

Sensitivity of the NEXT experiment to Xe-124 double electron capture

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ABSTRACT: Double electron capture by proton-rich nuclei is a second-order nuclear process analogous to double beta decay. Despite their similarities, the decay signature is quite different, potentially providing a new channel to measure the hypothesized neutrinoless mode of these decays. The Standard-Model-allowed two-neutrino double electron capture ($2\nu ECEC$) has been predicted for a number of isotopes, but only observed in ^{78}Kr , ^{130}Ba and, recently, ^{124}Xe . The sensitivity to this decay establishes a benchmark for the ultimate experimental goal, namely the potential to discover also the lepton-number-violating neutrinoless version of this process, $0\nu ECEC$. Here we report on the current sensitivity of the NEXT-White detector to ^{124}Xe $2\nu ECEC$ and on the extrapolation to NEXT-100. Using simulated data for the $2\nu ECEC$ signal and real data from NEXT-White operated with ^{124}Xe -depleted gas as background, we define an optimal event selection that maximizes the NEXT-White sensitivity. We estimate that, for NEXT-100 operated with xenon gas isotopically enriched with 1 kg of ^{124}Xe and for a 5-year run, a sensitivity to the $2\nu ECEC$ half-life of 7×10^{22} y (at 90% confidence level) or better can be reached.

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1 Introduction

Ever since the discovery of neutrino oscillations [1–3], and hence neutrino mass, there has been a sustained interest in searches for neutrinoless double beta decay processes. Such second-order weak interactions are generally considered to be the most promising way to test whether neutrinos are massive Majorana particles, identical to their anti-particles. Four related double beta processes have been proposed [4]. The neutrinoless double β^- emission process ($0\nu\beta\beta$, $(A, Z) \rightarrow (A, Z + 2) + 2e^-$) is possible in neutron-rich nuclei. This is, by far, the double beta process that has been explored the most both from an experimental and from a theoretical point of view. In proton-rich nuclei, up to three competing processes may be kinematically available: the neutrinoless modes of double β^+ emission, single β^+ emission plus single electron capture, and double electron capture ($0\nu ECEC$, $(A, Z) + 2e^- \rightarrow (A, Z - 2)$). Despite the much lower isotopic abundances of proton-rich nuclei undergoing double beta processes, $0\nu ECEC$ may provide an interesting alternative to $0\nu\beta\beta$ searches. Particular interest in $0\nu ECEC$ has been triggered by the special case in which the energy of the initial state matches precisely the energy of the (excited) final state [5, 6]. If this resonance condition is met, the $0\nu ECEC$ rate is expected to be increased by several orders of magnitude compared to the non-resonant (radiative) case.

A fundamental step toward sensitive $0\nu ECEC$ searches is the unambiguous measurement of the two-neutrino double electron capture ($2\nu ECEC$, $(A, Z) + 2e^- \rightarrow (A, Z - 2) + 2\nu_e$). This process is allowed in the Standard Model of particle physics, yet it is predicted to be extremely rare. The $2\nu ECEC$ predictions use similar many-body techniques and nuclear models as the ones employed for $0\nu ECEC$. Hence, a measurement of $2\nu ECEC$ rates is also relevant for interpreting $0\nu ECEC$ results. In $2\nu ECEC$, the excess energy is largely carried away by the two undetected neutrinos, with the recoil nucleus kinetic energy being

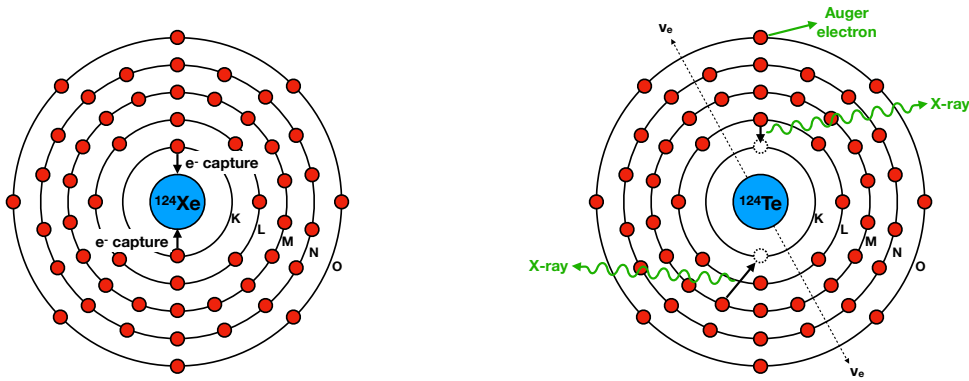


Figure 1. Schematic of the $2\nu ECEC$ process in ^{124}Xe . Left: two orbital electrons from the K shell are captured by the ^{124}Xe nucleus. Right: the resulting ^{124}Te atom de-excites via X-ray emission (two quanta in this example, from L→K and M→K transitions, respectively) or Auger electrons from the outer shells. The two electron neutrinos produced in the nuclear capture escape undetected.

Table 1. Summary of ^{124}Xe $2\nu ECEC$ results, for electrons captured from the K shell. For each experiment, the mass of ^{124}Xe in the fiducial volume, the live time, the exposure and the half-life result are given. Lower limits are given at 90% confidence level.

Experiment	^{124}Xe mass (kg)	Live time (yr)	Exposure (kg·yr)	$T_{1/2}$ (10^{22} yr)
XENON100 [7]	0.029	0.615	0.018	> 0.07
XMASS-I [8]	0.311	2.190	0.681	> 2.1
Gavriljuk <i>et al.</i> [9]	0.059	1.760	0.103	> 0.77
XENON1T [10]	1.493	0.487	0.726	1.8 ± 0.5

too low (~ 10 eV) to be detected either. The experimental signature is hence solely given by a cascade of X-rays and Auger electrons. This cascade is a consequence of the readjustment of the electron configuration of the atom that follows the capture by the nucleus of the two orbital electrons, typically from the K shell. The signature therefore lies in the tens of keV energy range, with all X-rays and Auger electrons produced at the same spatial location. A schematic representation of this process is shown in Figure 1, taking capture in ^{124}Xe as an example.

