Suppressing and Tagging $^{42}Ar/^{42}K$ Surface Beta Events in LEGEND Using Semi-Supervised Latent Density Estimation

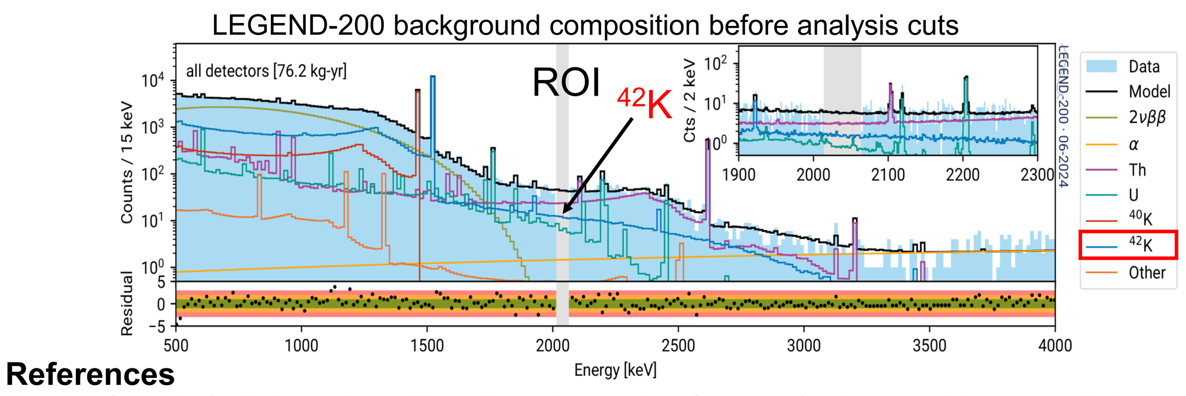
Niko Lay[1], Christoph Vogl[1], Konstantin Gusev[1], Nadezda Rumyantseva[1], Baran Hashemi[1], Lukas Heinrich[1], Moritz Neuberger[1], Mario Schwarz[1], Patrick Krause[1], Tommaso Comellato[1], Andreas Leonhardt[1], Brennan Hackett[2], Béla Majorovits[2], and Stefan Schönert[1]

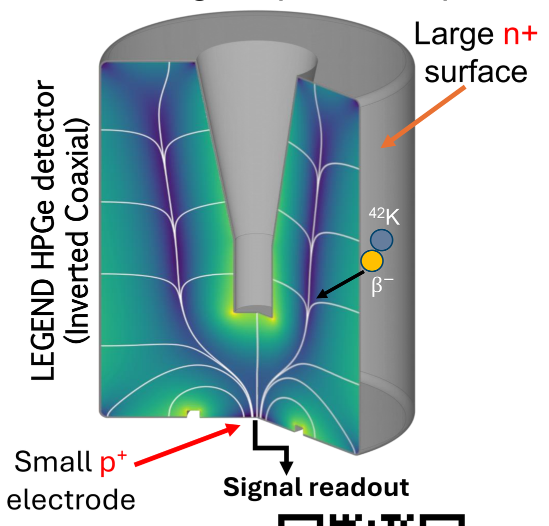
[1]Physics Department, School of Natural Sciences, Technical University of Munich, James-Franck-Str. 1, 85748 Garching, Germany – [2]Max Planck Institute for Physics, Boltzmannstr. 8, 85748 Garching, Germany

Digital Version

[1] Motivations

- The LEGEND experiment operates high-purity germanium (HPGe) detectors immersed in liquid argon (LAr) to search for neutrinoless double beta decay (0νββ) of ^{76}Ge.
- LEGEND-1000 background index goal: **< 10^{-5} cts / (keV kg yr)** at ROI.
- Without additional measures, **^{42}K n⁺-surface events** would be the **dominant background** in LEGEND-1000.
- Baseline mitigation: underground-sourced LAr (UGLAr) is depleted in ^{42}Ar.
- In case UGLAr is not available, combined detector enclosures and machine learning for pulse-shape classifications offer a promising alternative.
- The challenge:
  - n⁺ surface events are **challenging to simulate**
  - In real LEGEND-200 data: **very few labeled examples** to train on



