\pi a_0 m_0 v^2} \cdot OELF(\hbar\omega) \cdot \ln\left(1 + \left(\frac{\beta}{\theta(\hbar\omega)}\right)^2\right)$$

$$\theta(\hbar\omega) = \frac{\hbar\omega}{\gamma m_0 v^2}$$

  with incoming intensity I_0, sample thickness t, collection semi-angle β, speed v and mass m_0 of incident electron, and the characteristic scattering angle θ

- Normalization factors I_0 and t are determined via Kramers–Kronig analysis and the known optical refractive index n [Stöger-Pollach2008]:

$$Re\left[\frac{1}{\epsilon(\hbar\omega, 0)}\right] = 1 - P\,\frac{2}{\pi}\int_0^\infty OELF(\hbar\omega)\,\frac{\mathrm{d}\,\hbar\omega}{\hbar\omega} = \frac{1}{n^2}$$

  where P represents the Cauchy principle part of the integral

OELF → ELF

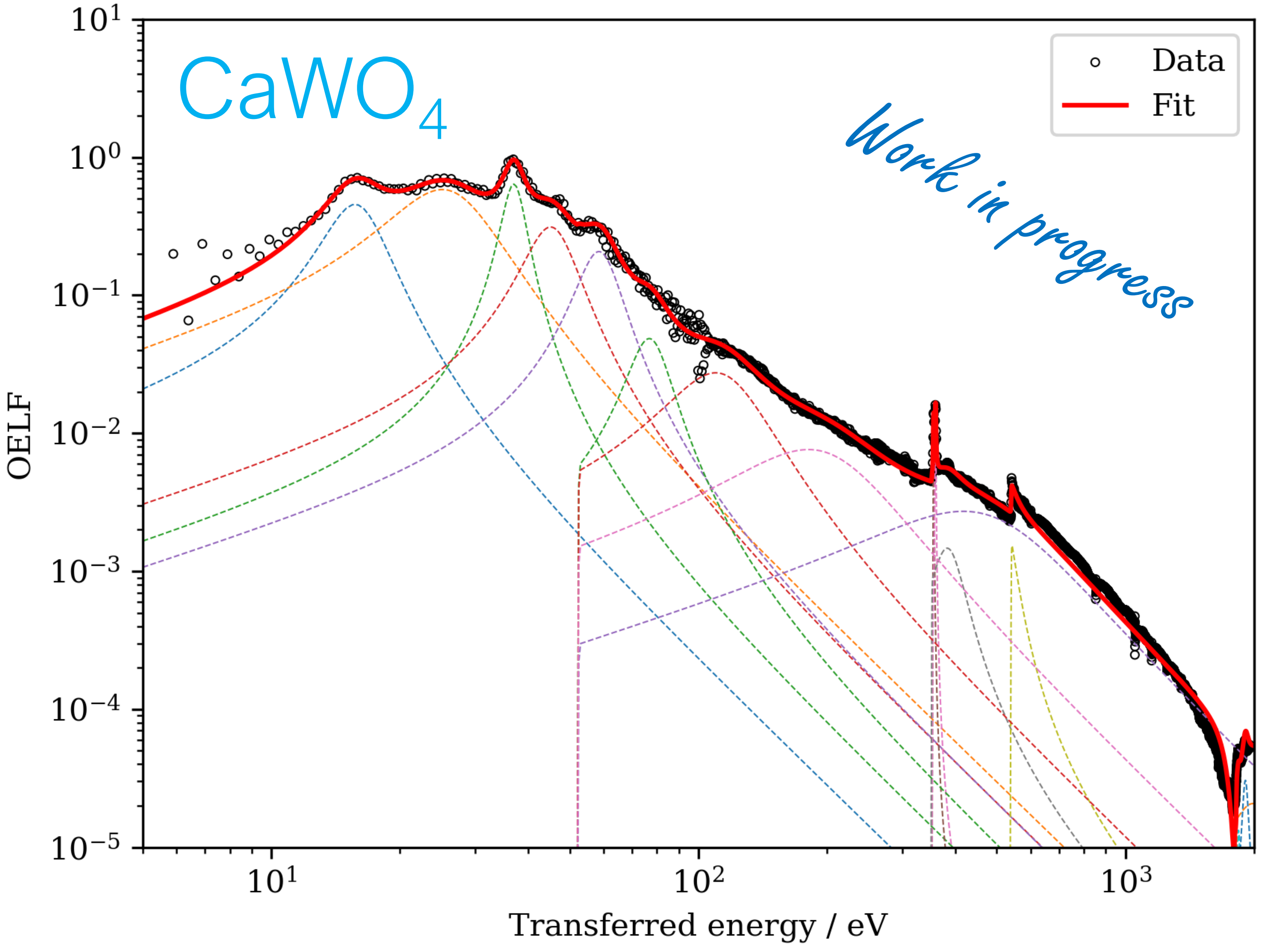
- Decompose the obtained OELF by fitting it with a sum of **Drude oscillators** [Ritchie1977]