Three experimental indications of $2\nu ECEC$ exist to date. A possible evidence for $ECEC$ has been reported in ^{130}Ba from geochemical measurements of the ^{130}Xe daughter, with half-life values in the $(5 - 30) \times 10^{20}$ yr range [11, 12]. However, the half-lives of the two quoted ^{130}Ba measurements are incompatible with each other. In addition, these measurements cannot separate possible contributions from the three competing double beta decay processes mentioned above, nor contributions from two-neutrino and neutrinoless modes. An indication with 4σ significance has been reported for direct evidence of $2\nu ECEC$ in ^{78}Kr with a gas proportional chamber, with a half-life of $T_{1/2}(^{78}\text{Kr}) = (1.9_{-0.7}^{+1.3} \pm 0.3) \times 10^{22}$ yr [13]. Recently, an observation with 4.4σ significance has also been reported in ^{124}Xe by the XENON1T Collaboration using a detector originally designed for direct dark matter searches, with $T_{1/2}(^{124}\text{Xe}) = (1.8 \pm 0.5 \pm 0.1) \times 10^{22}$ yr [10]. Details of recent $2\nu ECEC$ searches in ^{124}Xe are given in Table 1. Such searches have been performed either using large liquid xenon detectors [7, 8, 10] with a ^{124}Xe isotopic abundance close to the one of natural xenon (9.52×10^{-4} [14]), or using gas proportional counters using ^{124}Xe -enriched xenon [9]. Recent predictions from nuclear structure calculations [15–17] show good agreement with the ^{124}Xe half-life measurement by XENON1T. In ^{124}Xe , a 76.7% fraction of all double electron captures are expected to originate from two K shell electrons [18]. The majority of these double K shell captures are expected to produce two characteristic X-rays per event.

We argue in this paper that the xenon-based high-pressure gas time projection chambers (TPCs) being developed by the NEXT Collaboration for ^{136}Xe $0\nu\beta\beta$ searches are ideally suited to also search for double electron capture in ^{124}Xe , provided that a gas with sufficient ^{124}Xe fraction is used. From simulated signal data and background data taken with the NEXT-White detector we optimize the data selection cuts that provide the best sensitivity

to the $2\nu ECEC$ decay. These data are finally used to extrapolate the sensitivity to the NEXT-100 detector.

The paper is organized as follows. Section 2 describes the NEXT experimental program, with special emphasis in the NEXT-White detector used in this feasibility study. Section 3 describes the background data and signal simulation samples employed. The event selection and the sensitivity projections are presented in Sections 4 and 5, respectively. We conclude in Section 6.

2 The NEXT experimental program

The NEXT detectors rely on the technology of high-pressure (10–15 bar) xenon gas time projection chambers (TPCs) with electroluminescent (EL) amplification and optical readout. The gas TPC provides a homogeneous and low-density detector active volume. Electroluminescence provides a nearly noiseless amplification of the ionization electrons reaching the TPC anode, key for excellent energy resolution capabilities. The optical signals induced by xenon primary (S_1) and electroluminescent (S_2) scintillation are detected by readout planes at opposite ends of the detector’s cylindrical volume, behind transparent cathode and anode planes, capable of providing a full 3D image of the events. The so-called tracking plane is composed of a large number of silicon photomultipliers (SiPMs) placed on a 2D lattice, and is located a few mm away from the anode and the EL region. The tracking plane detects the forward-going S_2 light, providing an unambiguous 2D image for each TPC time slice. The so-called energy plane is composed of photomultiplier tubes (PMTs) and is located behind the cathode, away from the EL region. The energy plane detects the nearly uniform backward-going S_2 light, providing an accurate energy measurement. The energy plane also detects the prompt S_1 light produced in the drift volume, enabling an accurate event t_0 determination.

The NEXT detection concept applied to $2\nu ECEC$ signals is depicted schematically in Figure 2. Each X-ray interaction in the active volume may give rise to a separate S_2 signal, some millimeters or centimeters away from the event vertex. For example, tellurium K_α X-rays from $L\rightarrow K$ transitions produced by ^{124}Xe double electron capture, with an energy of 27.5 keV, have a linear attenuation coefficient of 1.6 cm in xenon at 10 bar. A weaker S_2 signal from Auger electrons at the event vertex may also be reconstructed. The S_2 signals have a pulse shape characteristic of point-like energy deposits, with a time width primarily affected by diffusion effects along ionization electron drift. Regardless of the number of S_2 signals, a single (narrower) S_1 signal characteristic of the full event energy deposition is also present in the event PMT waveforms.

The strengths of the NEXT approach are threefold. First, NEXT TPCs feature a better energy resolution in the energy region of interest compared to the liquid xenon scintillators or gas proportional counters listed in Table 1. Second, NEXT provides full 3D position reconstruction capabilities to suppress external background events. This is also the case of liquid scintillators (which also provide xenon self-shielding), but only partially the case for the gas proportional counter of reference [9]. Third, the low density of the detector and its 3D imaging capabilities allow NEXT to spatially separate the X-ray conversions or Auger

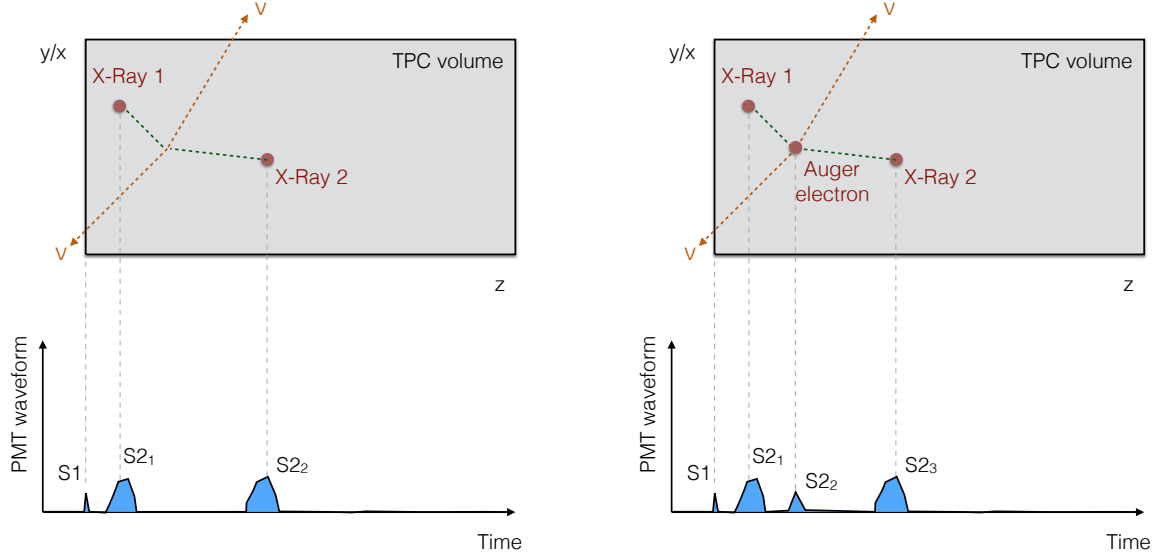


Figure 2. Schematic of $2\nu ECEC$ signature in NEXT. Two golden samples are considered, with two (left panel) and three (right panel) separate energy depositions per event, respectively.

electron deposits for a significant fraction of all $2\nu ECEC$ events. This is not possible in the higher-density liquid xenon, and only partially possible (that is, along the drift direction) in a gas proportional counter.