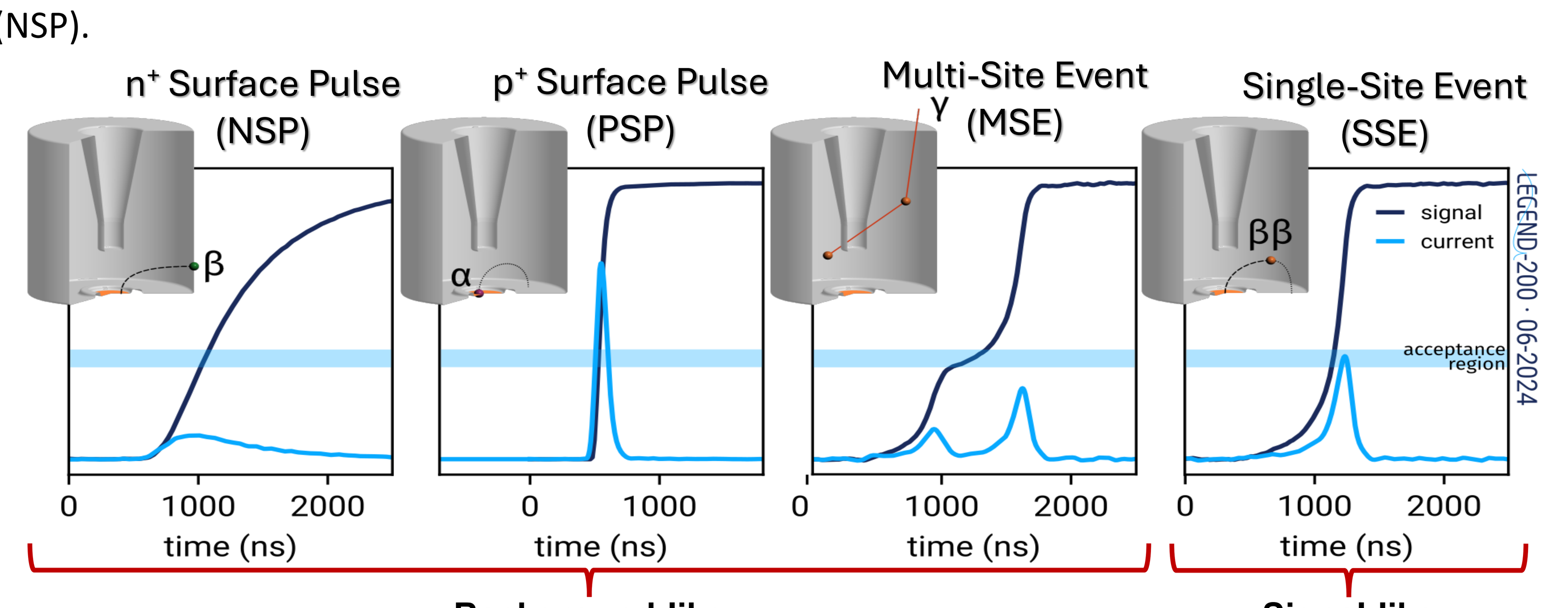


References
1. LEGEND Collaboration, *First Results on the Search for Lepton Number Violating Neutrinoless Double Beta Decay with the LEGEND-200 Experiment*, arXiv:2505.10440 [hep-ex], 2025.
2. LEGEND Collaboration, *LEGEND-1000 Preconceptual Design Report*, arXiv:2107.11462 [physics.ins-det], 2021.