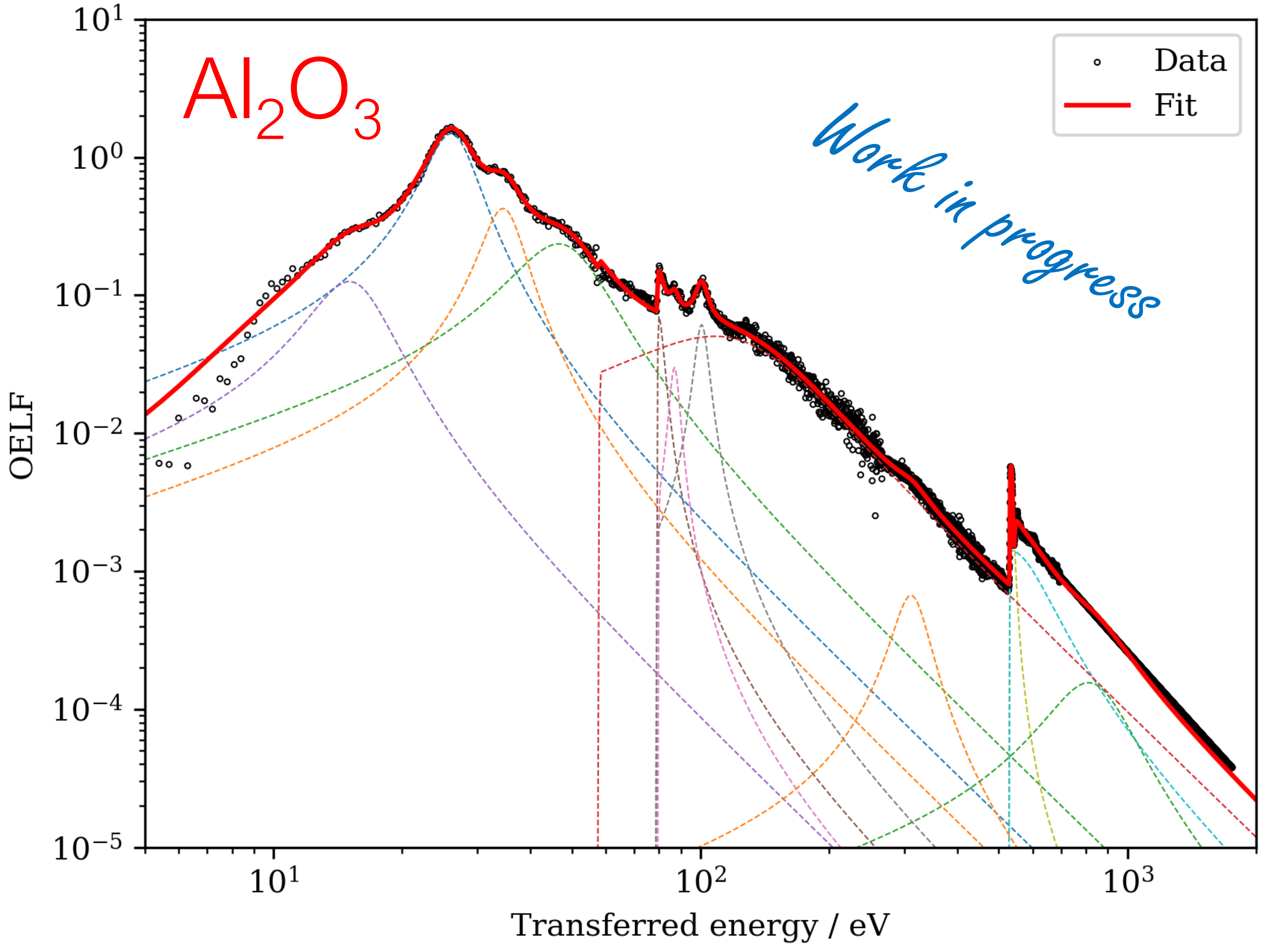
$$OELF(\hbar\omega) = \sum_i a_i \cdot \frac{\gamma_i \cdot \hbar\omega}{\left((\hbar\omega)^2 - (\hbar\omega_i)^2\right)^2 + (\gamma_i \cdot \hbar\omega)^2}$$

  with the resonance frequency ω_i, damping γ_i, and strength a_i of the i-th oscillator