The first phase of the NEXT experimental program started in 2009 with the construction, commissioning and operation of two EL prototypes, NEXT-DEMO [19] and NEXT-DBDM [20], with xenon active masses of about 1 kg. These prototypes demonstrated the robustness of the technology, its excellent energy resolution and its unique topological signature. The NEXT-White demonstrator [21], deploying 4 kg of xenon in its active volume, implements the second phase of the program. This detector has been operating underground at the Laboratorio Subterráneo de Canfranc (LSC, Spain) since 2016. NEXT-White is also the first radiopure detector in the NEXT series. Its main goals are a detailed assessment of the backgrounds for ^{136}Xe double beta decay searches, the measurement of the ^{136}Xe $2\nu\beta\beta$ half-life and the characterization of the detector performance at energies close to the ^{136}Xe energy region of interest (about 2.5 MeV). The NEXT-100 detector, currently under construction, constitutes the third phase of the program. With a ^{136}Xe active mass approaching 100 kg, NEXT-100 will perform the first sensitive $0\nu\beta\beta$ search in xenon gas [22]. The fourth phase of the program contemplates tonne-scale xenon gas detectors. Two R&D lines are being pursued in parallel. The NEXT technology can be scaled up to $0\nu\beta\beta$ source masses in the tonne scale introducing several technological advancements already available [23, 24]. The NEXT Collaboration is also pursuing a more radical approach to a tonne-scale experiment based on the efficient detection of the Ba^{++} ion produced in the $0\nu\beta\beta$ decay of ^{136}Xe using single-molecule fluorescence imaging (SMFI) [24–29].

3 Data samples

For a given ^{124}Xe mass in the detector, a reliable evaluation of the experimental sensitivity to ^{124}Xe $2\nu ECEC$ relies on two factors: a good description of the backgrounds and a realistic estimate of the efficiency in reconstructing and selecting $2\nu ECEC$ signal events. The lower the background rate and the higher the signal efficiency, the better the ^{124}Xe $2\nu ECEC$ sensitivity and the prospects for its observation. For this analysis, we combine a background dataset from the NEXT-White detector adding up to 5 months of data-taking (Section 3.1) with a custom Monte-Carlo (MC) simulation of the $ECEC$ signal (Section 3.2).

3.1 Background data sample

The background sample used in this analysis was taken in 2019 between February 25th and July 10th and between September 13th and November 6th, as part of Run Va and Run Vb of the NEXT-White detector, which was filled with ^{136}Xe -enriched gas. The amount of ^{124}Xe present in the source is negligible, as shown in Figure 3, which makes this run configuration perfect for background characterization. The total accumulated exposure in this period is 125.9 days.

The events considered in the analysis are those taken by the low-energy trigger of the detector, which is set to record events between approximately 8 keV and 80 keV. This background dataset constitutes a total of 2.2×10^8 low-energy triggers. Detector conditions were stable during the whole data-taking period. The pressure was 10.13 bar, with voltages of 30 kV and 7.7 kV in the cathode and gate. The drift velocity of the electrons in the gas [30] remained fairly constant at ~ 0.91 mm/ μs . The electron lifetime during this period of data-taking varied between 5 and 9.5 ms, many times greater than the maximum drift time. The smooth variations in the detector conditions are accounted for using $^{83\text{m}}\text{Kr}$ calibration data, which allows for a continuous monitoring of the electron lifetime and other detector properties [31].

Due to the low-energy nature of these events, the data are processed to obtain a full 3D point-like reconstruction for each separate energy deposit in the event. The waveforms from the PMTs are summed to identify S_1 and S_2 signals. The integral of each S_2 signal is used to determine the deposited energy in each site. The waveforms of the SiPM sensors are combined to perform a 2D reconstruction of each S_2 signal separately, which is in turn aggregated with the drift time to have one point-like 3D reconstruction per S_2 signal. The energy of each S_2 signal is finally corrected by lifetime and geometry effects and converted to keV on a run-by-run basis. For more details on NEXT-White low-energy data processing and calibration procedures, see reference [31].

3.2 Signal simulation sample

The only particles emitted in the $ECEC$ process are neutrinos, which are undetectable. Hence, the simulation of the decay is focused on the daughter nucleus, which for ^{124}Xe is ^{124}Te . Although electrons of any shell can be captured, K shell electrons have the highest probability. Thus, the aim is to study ^{124}Te atoms with a double K shell vacancy, which relax by emitting X-rays or Auger electrons. The simulation is based on the atomic

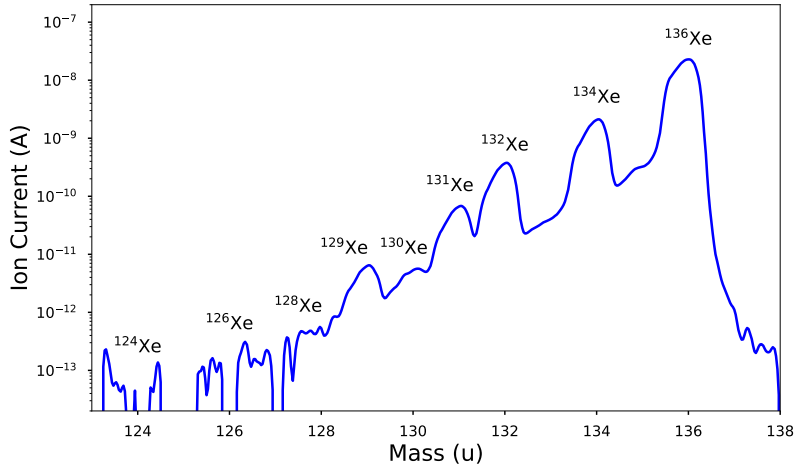


Figure 3. Isotopic composition of NEXT ^{136}Xe -enriched gas.

relaxation package of Geant4 v10.04 [32]. Geant4 uses the Livermore Evaluation Atomic Data Library (EADL) [33], that contains data to describe the relaxation of atoms back to neutrality after they are ionized. Since the package does not provide a mechanism to generate *ECEC* events, we approximate our simulation by generating two independent ^{124}Te atoms with a single K shell vacancy and at the same spatial location per event, as done in reference [8].

Albeit the energy of two single K shell vacancies (63.63 keV [34]) is not the same of that of a double vacancy (64.46 keV [35]), we consider the difference, 0.8 keV, negligible.

Each atom in the simulation de-excites independently according to the X-ray and Auger emission probabilities. The observed emission probabilities, derived from the number of primary gammas in the simulation shown in the left panel of Figure 4 are consistent with the fluorescence yield of ^{124}Te [36]. The energy of the emitted gammas matches also the atomic energy levels of the ^{124}Te atom, as shown on the right panel of Figure 4.