https://legend-exp.org/

[2] Pulse shapes in HPGe detectors

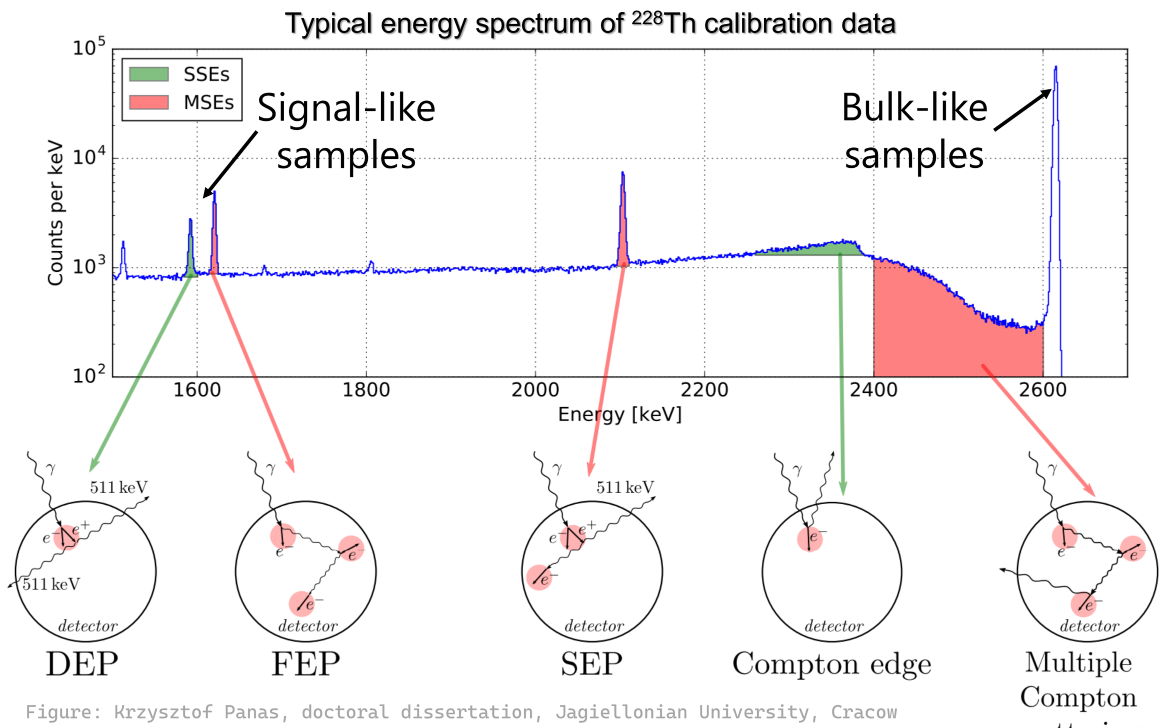
Depending on the physical origins, four main types of pulse shapes are induced when ionizing radiation deposits energy in an HPGe detector. 0νββ-signal is expected to be single-site. $^{42}Ar/^{42}K$ beta backgrounds are mainly n⁺ surface pulses (NSP).

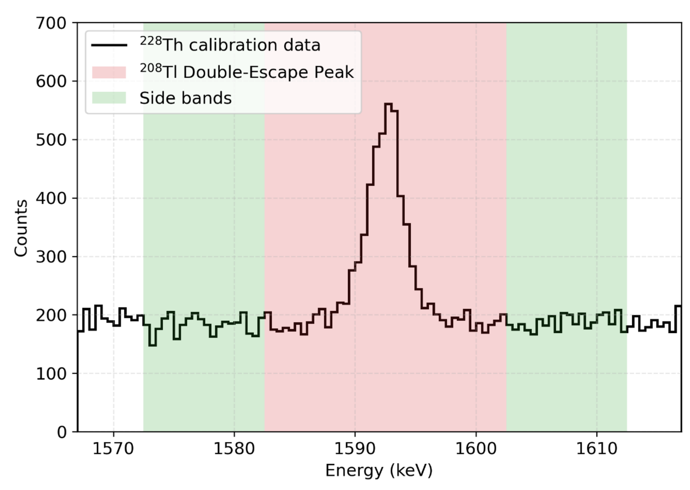


[3] Available signal and background proxies from ^{228}Th calibration

Different physical interactions of the 2.6 MeV ^{208}Tl line with the detector induces enhanced pulse-shape populations at different energies:

- Double-Escape Peak (DEP): 0νββ-like (signal) (single-site / SSE)
- Full-Energy Peak (FEP) and Single-Escape Peak (SEP): multi-site (MSE)





Available **SSE and MSE samples** are a **mixture** between Compton continuum events and the true events in the peaks

No/very few explicit labels available for the surface events: n⁺ surface pulses (NSP) and p⁺ surface pulses (PSP)

[4] Modeling the likelihood of the data under the peak and the side-band hypotheses

- The data distribution at the peak energy consists of a superposition between the true events from the peak and a background component.
- The data distribution from the background at the peak energy resembles that from the side-bands.
- Provide a guess $p(z \mid H_2)$ with a known functional form.