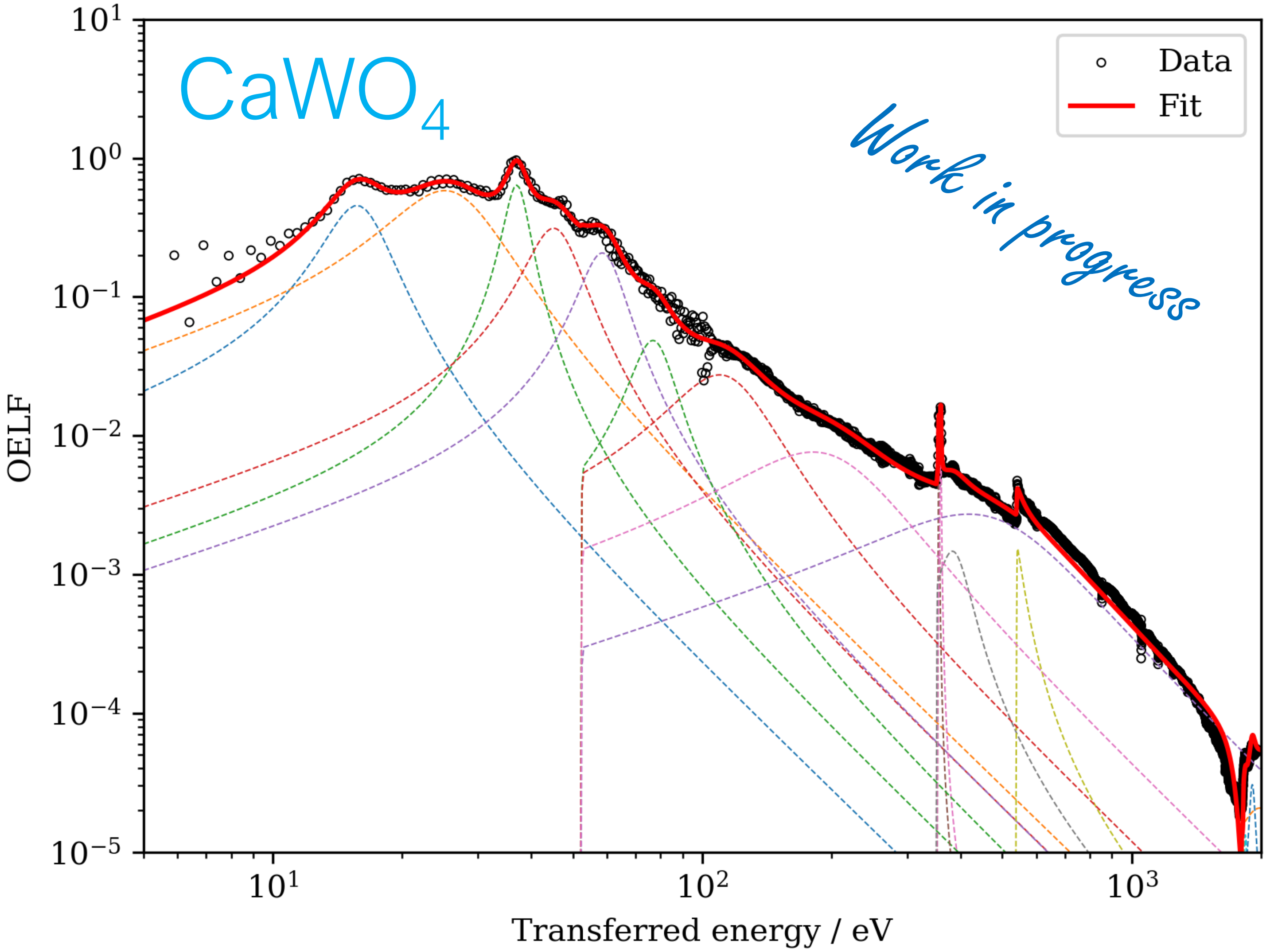
- Allow arbitrary **virtual oscillators**, also with negative strength, to describe also non-free electron materials [Da2022]