The interactions of electrons and gammas in the volume of the detector are simulated according to the *G4EmStandardPhysics_option4* package of Geant4. Then, we simulate the electron drift (with realistic electron diffusion and negligible electron attachment), the light emission using parametrized models of the detector and the electronics response (including noise) to finally produce a set of sensor waveforms, equivalent to that of the real detector. These waveforms are then processed identically as detailed in Section 3.1.

The full signal dataset is composed of 10^8 events distributed homogeneously over the active volume of the NEXT-White detector.

4 Event selection

Signal and background events produce different signatures in the detector. At low energies (<100 keV), the events in the chamber are primarily small-angle Compton scatterings of background gamma-rays, photoelectric interactions of low-energy gamma-rays, isolated

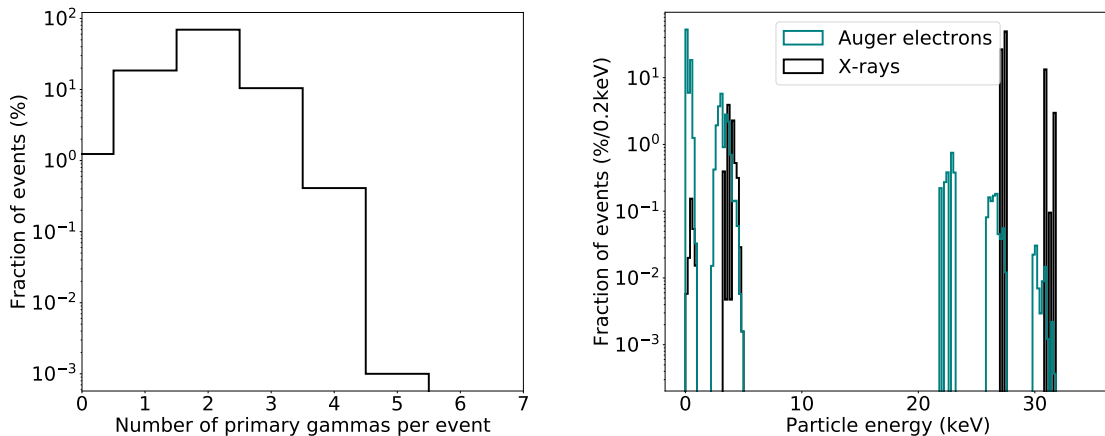


Figure 4. Monte-Carlo truth distributions of ^{124}Xe *ECEC* signal events. Left: number of primary gammas (X-rays) per simulated event. Right: distribution of simulated X-ray energies.

xenon X-rays and, mostly, decays of metastable $^{83\text{m}}\text{Kr}$ atoms introduced in the active volume as a calibration source [31]. These events are characterized by having a single-site interaction and thus producing one S_1 and one S_2 signals. On the other hand, the vast majority of $2\nu ECEC$ events consist of at least two interactions, regardless of whether they come from X-rays or Auger electrons. This can be inferred for example from the left panel of Figure 4, showing that approximately 99% of $2\nu ECEC$ events are expected to produce at least one X-ray. Hence, the event topology provides a key feature to discriminate background events from signal.

Notwithstanding, there are two cases in which this feature is not as useful. First, pile-up of different events in the DAQ window could in principle mimic the signature of a *ECEC* event, if only one S_1 signal is reconstructed. However, the energies of the individual S_2 signals rarely match the ones expected from our signal events. Second, the two X-rays or Auger electrons from a *ECEC* event can interact very close to the originating vertex, meaning that both signals merge into a single S_2 , spoiling the topological signature of the process. A fraction of these events could be recovered by improving and customizing the reconstruction algorithms for this particular case, see discussion in Section 5.2.

In order to optimize the signal and minimize the background, we perform a number of selections in the data. These selections are based both on topology and energy considerations. First, we reduce the data size by selecting a broad energy window around the region of interest (ROI), which eliminates most of the events coming from the $^{83\text{m}}\text{Kr}$ source, see Section 4.1. Second, we apply data quality cuts in Section 4.2. In Section 4.3 we discuss the fiducial cuts. We then select the optimal energy ROI for the search, see Section 4.4. We finally apply the multi-site event selection in Section 4.5. Each selection is done separately and based on the optimization of the following figure of merit:

$$\text{FOM} = \frac{\varepsilon_{\text{sig}}}{\sqrt{\varepsilon_{\text{bkg}}}}, \quad (4.1)$$

Table 2. Event selection summary. Cumulative signal and background efficiency as a function of the various event selection criteria.

Processing/selection step	Fraction of background data (%)	Fraction of signal MC (%)
DAQ triggers or MC simulated events	100	100
Event reconstruction	83.564 ± 0.003	89.10 ± 0.10
$^{83\text{m}}\text{Kr}$ veto	$(40.53 \pm 0.04) \times 10^{-2}$	83.50 ± 0.12
Data quality	$(13.99 \pm 0.02) \times 10^{-2}$	35.76 ± 0.15
Fiducial	$(4.06 \pm 0.04) \times 10^{-3}$	25.42 ± 0.14
Event energy	$(5.28 \pm 0.15) \times 10^{-4}$	24.39 ± 0.13
Multi-site	$(1.15 \pm 0.07) \times 10^{-4}$	22.90 ± 0.13

where ε is the relative efficiency of the cut defined as

$$\varepsilon = \frac{\# \text{ events after the cut}}{\# \text{ events before the cut}}. \quad (4.2)$$

A data reduction summary for signal and background events and as a function of the various sequential cuts is given in Table 2 and discussed in Section 4.6.

4.1 $^{83\text{m}}\text{Kr}$ veto requirement

The $^{83\text{m}}\text{Kr}$ calibration source used in the experiment represents about 73% of the low-energy triggers. The decay of this isotope produces 41.5 keV single-site events. Since the energy resolution FWHM at these energies is around 2 keV [31], we can reduce these events to the minimum by requiring the energy of the whole event to be in a broad window above the $^{83\text{m}}\text{Kr}$ peak.

As shown in Figure 5, the energy spectrum is dominated by the $^{83\text{m}}\text{Kr}$ peak at 41.5 keV and, to a lesser extent, by the coincidence of two $^{83\text{m}}\text{Kr}$ events in the same waveform at 83 keV. We remove these data from our sample by selecting the events with a total energy between $50 \text{ keV} < E_{\text{evt}} < 80 \text{ keV}$. The combined requirement of successful event reconstruction plus $^{83\text{m}}\text{Kr}$ veto keeps 0.4% of the background data, hence reducing the size of the data sample by a factor of 200, while keeping 83.5% of the simulated $2\nu\text{ECEC}$ signal events.