Formally:

- $p(z \mid \widetilde{H}_0) = p(z \mid H_0) \cdot p(H_0 \mid \widetilde{H}_0) + p(z \mid H_1) \cdot p(H_1 \mid \widetilde{H}_0)$
- $p(z \mid \widetilde{H}_1) = p(z \mid H_1)$
- $p(z \mid \widetilde{H}_2) = p(z \mid H_2)$

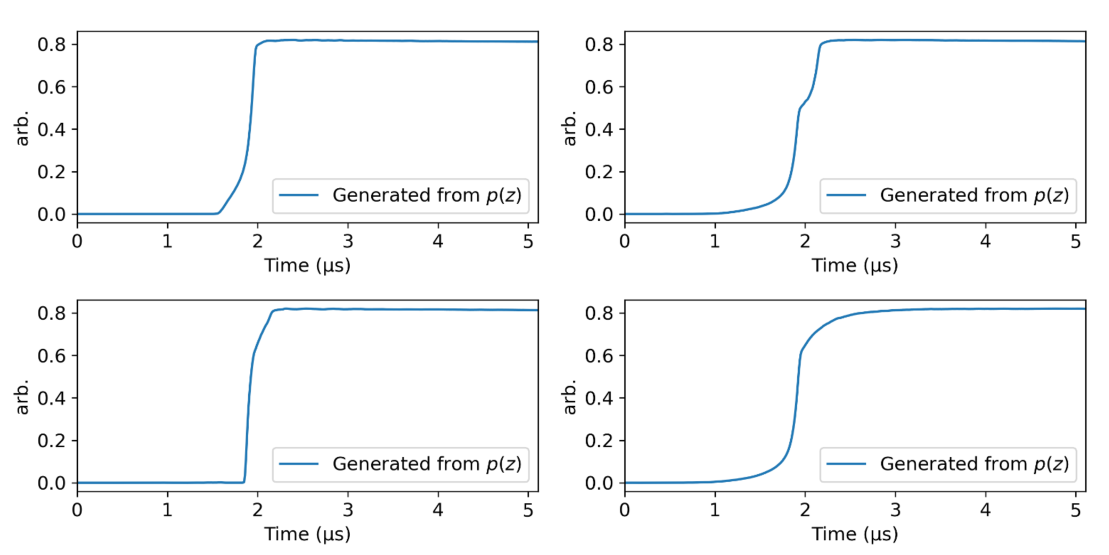
$$p(H_i \mid \widetilde{H}_j) = \begin{bmatrix} \frac{N_{peak} - N_{SB}}{N_{peak}} & 0 & 0 \\ \frac{N_{SB}}{N_{peak}} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Notation:
- H_0: true events from the peak
- H_1: true events from the side-band
- H_2: events randomly sampled from a guess distribution
- $\widetilde{H}_i$: mixture of events that correspond to the transition probabilities $p(H_i \mid \widetilde{H}_j)$.

Obtain an initial guess by training a denoising Variational AutoEncoder (VAE), trained using the InfoVAE loss with $\alpha = 1$.

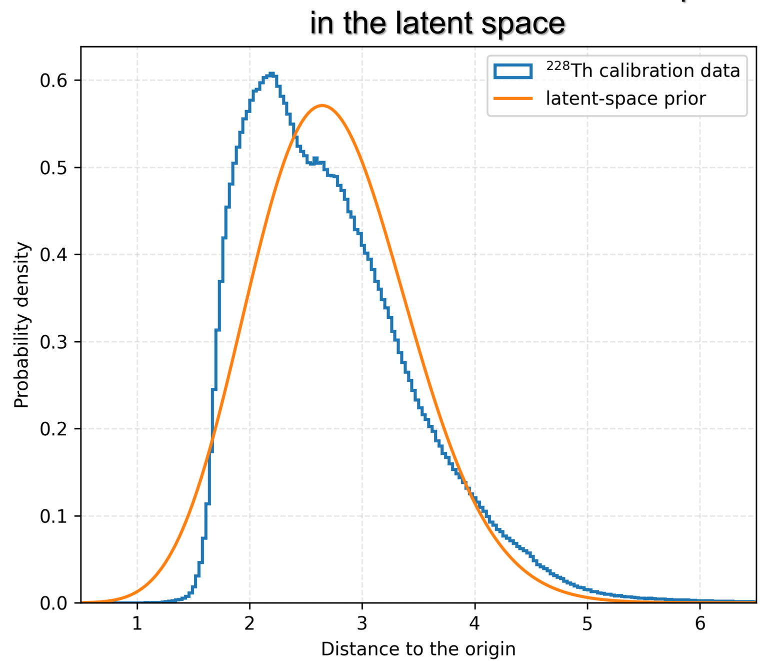
$$L = \mathbb{E}_{p(x)}\mathbb{E}_{q_\varphi(z \mid x)}[\log p_\theta(x \mid z)] - (1-\alpha)\mathbb{E}_{p(x)} D_{KL}\big(q_\varphi(z \mid x) \,\|\, p(z)\big) - (\alpha + \lambda - 1) D_{KL}\big(q_\varphi(z) \,\|\, p(z)\big)$$