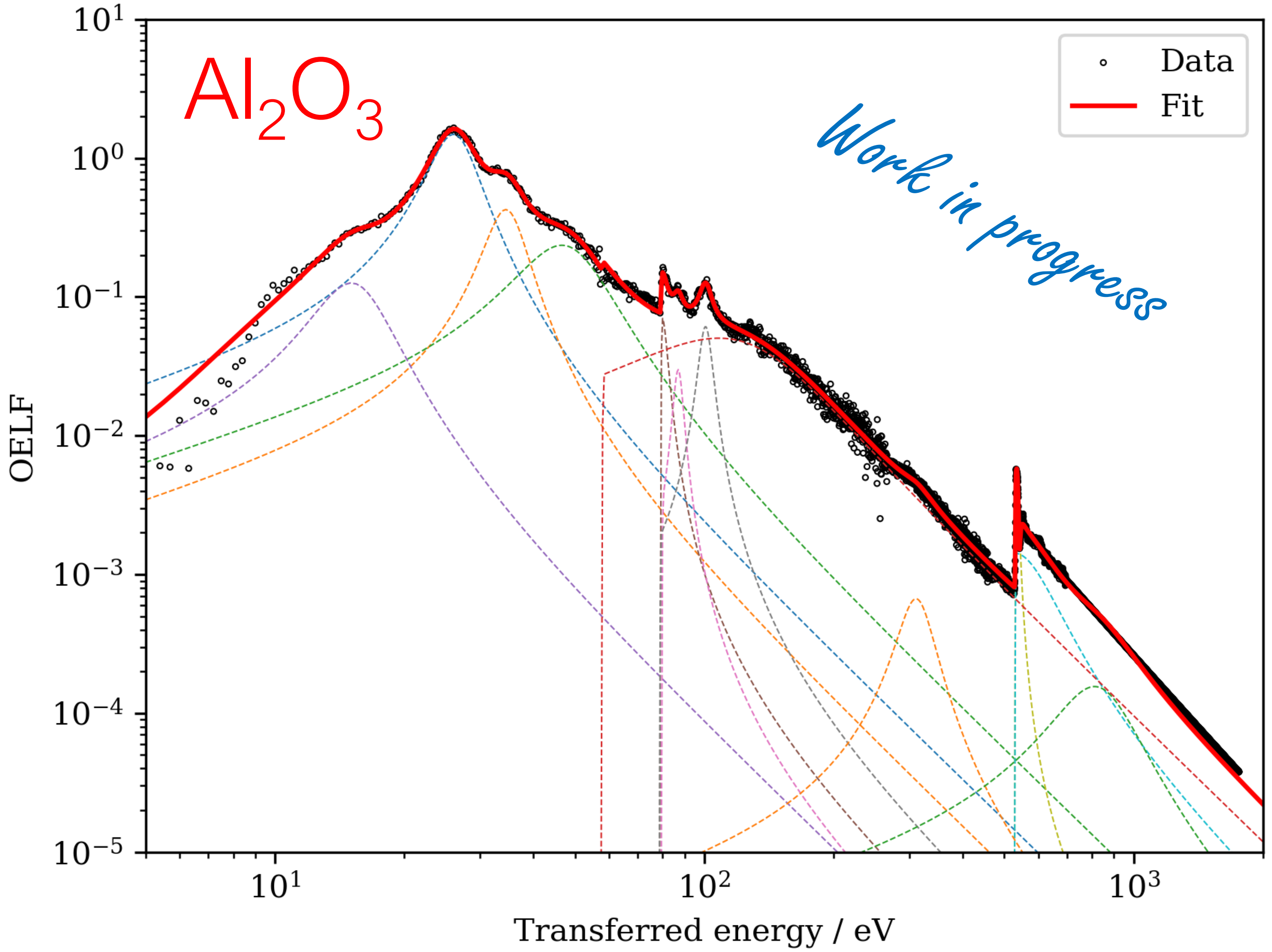
OELF of $CaWO_4$ and Al_2O_3





OELF of $CaWO_4$ and Al_2O_3





➔Good fit down to ~20 eV

OELF → ELF

- Decompose the obtained OELF by fitting it with a sum of **Drude oscillators** [Ritchie1977]

$$OELF(\hbar\omega) = \sum_i a_i \cdot \frac{\gamma_i \cdot \hbar\omega}{\left((\hbar\omega)^2 - (\hbar\omega_i)^2\right)^2 + (\gamma_i \cdot \hbar\omega)^2}$$

  with the resonance frequency ω_i, damping γ_i, and strength a_i of the i-th oscillator

- Allow arbitrary **virtual oscillators**, also with negative strength, to describe also non-free electron materials [Da2022]

- **Extend OELF to ELF** at finite k-values by assuming a free-electron dispersion relation [Ritchie1977]:

$$\omega_i \to \omega_i + \frac{(\hbar k)^2}{2m_e}$$

  (impact of other extensions, e.g. based on Mermin‘s dielectric function [Abril1998], are currently investigated)

ELF → Differential Cross Section

- The differential cross section for an incident electron of energy E to lose energy $\hbar\omega$ is related to the ELF via [Raine2014]:

$$\frac{\mathrm{d}\sigma(E,\hbar\omega)}{\mathrm{d}\hbar\omega} = \frac{1}{\pi N a_0 E}\int_{k_-}^{k_+} ELF(\hbar\omega,\hbar k)\frac{\mathrm{d}k}{k} + r.c.$$

  with the atomic density if the target N

- To be applicable also to energies above ~10keV, relativist corrections (r.c.) have to be considered [Raine2014]:

$$r.c. = \frac{1}{\pi N a_0 \beta^2 m_e c^2} OELF(\hbar\omega)\left(ln\left(\frac{1}{1-\beta}\right)-\beta^2\right)$$

$$k_\pm = \frac{1}{c}\left(\sqrt{E(E+2m_e c^2)} \pm \sqrt{(E-\hbar\omega)(E-\hbar\omega+2m_e c^2)}\right)$$

$$\mathrm{E} \rightarrow \beta^2 m_e c^2 \text{ with } \beta = \sqrt{1-\left(1+\frac{E}{m_e c^2}\right)^{-2}}$$