4.2 Data quality selections

Data quality criteria are imposed based on the multiplicity of reconstructed S_1 and S_2 signals per event. First, we remove all events with no or multiple S_1 signals. Events with no S_1 signals are not reconstructed along the drift coordinate¹. Therefore, they cannot be selected according to fiducial volume criteria nor their energy corrected for electron lifetime effects along drift. Events with more than one S_1 signal on the other hand introduce an

¹The drift time can also be estimated from the width of the S_2 signal. This method is less accurate, but it might be required in larger detectors where the S_1 detection efficiency is smaller.

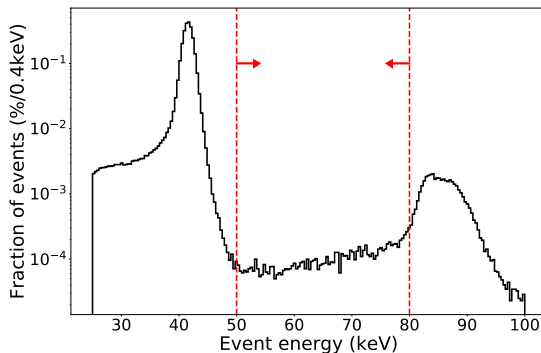


Figure 5. Event energy spectrum of fully reconstructed low-energy triggers from a 26.6 h low-background run of NEXT-White. Red lines indicate the broad energy window for the $^{83\text{m}}\text{Kr}$ veto.

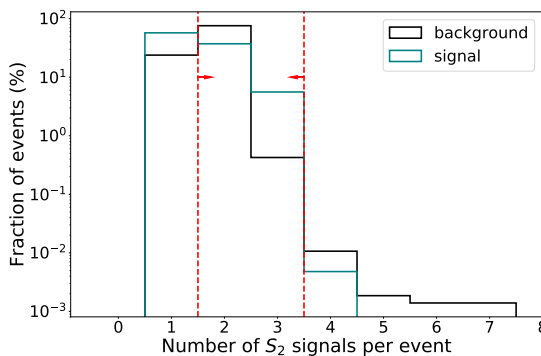


Figure 6. S_2 multiplicity per event for signal and background events after the $^{83\text{m}}\text{Kr}$ veto. Red lines indicate the limits of the range of accepted values.

ambiguity in the drift coordinate determination, resulting in the same limitations as events with no S_1 signals. Additionally, such events may originate from event pile-up. The single S_1 condition keeps 45.3% of the background data and 100% of the simulated signal.

Second, we require each event to have either two or three S_2 signals. This condition is based on the topology of $2\nu ECEC$ events, which should produce two or three separate energy depositions in most cases, see Figures 2 and 4. Thus, this requirement selects events in which at least two of them are spatially distinguishable along the drift coordinate. This cut keeps 42.8% of the signal events and 76% of the background events. Despite losing a significant fraction of signal events, for this study we assume that energy depositions that overlap in Z are not separable as doing so would require dedicated reconstruction algorithms as discussed in Section 5.2. As shown in Figure 6, the probability to reconstruct three S_2 signals per event after the $^{83\text{m}}\text{Kr}$ veto is higher in signal than in background, while the opposite is true for two- S_2 events.

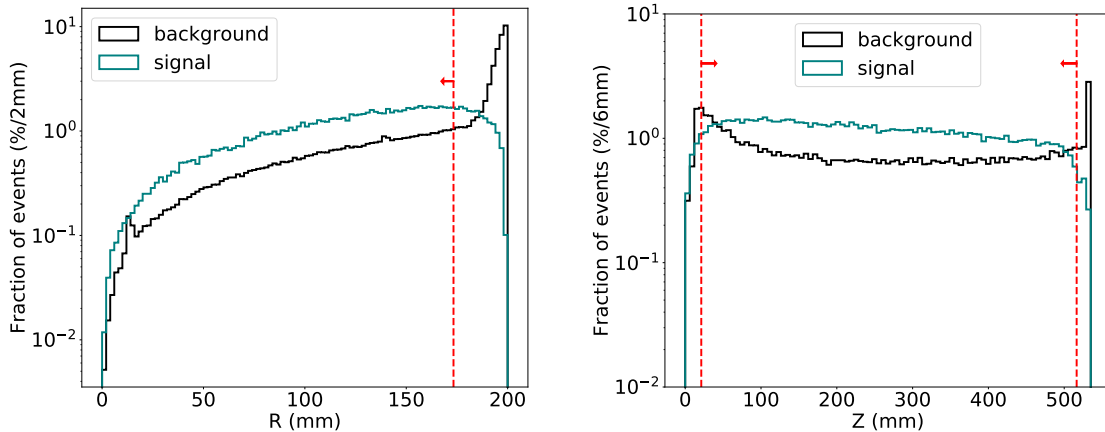


Figure 7. Event selection based on spatial information. One entry per reconstructed S_2 signal is shown. Left: signal and background distributions along the radial detector coordinate, with optimal R_{\max} cut position (red lines). Right: signal and background distributions along the drift coordinate and after the fiducial radius selection, with optimal Z_{\min} and Z_{\max} cut positions (red lines).

4.3 Fiducial selection

Signal events are homogeneously distributed over the entire active volume. On the other hand, background events tend to be reconstructed on the borders of the detector. Thus, we define a fiducial volume of the detector that maximizes the sensitivity to our search. An event is considered to pass the fiducial cut if and only if all of the S_2 signals satisfy the condition. Three cut variables are separately optimized to define the fiducial selection: the maximum radial position R_{\max} , the minimum drift distance Z_{\min} and the maximum drift distance Z_{\max} of all S_2 signals in the event. In order to obtain the optimal selection we evaluate the figure of merit in Eq. (4.1) for each variable independently within a sensible range of values for the cut variables.

For the radial coordinate we only set an upper limit. The optimal value is found to be $R_{\max} = 183.5$ mm, to be compared with the NEXT-White active volume radius of $R = 198$ mm. The radial distributions of signal and background S_2 signals are shown in the left panel of Figure 7, together with the cut position. With this cut we keep 76% of the simulated signal events and 9% of the background events.

For the longitudinal coordinate we set both a lower and an upper limit. The optimal values are $Z_{\min} = 44$ mm and $Z_{\max} = 512.5$ mm, respectively. The TPC active volume boundaries along drift are $Z = 0$ (anode) and $Z = 530.3$ mm (cathode). The drift distance distributions of signal and background S_2 signals are shown in the right panel of Figure 7, together with the cut positions. Combining the lower and upper edges of the cut we end up keeping 93.5% of the signal events and 32% of the background events.