The VAE prior (standard normal) serves as an initial guess



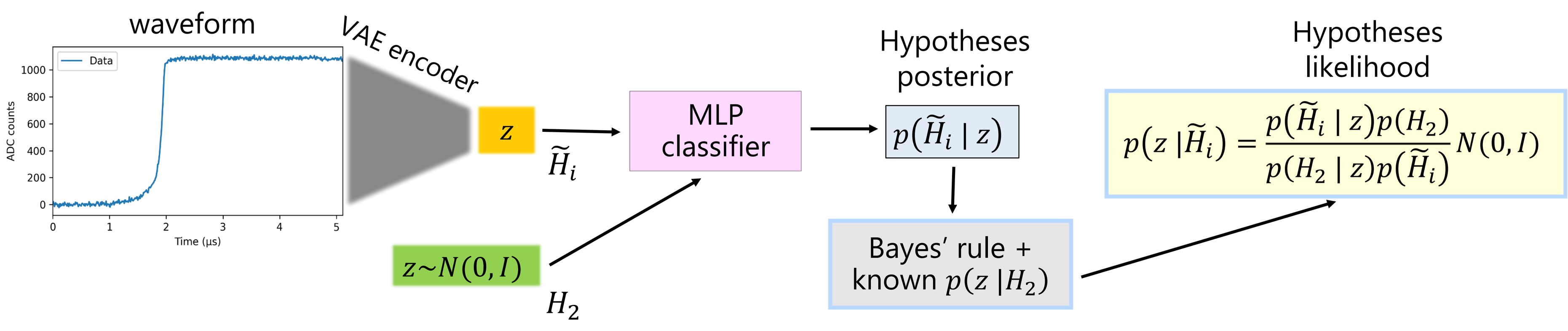
Waveforms sampled randomly from the prior

Radial distribution of data and the VAE prior in the latent space



[5] Gamma peak vs. side-bands vs. VAE prior classification

- Instead of classifying signal-like vs. n⁺ surface waveforms (labeled events are scarce/unavailable), we train a small MLP using cross-entropy loss to classify events from a peak ($\widetilde{H}_0$), the side-bands ($\widetilde{H}_1$), and the guess (H_2) from ^{228}Th calibration data.
- Obtain the likelihood of the data in the latent space $p(z \mid \widetilde{H}_i)$ under the peak/side-bands hypotheses using Bayes' rule.



- The **likelihood** of the data from the **true events in a peak of interest** is obtained using the peak and side-bands modeling (side-bands subtraction of the distributions in the latent space):