Differential Cross Section → Stopping Power

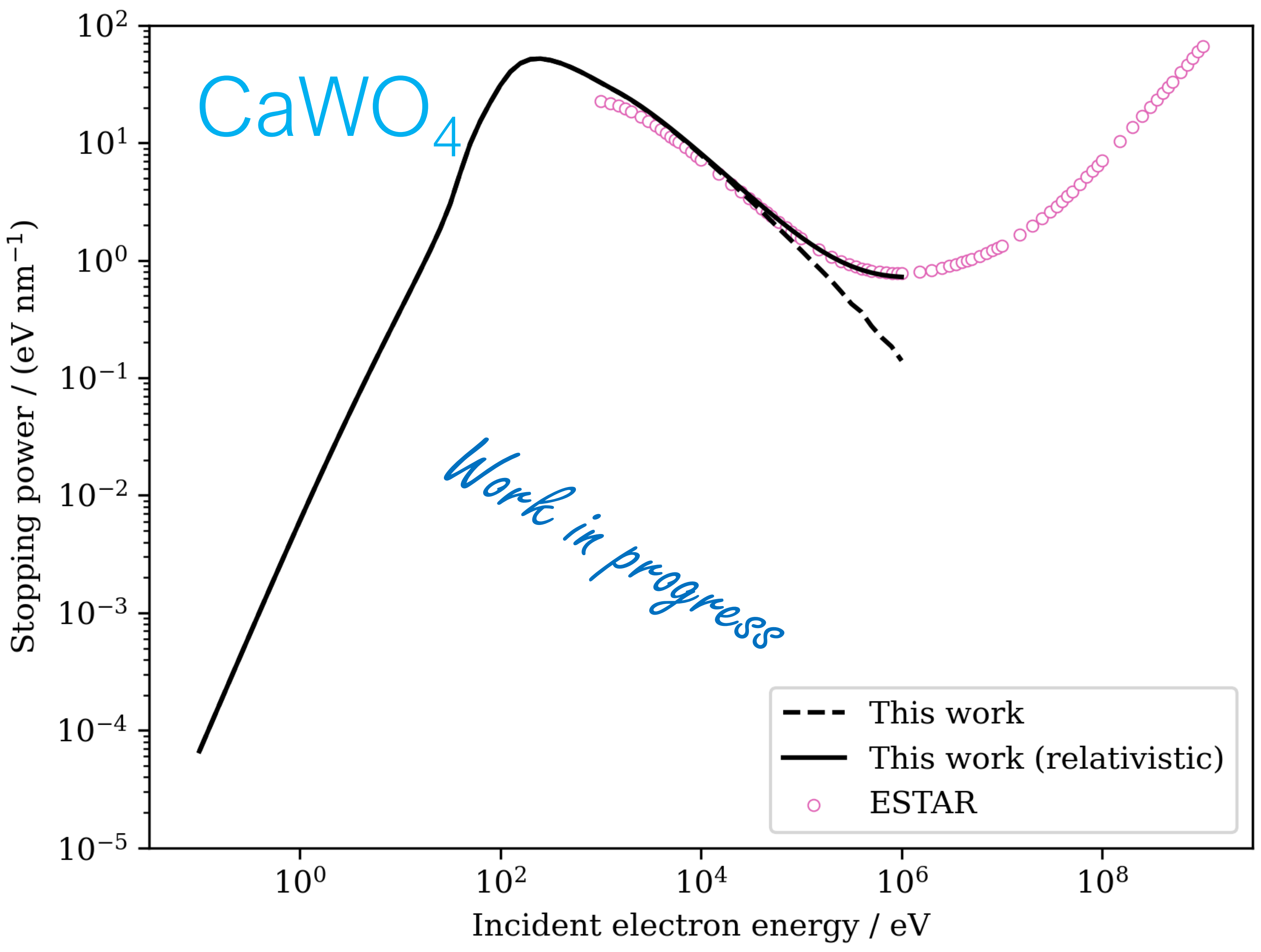
- Finally, the stopping power for an incident electron with energy E is obtained via [Raine2014]:

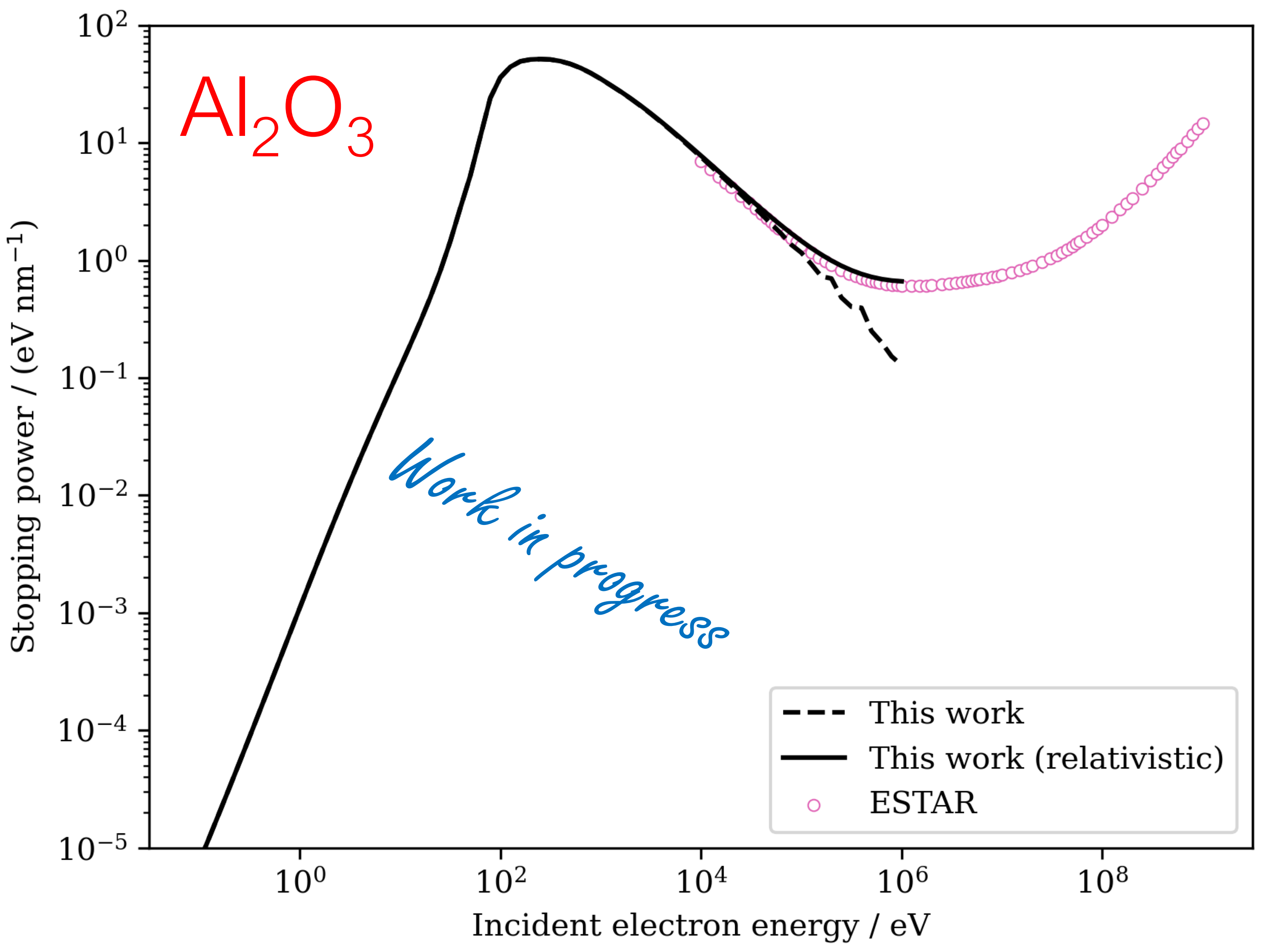
$$S(E) = N \int_{\omega_-}^{\omega_+} \frac{\mathrm{d}\sigma(E,\hbar\omega)}{\mathrm{d}\hbar\omega} \mathrm{d}\hbar\omega$$