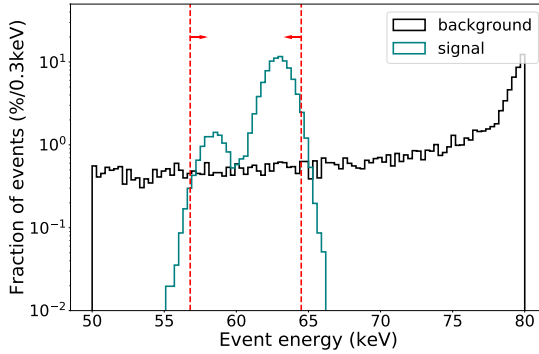


Figure 8. Event energy E_{evt} signal and background distribution after fiducial selection, with optimal E_{evt} cut positions (red lines).

4.4 Event energy selection

As mentioned in Section 3.2, the energy released in our simulated ^{124}Xe $2\nu\text{ECEC}$ events is 63.63 keV. Considering the good energy resolution of the detector, it is rather convenient to restrict the energy ROI beyond that already done by the $^{83\text{m}}\text{Kr}$ veto requirement of Section 4.1.

The maximum and minimum allowed event energies are separately optimized to define the energy ROI $E_{\text{evt},\text{min}} < E_{\text{evt}} < E_{\text{evt},\text{max}}$. The optimal value for the upper limit is found to be $E_{\text{evt},\text{max}} = 64.6$ keV, and for the lower limit $E_{\text{evt},\text{min}} = 56.4$ keV. The combined requirement of both limits yields a 96% efficiency for signal events and a 13% efficiency for background events. Event energy distributions for signal and background fiducial events are shown in Figure 8. As can be seen in the figure, the cut optimization selects a bimodal distribution for signal events: a primary peak corresponding to the full energy deposit being correctly reconstructed, plus a secondary peak where an energy of 4–5 keV either escapes the active volume or is not reconstructed. As shown in Figure 4, X-ray lines of 4–5 keV are indeed expected. Background events are found to have a flat energy distribution in the ROI.

4.5 Multi-site selection

We account for two signal sub-samples in our analysis: both a two- S_2 sub-sample and a three- S_2 sub-sample. For the two- S_2 sub-sample not all events are selected, but only those where both energy depositions in the event satisfy a certain energy requirement $E_{S_2,\text{min}} < E_{S_2} < E_{S_2,\text{max}}$. As observed in Figure 4 (right), for signal we expect most isolated energy deposits to be due to tellurium K_α (L \rightarrow K) X-rays, with a S_2 energy of 27.5 keV. As shown in the same figure, higher-energy X-rays of 31–32 keV from initial electrons in outer shells are also possible.

Figure 9 shows the S_2 energy spectrum of the two- S_2 signal and background sub-samples. After evaluating the figure of merit we obtain $E_{S_2,\text{min}} = 26.0$ keV and $E_{S_2,\text{max}} = 37.3$ keV

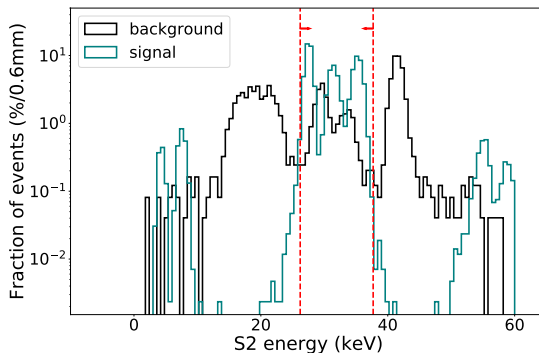


Figure 9. S_2 energy E_{S_2} signal and background distribution in two- S_2 sub-sample, with optimal E_{S_2} cut positions (red lines).

as the optimal limits. The combined effect of both limits keeps 94% of the signal events and 21.7% of the background events with 2 S_2 signals.

As far as the three- S_2 sub-sample is concerned, no E_{S_2} energy selection is performed and all events in the sub-sample are kept. As shown in Figure 6, the probability to have three- S_2 events is an order of magnitude higher in signal than in background even without a E_{S_2} requirement. After all cuts, the events with three- S_2 signals represent a 12.7% of the selected signal events and 0.5% of the selected background events.

4.6 Event selection summary

The cumulative efficiencies after each data processing step are shown in Table 2 for both background data and signal MC events. We estimate a final efficiency of $(22.90 \pm 0.13)\%$ for simulated double K shell captures, to be compared with an acceptance of $(1.15 \pm 0.07) \times 10^{-6}$ measured in ^{124}Xe -depleted background data. The latter number corresponds to a total background rate of $24.7 \mu\text{Hz}$, or 780 counts/yr.

We also analyze the dependence of the background rate after all selections on the initial rate of events. Since the background sample is dominated by the $^{83\text{m}}\text{Kr}$ calibration source, we divide the full dataset into smaller samples with approximately the same $^{83\text{m}}\text{Kr}$ rate. The optimized selections from the full dataset are then applied to these samples. Figure 10 shows the background rate after all selections as a function of the average $^{83\text{m}}\text{Kr}$ rate in each sample. Clearly, the background rate does not depend on the $^{83\text{m}}\text{Kr}$ rate, proving that the selection is robust and can be used in a variety of detector conditions.

While our data-driven approach to the background estimate implies that a full understanding of the background composition is *a priori* not known, much can be inferred from the background data distributions. On the one hand, Figure 10 excludes $^{83\text{m}}\text{Kr}$ -related events as a dominant background source. On the other hand, Figures 8 and 9 point to multi-site gamma interactions with a flat gamma energy spectrum in the energy region of interest, and where one of the energy deposits is a xenon K-shell X-ray at 29.7 keV or 33.8 keV. Background events are therefore likely dominated by low-energy gamma rays produced

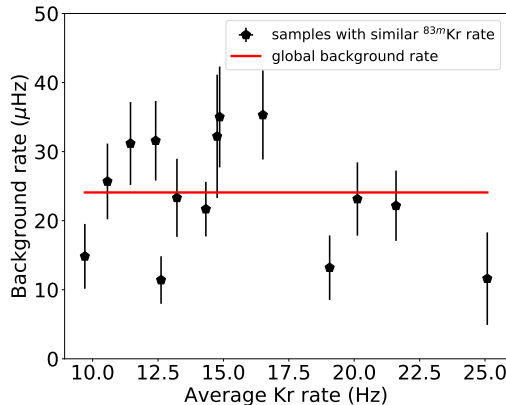


Figure 10. Background rate after all selections as a function of the $^{83\text{m}}\text{Kr}$ rate for different samples of the full background dataset. The values oscillate around the overall background rate (solid line).

by radioactive impurities in the detector materials, undergoing Compton scattering prior to entering the active volume, and producing photo-electrons and xenon X-rays in the active volume. We cannot be certain about which gamma-ray emitting isotope is primarily responsible for the overall background rate. Based on findings from other experiments [8, 10] as well as from NEXT measurements at higher energies [37], ^{60}Co , ^{40}K , and isotopes in the ^{238}U and ^{232}Th decay chains are the likely main contributors.