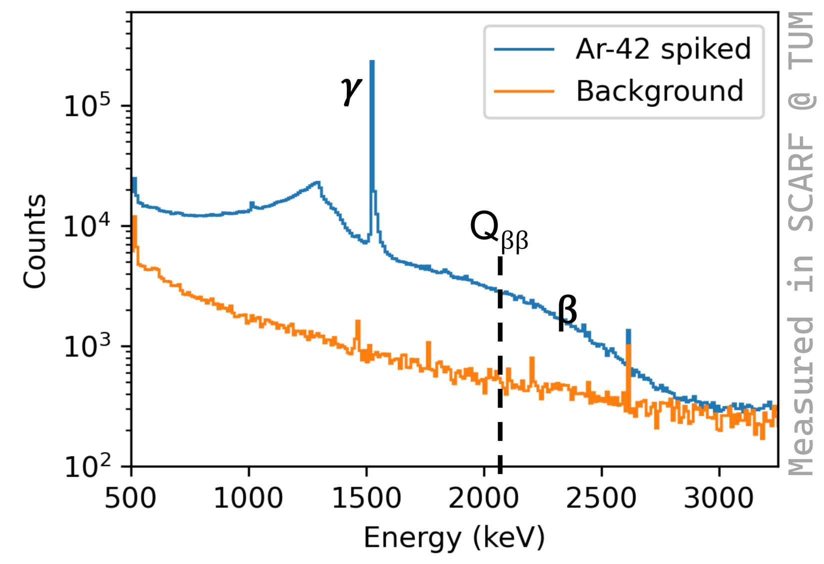
$$p(z \mid H_0) = \frac{1}{p(H_0 \mid \widetilde{H}_0)}\left\{\frac{p(\widetilde{H}_0 \mid z)p(H_2)}{p(H_2 \mid z)p(\widetilde{H}_0)} - \frac{p(\widetilde{H}_1 \mid z)p(H_2)}{p(H_2 \mid z)p(\widetilde{H}_1)} p(H_1 \mid \widetilde{H}_0)\right\} N(0, I)$$

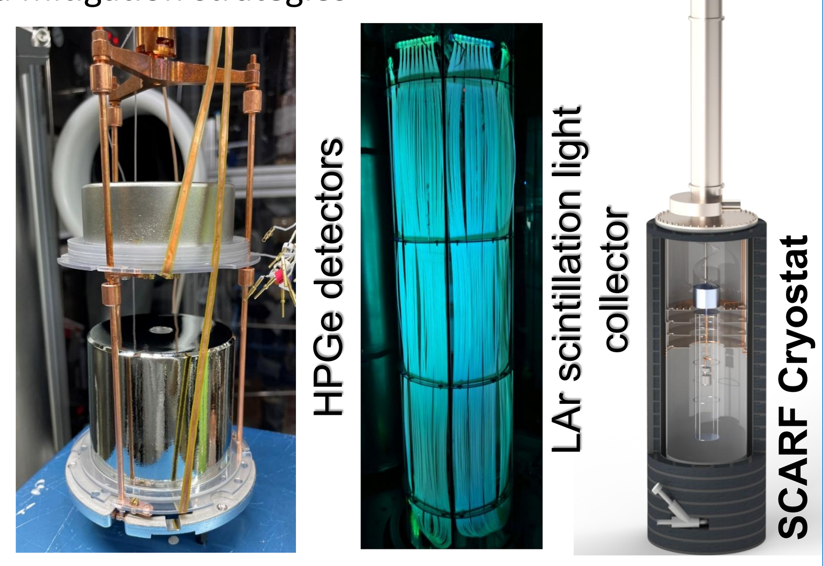
- Similarly for the **side-bands**:

$$p(z \mid H_1) = \frac{p(\widetilde{H}_1 \mid z)p(H_2)}{p(H_2 \mid z)p(\widetilde{H}_1)} N(0, I)$$

[6] Dataset enhanced in ^{42}K n⁺ surface betas measured in SCARF at TUM for benchmarking

- SCARF: LAr test facility at TU Munich (TUM)
- Measurements of HPGe detectors in one-ton of LAr before and after ^{42}Ar-spiking (435 Bq) in different configurations for studies of $^{42}Ar/^{42}K$ background mitigation strategies