  with integration boundaries for the energy loss of

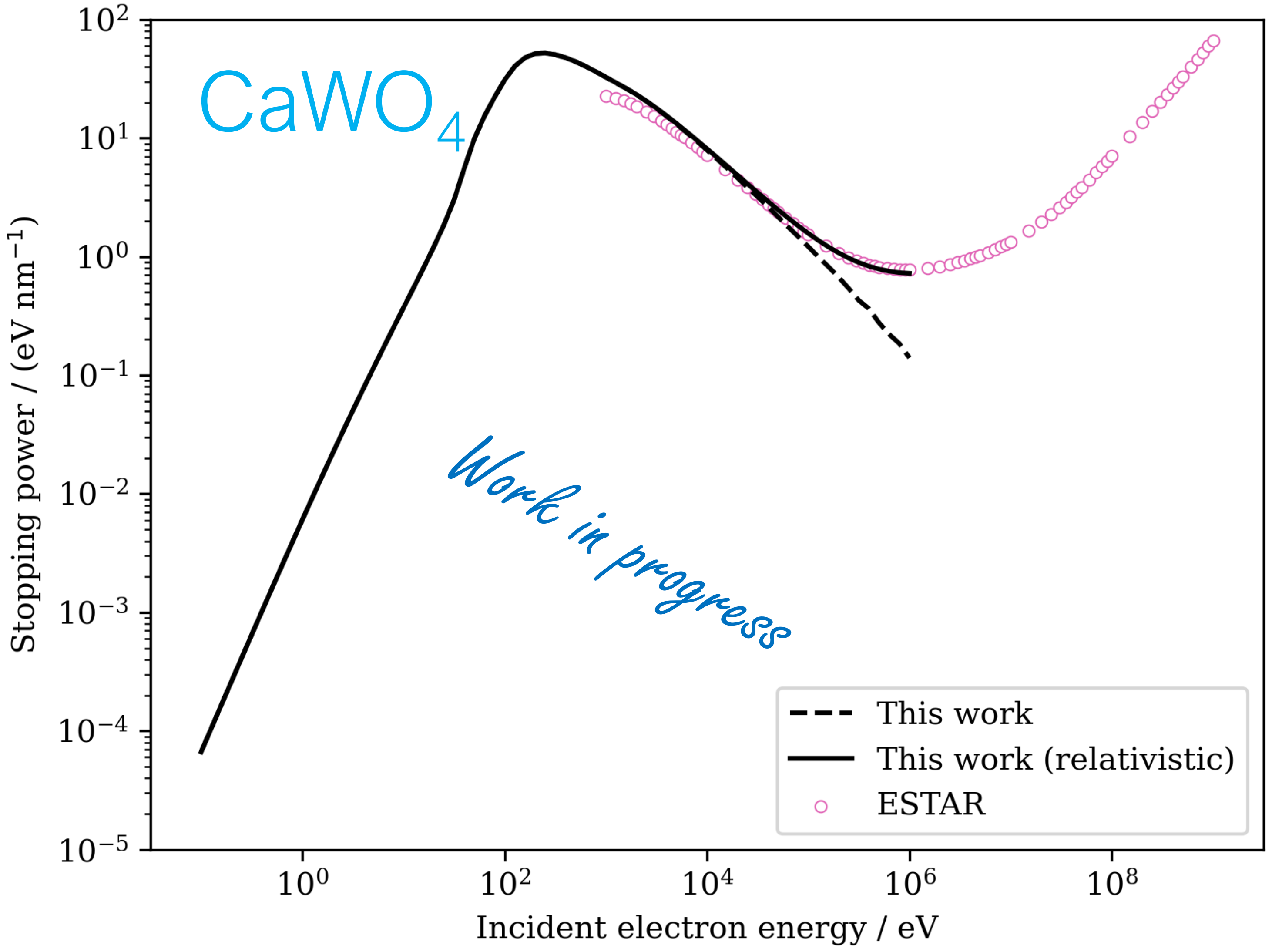
$$\omega_- = 0$$
$$\omega_+ = E/(2\hbar)$$