5 Sensitivity projections

The data-driven background evaluation and the corresponding $2\nu ECEC$ signal efficiency study of Section 4 have been done using NEXT-White data. However, our purpose is to study the feasibility of detecting K shell $2\nu ECEC$ events in the forthcoming NEXT-100 detector (see Section 2), if a significant ^{124}Xe mass were added to its ^{136}Xe -enriched xenon gas. The NEXT-100 detector is designed to hold approximately 100 kg of xenon with an enrichment fraction of 90% in the ^{136}Xe isotope. The natural abundance of ^{124}Xe is 0.095%, or about 100 g of ^{124}Xe in 100 kg of natural xenon. In the ^{136}Xe -enriched xenon to be used in NEXT-100, the amount of ^{124}Xe mass would be even less, as shown in Figure 3. Such ^{124}Xe masses are too small for a competitive ^{124}Xe $2\nu ECEC$ search. The objective of this study is therefore studying whether the addition of about 1 kg of highly ^{124}Xe -enriched xenon to the 100 kg of ^{136}Xe -enriched gas could yield a promising $2\nu ECEC$ sensitivity in NEXT-100. In the following, we assume that NEXT-100 will contain 1 kg of ^{124}Xe in its active volume. The mixing of ^{136}Xe and ^{124}Xe would not affect the performance of the detector in any way, nor would it impact the program of ^{136}Xe $\beta\beta$ searches in NEXT-100. The ^{136}Xe mass in the active volume would remain essentially the same after mixing this relatively small amount of ^{124}Xe . The NEXT gas system is already prepared to perform such mixing operation, if a ^{124}Xe gas bottle were acquired.

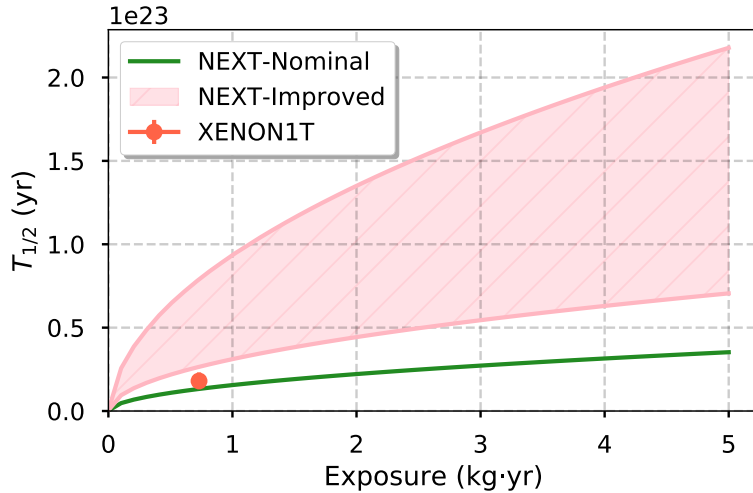


Figure 11. NEXT nominal (green curve) and improved (red band) half-life sensitivity to ^{124}Xe $2\nu ECEC$ versus exposure, compared with the XENON1T measurement in reference [10] (red marker).

The sensitivity to the ^{124}Xe $2\nu ECEC$ half-life $T_{1/2}$, where both electrons are captured from the K shell, is computed as [4]:

$$T_{1/2} = \ln 2 \cdot \frac{N_A \cdot \varepsilon_s \cdot M \cdot t}{W \cdot N_s} \quad (5.1)$$

where N_A the Avogadro's number, $\varepsilon_s = (22.90 \pm 0.13)\%$ is the $2\nu ECEC$ signal efficiency estimated in Section 4, M is the ^{124}Xe mass in the NEXT-100 active volume, t is the exposure time, $W = 123.9$ g/mol is the molar mass of the ^{124}Xe isotope, and N_s is the maximum number of $2\nu ECEC$ signal events that would be compatible with a background-only measurement. Note that the average upper limit N_s depends on the number of background events for an exposure time t , which has been estimated in Section 4, and on the confidence level value assumed. In the following, we use the customary 90% confidence level value. There are various prescriptions to evaluate N_s given a certain background prediction. In this case, we use the standard Feldman-Cousins prescription [38]. The $2\nu ECEC$ sensitivity of Eq. (5.1) refers specifically to the double K shell capture process in ^{124}Xe , as the event selection would be different for different capture configurations.

5.1 Nominal sensitivity

The NEXT half-life sensitivity to ^{124}Xe $2\nu ECEC$ is shown as a function of accumulated exposure (in kg·yr) as the green line in Figure 11. A sensitivity of 1.6×10^{22} yr at 90% CL, comparable to the central value of the recent XENON1T measurement [10], is expected to be reached after an exposure of 1 kg·yr in NEXT-100. This is one year livetime of NEXT-100 operated with 1 kg of ^{124}Xe mass in its active volume. In five years of operation in the same conditions, a sensitivity of 3.5×10^{22} yr at 90% CL could be reached. We

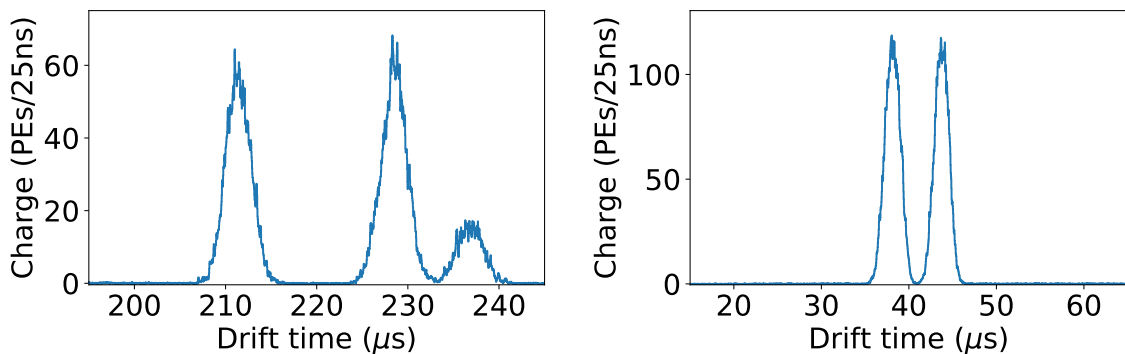


Figure 12. Examples of PMT waveforms of simulated $2\nu ECEC$ signal events that are incorrectly identified by NEXT standard reconstruction algorithms. Left panel: event with three separate energy deposits, reconstructed as having two S_2 signals at times 211 and 228 μs , respectively. Right panel: event with two separate energy deposits, reconstructed as having one S_2 signal at time 38 μs .

consider this nominal sensitivity to be conservative, as it assumes the background rate measured in NEXT-White and the $2\nu ECEC$ signal efficiency achieved in this work, as presented in Section 4. In the following, we justify how more favorable assumptions for background rate and signal efficiency are plausible for NEXT-100.