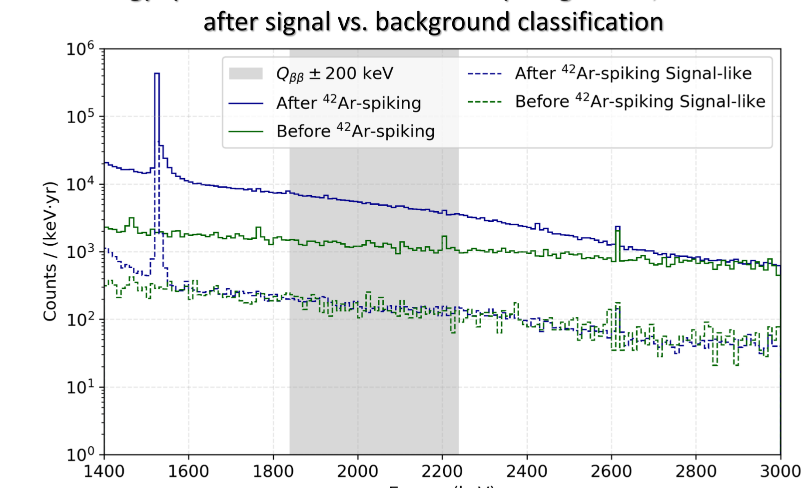




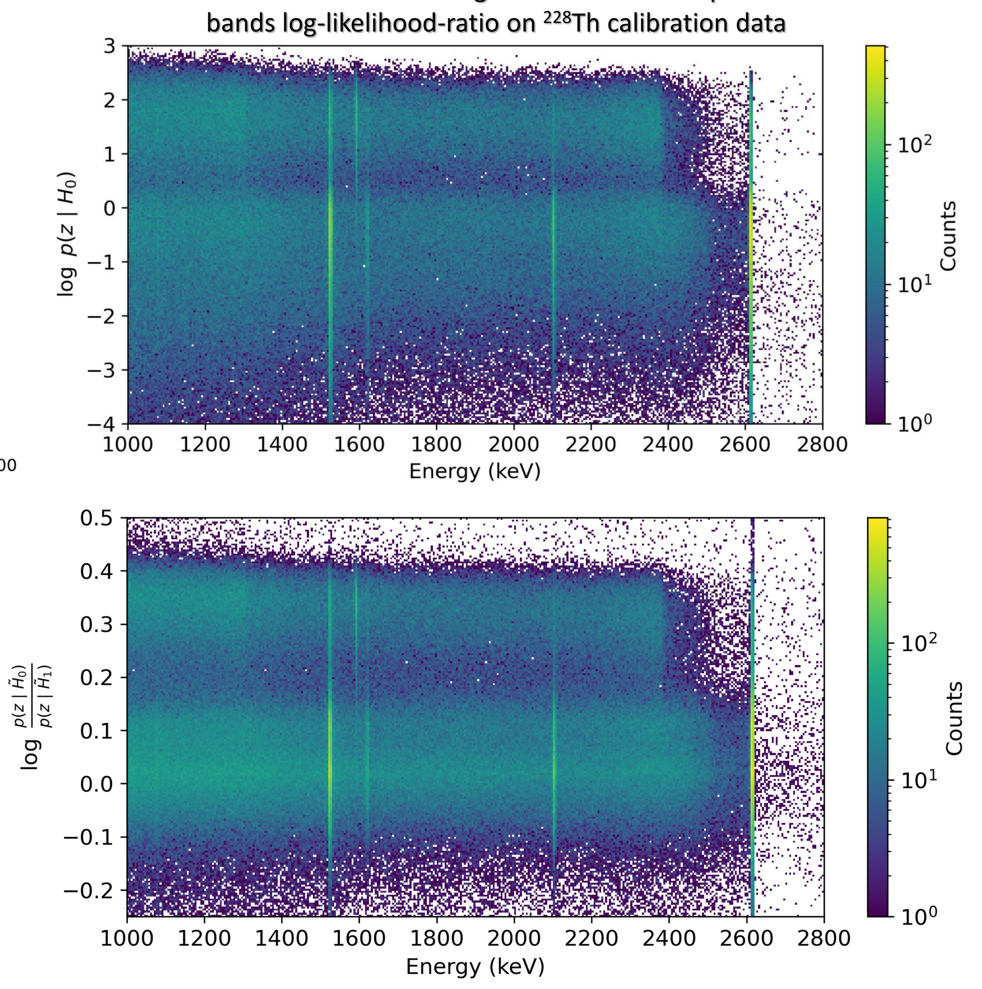
[7] Signal- vs. Background-like identification (preliminary)

Data from the ^{208}Tl DEP and its side-bands from ^{228}Th calibration data are used to tag signal-like events and suppress backgrounds using the estimated likelihoods.