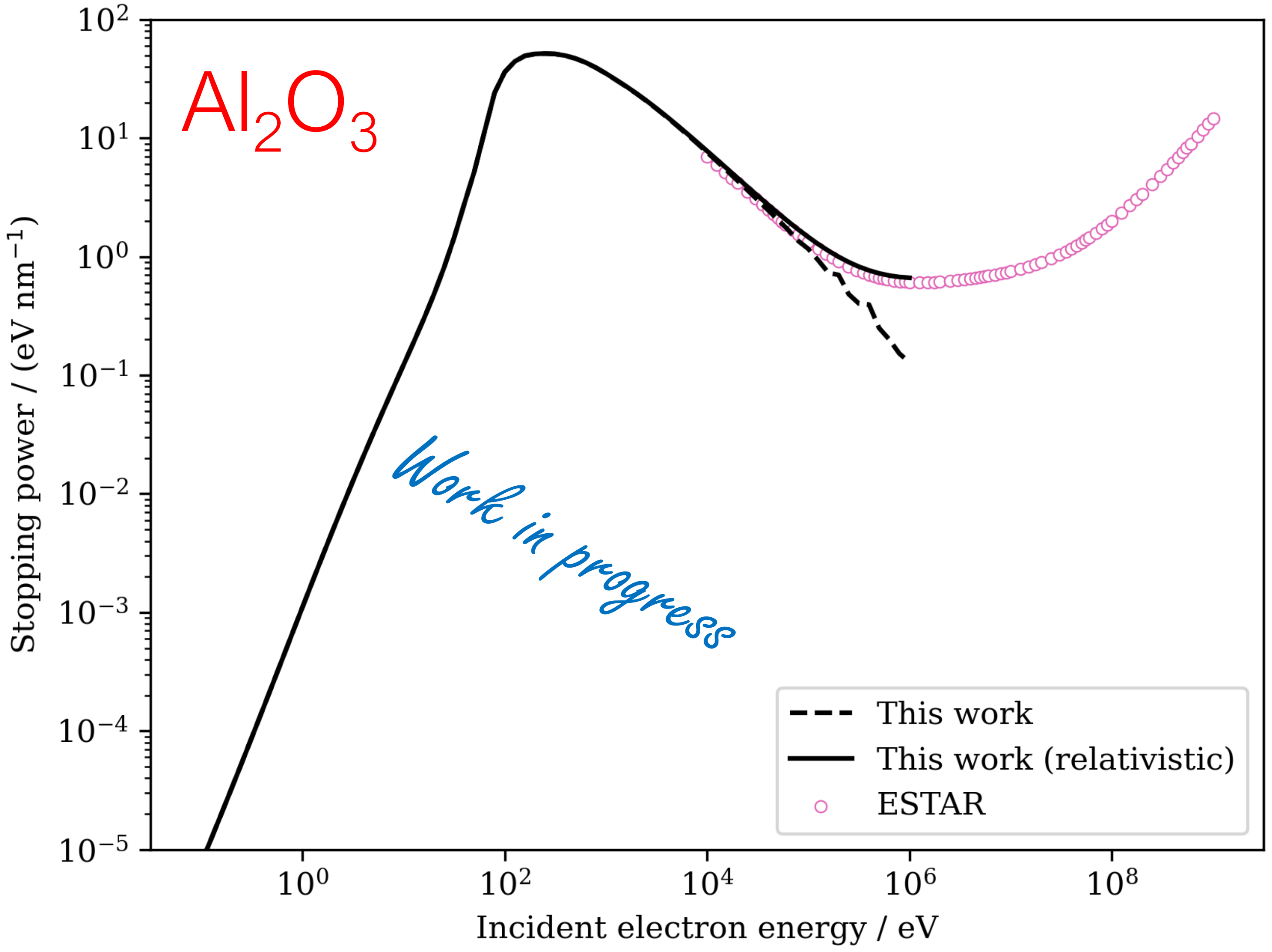
Stopping Power of $CaWO_4$ and Al_2O_3





Stopping Power of $CaWO_4$ and Al_2O_3





→Very good agreement with ESTAR >1 keV

→$CaWO_4$ - first measured stopping power at sub-keV range

Summary and Outlook

Summary

- ELOISE obtained **sub-keV reference data** for e^- ionisation in Al_2O_3 and $CaWO_4$ via **EELS measurements**
- First **qualitative comparison** with Geant4 10.6.3
  - **Rough overall agreement** but differences in spectral features
  - Activation of **PAI seems to improve agreement w.r.t** default G4EmStandardPhysics_option4
- Obtained cross sections from EELS measurements for further studies
  - Obtained Optical Energy Loss Functions (OELF) for Al_2O_3 and $CaWO_4$
  - Preliminary extension of OELFs to full Energy Loss Functions at finite momentum transfer
  - **First stopping power spectrum for $CaWO_4$ at sub-keV energies**
  - **Perfect agreement with ESTAR** reference data above 1 keV

Outlook

- **Publication** of EELS data sets and results **under preparation**
- **Established workflow** usable also for further (solid) target materials
- Study possibility to **extend Geant4/MicroElec** with the sub-keV cross section data for Al_2O_3 and $CaWO_4$

Bibliography

- [ESTAR] M. J. Berger et al., NIST Standard Reference Database 124
- [Ritchie1977] R. H. Ritchie & A. Howie, *Philos. Mag.*, 36.2 (1977) 463-481
- [Abril1998] I. Abril at al., *Phys. Rev. A*, 58.1 (1998) 357-366
- [Apostolakis2000] J. Apostolakis et al., *Nucl. Instrum. Methods Phys. Res. Sect. A*, 453 (2000) 597-605
- [Stöger-Pollach2008] M. Stöger-Pollach et al., *Ultramicroscopy*, 108.5 (2008) 439-444
- [Raine2014] M. Raine et al., *Nucl. Instrum. Methods Phys. Res. Sect. B*, 325 (2014) 97-100
- [Gibaru2021] Q. Gibaru et al., *Nucl. Instrum. Methods Phys. Res. Sect. B*, 487 (2021) 66-77
- [Da2022] B. Da et al., *J. Appl. Phys.*, 131 (2022) 175301
- [HK2023] H.Kluck, *SciPost Phys. Proc.*, 12 (2023) 64, arXiv:2212.12634