5.2 Potential improvements

The first potential improvement going from NEXT-White to NEXT-100 is the size of the detector. As the radius and length of the TPC are increased, the fiducial regions described in Section 4.3 represent a larger fraction of the active volume. Thus, a larger fraction of the ^{124}Xe mass is kept, which translates into an increase in signal rate.

The second improvement comes from changes in detector design that reduce the background rate. Compared to NEXT-White, NEXT-100 is being built from more radiopure materials and with a thicker inner shielding. In NEXT-100, the inner shielding is made of 12 cm of ultra-pure copper, to be compared with the 6 cm copper shielding of NEXT-White. The shielding is expected to be particularly important for the low-energy backgrounds relevant to $2\nu ECEC$ searches. Hence, despite the larger detector mass, it is possible (although not guaranteed) that the total background rate in NEXT-100 will be lower than the value measured in NEXT-White.

Third, improvements in low-energy event reconstruction should significantly increase the $2\nu ECEC$ signal efficiency in NEXT-100, and possibly also reduce the background rate. NEXT reconstruction algorithms used in Section 3 and Section 4 were developed for the higher-energy $\beta\beta$ searches. Dedicated low-energy reconstruction algorithms are likely to perform better. We show in Figure 12 examples of PMT waveforms for simulated $2\nu ECEC$ events that are incorrectly reconstructed by the current algorithms. As it is apparent from the waveforms, the reconstruction tends to merge into the same S_2 signal energy deposits that are visually separable from each other. This is due to the proximity of energy deposits along the drift direction and to the longitudinal diffusion, partially merging the nearby

deposits together. As noted earlier (Section 2), spatial separations of order 10–20 mm among energy deposits in the same event are common, in the $2\nu ECEC$ case. In particular, a large inefficiency results from signal events that are mis-reconstructed as single S_2 signal events, which are discarded as background-like in our analysis. It is therefore plausible to obtain a twice as large overall signal efficiency thanks to a dedicated low-energy reconstruction combined with the larger active volume of NEXT-100.

Fourth, event selection might also be improved in NEXT-100. One possibility would be to adopt a multi-variate selection as opposed to sequential cuts as done in Section 4. In this case the selection would be optimized in a multi-dimensional space of observables, for example in $(R, Z, E_{\text{evt}}, E_{S_2})$ space, accounting for correlations among them. On the other hand, another possibility to improve the signal/background event classification is by using deep learning techniques. This technique is already being used in NEXT for $0\nu\beta\beta$ searches, yielding promising results [39].

To conclude, we believe that an improved half-life sensitivity in NEXT-100 is plausible, compared to the nominal sensitivity obtained from NEXT-White detector performance and backgrounds. This improved sensitivity is shown in Figure 11 as a filled red band. The lower limit of the band solely assumes a factor of 2 increase in $2\nu ECEC$ efficiency, ε_s . The upper limit of the band assumed both a factor of 2 increase in ε_s and a factor of 10 reduction in background rate. Sensitivities in the $0.7\text{--}2.2 \times 10^{23}$ yr range at 90% CL and after 5 years of operation appear possible. While this study focuses on ^{124}Xe $2\nu ECEC$, an accurate measurement of the two-neutrino mode would set the stage for a sensitive search of the lepton number-violating $0\nu ECEC$ mode of ^{124}Xe , which would be the ultimate goal for double electron capture searches in NEXT.

6 Conclusions

The potential discovery of the Majorana nature of massive neutrinos via the observation of the neutrinoless decay modes of double beta decay processes is one of the most important questions in neutrino physics today. Neutrinoless double electron capture on proton-rich nuclei is a promising and alternative process compared to the far more exploited neutrinoless double β^- decay of neutron-rich nuclei. Yet, this process is significantly less understood both from the theoretical and the experimental points of view. The measurement of the Standard Model-allowed two-neutrino double electron capture is a first important step toward sensitive neutrinoless double electron capture searches. Two-neutrino double electron capture is a process in which two orbital electrons are simultaneously captured, typically from the K shell, by a proton-rich nucleus. The experimental signature is given by the emission of X-rays and Auger electrons from the de-excitation of the daughter atom.

In this paper, we establish that the high-pressure xenon gas TPC technology developed by the NEXT Collaboration for ^{136}Xe double β^- decay searches is ideally suited to perform ^{124}Xe double electron capture searches as well. The reasons are the excellent energy resolution of the technology at the energy region of interest near 64 keV, its 3D imaging capabilities to suppress external backgrounds, and its capability to spatially separate the X-ray conversions or Auger electron deposits for a significant fraction of all double electron

capture events. We have studied the feasibility to detect ^{124}Xe two-neutrino double electron capture in NEXT using actual NEXT-White background data and a detailed simulation of the signal in the same detector. The low-background data sample uses 125.9 days of NEXT-White low-energy triggers, originally designed for $^{83\text{m}}\text{Kr}$ detector calibrations, with the detector filled with ^{124}Xe -depleted xenon gas ($< 10^{-5}$ isotopic abundance). Both background data and simulated signal are reconstructed with NEXT standard reconstruction algorithms. An optimal event selection for ^{124}Xe two-neutrino double electron capture searches has been developed, maximizing the signal efficiency over the square root of background acceptance as the figure of merit. The event selection relies on the total event energy, on the multiplicity of xenon primary (S_1) and charge-induced (S_2) scintillation signals per event, and on the spatial location and energy of the individual energy depositions reconstructed in the event. As a result, a total background rate of $24.7 \mu\text{Hz}$ (780 counts/yr) is measured in NEXT-White, for a total signal efficiency of 22.9%. Extrapolating this background rate and signal efficiency to NEXT-100 and assuming it is operated with 1 kg of ^{124}Xe in its active volume, an option that is technically feasible if a bottle with sufficient ^{124}Xe -enriched gas quantity were procured, a sensitivity of 1.6×10^{22} yr at 90% CL could be obtained after one year of operations. This sensitivity is comparable to the recent measurement of ^{124}Xe by the XENON1T Collaboration, $(1.8 \pm 0.5) \times 10^{22}$ yr [10]. We use this result as a basis to assess the case for a ^{124}Xe two-neutrino double electron capture measurement in the NEXT-100 detector, currently under construction. We expect that a dedicated double electron capture reconstruction capable of better discerning separate energy deposits could increase the signal efficiency by as much as a factor of two. With this improvement alone, we predict a two-neutrino double electron capture sensitivity of 7×10^{22} yr after 5 years of operation, for the same background rate (780 counts/yr) and the same ^{124}Xe active mass (1 kg). Other NEXT-100 detector design and analysis improvements compared to NEXT-White may yield further improvements in background reduction, resulting in even better sensitivities.

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