Energy spectra before and after the spiking of ^{42}Ar, before and after signal vs. background classification



The distribution of the DEP log-likelihood and the peak to side-bands log-likelihood-ratio on ^{228}Th calibration data



Gamma lines survival fraction after setting a 90% threshold on the log-likelihood and a 95% threshold on the log-likelihood-ratio

Peak	Energy (keV)	Survival Fraction (%)
^{208}Tl DEP	1592.5	87.8 ± 1.7 ↑
^{212}Bi FEP	1620.7	11.06 ± 0.91 ↓
^{208}Tl SEP	2103.5	6.87 ± 0.33 ↓
^{208}Tl FEP	2614.5	9.353 ± 0.051 ↓

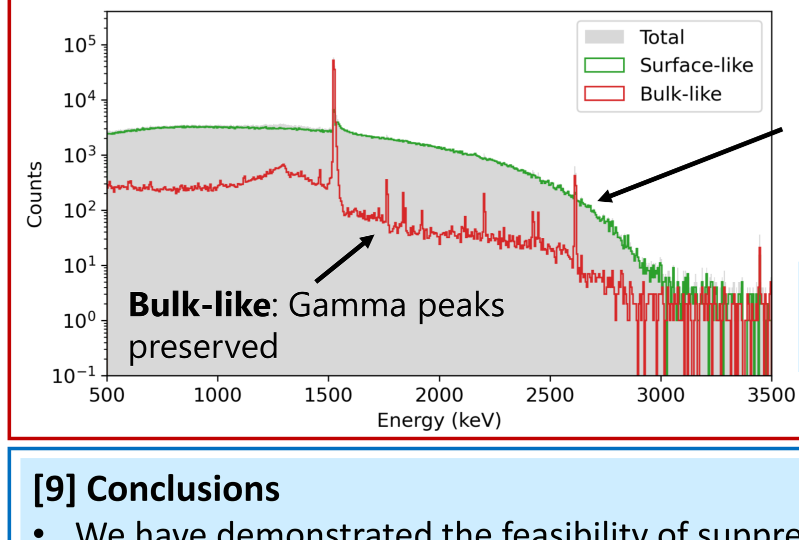
The suppression of ^{42}K n⁺ surface backgrounds is calculated from the change in signal-like counts before and after ^{42}Ar spiking. Obtained ^{42}K survival fraction:

$\mathbf{SF_{^{42}K} < 0.3\,\%}$ at 90% CL

[8] Bulk- vs. surface-like identification (preliminary)

Data from the ^{208}Tl 2.6 MeV FEP and its side-bands from ^{228}Th calibration data allows us to distinguish events depositing energy near the n⁺ surface (surface-like) vs. events with energy depositions in the detector bulk only (bulk-like). This is due to the energy loss near the n⁺ surface, resulting in a partial charge collection. Thus, events with n⁺ surface energy depositions would be shifted towards lower energy values with respect to the peak energy.

Energy spectrum after the spiking of ^{42}Ar of events with light in the LAr



Surface-like: Continuous beta-like spectrum

^{42}K survival fraction:
$\mathbf{SF_{^{42}K} = 1.49^{+0.080}_{-0.083}\,\%}$

Gamma lines survival fraction after setting a 95% threshold on the log-likelihood and a 95% threshold on the log-likelihood-ratio

Peak	Energy (keV)	Survival Fraction (%)
^{208}Tl DEP	1592.5	96.0 ± 2.0 ↑
^{212}Bi FEP	1620.7	88.1 ± 2.1 ↑
^{208}Tl SEP	2103.5	93.09 ± 0.94 ↑
^{208}Tl FEP	2614.5	90.66 ± 0.21 ↑

[9] Conclusions

- We have demonstrated the feasibility of suppressing and tagging n⁺ surface events without using labeled NSP.
- Flexibility: Once pulse-shape simulations of double-beta events are available, we can directly estimate the likelihood of data under a double-beta-like hypothesis using the method developed for all LEGEND detectors.
- Current ^{42}Ar SCARF measurements are not sufficiently sensitive to probe the target ^{42}K suppression of SF < 10^{-5} or similar for LEGEND-1000 .
- Future $^{42}Ar/^{42}K$ mitigation campaign with 100 times ^{42}Ar activity allows to probe SF down to 10^{-5}.